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DENSITY FUNCTIONALS FOR THE PAULI–FIERZ HAMILTONIAN

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Abstract. We develop a density-functional theory for the Pauli–Fierz Hamiltonian of nonrelativistic quantum electrodynamics in the spirit of the convex-analytic formulation of Lieb. We consider finitely many electrons, subject to external scalar and vector potentials, coupled to the full continuum of massless transverse photons with an ultraviolet cutoff. The natural basic variables are the standard electron density and a combined current density, the sum of the paramagnetic current density and a field-induced current density generated by the quantized vector potential. We prove representability results for these density–current pairs and show that the mixed-state constrained-search functional attains its infimum and coincides with the Lieb functional obtained by convex conjugation. Since arbitrarily soft photons purify mixed states at a negligible energy cost without changing their density and combined current density, the pure-state Levy–Lieb functional equals the Lieb functional and is therefore convex, even though its infimum need not be attained. In addition, we establish the zero-coupling limit, which recovers the mixed-state Vignale–Rasolt functional of current-density-functional theory. Finally, we consider the long-wavelength (dipole) limit and show that the limiting functional can be written as a constrained search for the well-known length-gauge dipole Hamiltonian.

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1. Introduction

Strong coupling of molecules and solids to the quantized electromagnetic field of an optical cavity has been reported to modify chemical and material properties [12, 5, 15, 6]. At the energy scales of chemistry and condensed-matter physics, such effects are described by nonrelativistic quantum electrodynamics (QED) in the form of the Pauli–Fierz Hamiltonian [40, 54], in which electrons are minimally coupled to the quantized transverse vector potential. To treat realistic systems, density-functional theory (DFT) has been extended to this setting as quantum-electrodynamical DFT (QEDFT) [57, 46, 45]. See [13, 49] for approximate functionals and [48, 47] for reviews. While the Pauli–Fierz Hamiltonian itself is well understood mathematically [22, 21, 2, 19, 34], the density-functional side has been analyzed in mathematical detail only for quantum-optical model systems such as the Rabi and Dicke models [39, 3, 4], in which the system is reduced to two-level systems coupled to finitely many field modes.

The mathematical structure of DFT was clarified by Lieb [33], who placed Levy's constrained search [28] into the framework of convex analysis (see [32, 41] for recent accounts). In the presence of magnetic fields, the density is supplemented by the paramagnetic current density $\mathbf{j}^{\mathrm{p}}$, which couples linearly to the external vector potential $\mathbf{A}$ in the current-density-functional theory (CDFT) of Vignale and Rasolt [58, 59]. Absorbing the diamagnetic term $\frac{1}{2}|\mathbf{A}|^2$ into the scalar potential makes the ground-state energy jointly concave in the potentials [56], which also leads to a convex formulation of CDFT [42]. Several cornerstones of DFT are more delicate here: the density–current pair does not in general determine the potentials uniquely [8, 26]. Furthermore, only sufficient conditions for N-representability are known, and it is open whether pure- and mixed-state N-representability coincide [35, 55, 10]. Lower semicontinuity of the (mixed-state) Vignale–Rasolt functional was proved only recently [24].

In this article, we develop density-functional theory for the Pauli–Fierz Hamiltonian itself, in the spirit of Lieb's analysis. We consider N spinless electrons in $\mathbb{R}^3$ coupled to the full continuum of massless transverse photons, with a fixed ultraviolet cutoff but no infrared cutoff, in an external scalar potential v and an external classical vector potential $\mathbf{A}$. The photon mode $\mathbf{k}$ couples proportionally to $e\widehat{\chi}(\mathbf{k})$, where $e \geq 0$ is the coupling constant and the form factor $\widehat{\chi}$ is any function satisfying (9), such as the hard cutoff $\mathbb{1}_{|\mathbf{k}|\leq\Lambda}/\sqrt{|\mathbf{k}|}$. We indicate these choices by the superscripts e, χ. A new feature compared with CDFT is that a finite-energy state may contain arbitrarily many photons of arbitrarily small energy. This infrared freedom causes the main technical difficulties, but it is also behind some of the most striking results.

The combined current density. For a finite-energy state Ψ,

$$\langle \Psi, H^{v,\mathbf{A}}\Psi\rangle = \langle \Psi, H^{0,0}\Psi\rangle + \langle v + \tfrac{1}{2}|\mathbf{A}|^2, \rho_\Psi\rangle + \langle \mathbf{A}, \mathbf{j}^{\mathrm{c}}_\Psi\rangle, \qquad \mathbf{j}^{\mathrm{c}}_\Psi = \mathbf{j}^{\mathrm{p}}_\Psi + \mathbf{j}^{\mathrm{ph}}_\Psi,$$

where $H^{0,0}$ is the Pauli–Fierz Hamiltonian without external potentials (26), ρ_Ψ is the electronic density, and $\mathbf{j}^{\mathrm{ph}}_\Psi(\mathbf{x}) = -eN\,\mathrm{Re}\langle \Psi, \mathfrak{A}(\mathbf{x})\Psi\rangle_{\mathbf{x}}$ is the *field-induced current density*, that is, $-e$ times the density-weighted mean of the quantized vector potential $\mathfrak{A}$ at the position $\mathbf{x}$ of an electron, the partial inner product being taken in all other variables. Thus the external potentials see a state only through ρ_Ψ and the *combined current density* $\mathbf{j}^{\mathrm{c}}_\Psi$, and these are our basic variables. The combined current density obeys a kinetic-energy bound similar to that for $\mathbf{j}^{\mathrm{p}}$ (Proposition 4.1),

but although $\operatorname{div}\mathfrak{A} = 0$, its field-induced part need not be divergence-free for entangled electron–photon states (Proposition 4.2). Ground states carry the magnetostatic fields of their own physical current density $\mathbf{j}^{\mathrm{c}} + \rho\mathbf{A}$ (Proposition 4.3).

Representability. The photon field purifies the electrons: the pairs $(\rho_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi)$ of pure electron–photon states with finite energy are exactly those of electronic *mixed* states with finite kinetic energy (Theorem 4.4). For $e > 0$, coherent photon displacements depending on the electron positions produce field-induced currents $-e\rho\mathbf{a}$, where the vector field $\mathbf{a}$ need not be transverse. Hence, every $(\rho, \rho\mathbf{v})$ with $\int_{\mathbb{R}^3}\rho = N$, $\sqrt{\rho} \in H^1(\mathbb{R}^3)$ and $\int_{\mathbb{R}^3}\rho(|\mathbf{v}|^2 + |\boldsymbol{\nabla}\mathbf{v}|^2) < \infty$ is a pure-state N-representable density–combined-current pair (Theorem 4.6 and Corollary 4.7).

Universal functionals. The Pauli–Fierz Levy–Lieb (PFLL) functional is the pure-state constrained search

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) = \inf_{\substack{\|\Psi\|=1 \\ \rho_\Psi = \rho \\ \mathbf{j}^{\mathrm{c}}_\Psi = \mathbf{j}^{\mathrm{c}}}} \langle \Psi, H^{0,0}\Psi\rangle,$$

and the Pauli–Fierz Lieb (PFL) functional $F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$ is the convex conjugate of the ground-state energy, reparametrized as in [56]. As in Lieb's theory, it is the lower semicontinuous convex envelope of $F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}})$. Our first main result (Theorem 4.8) is the counterpart of [33, 24]: the mixed-state constrained-search functional is lower semicontinuous, equals $F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$, and attains its infimum at a density matrix of finite mean photon number. Since an energy bound does not control the photon number, the proof removes soft photons and restores the combined current density exactly, at a controlled energy cost. Our second main result (Theorem 4.10) points in the opposite direction and sets QEDFT apart from DFT or CDFT: soft photons purify any finite-energy mixed state at arbitrarily small energy cost without changing $(\rho, \mathbf{j}^{\mathrm{c}})$, so that

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) = F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}).$$

Hence, unlike the Levy–Lieb functional of electronic DFT, which is not convex [33], the PFLL functional is convex and lower semicontinuous, and pure- and mixed-state N-representability coincide (Corollary 4.11). The price to pay is that the pure-state infimum is in general not attained. This is true already for one electron and at every coupling (Proposition 4.9). Optimizers need not be ground states, and in Section 4.6 we discuss which ground-state properties carry over to optimizers. Mixed-state optimizers contain few soft photons: for the hard cutoff, the expected number and energy of photons with frequency below κ are $O(\kappa)$ and $O(\kappa^2)$, respectively, so the probability of finding any such photon vanishes as $\kappa \downarrow 0$ (Proposition 4.16).

Zero-coupling and dipole limits. At $e = 0$, the photons still purify electronic mixed states, so that $F^{0,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{p}}) = F^{0,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{p}}) = F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}})$, the mixed-state Vignale–Rasolt functional (Theorem 4.17), and $F^{e,\chi}_{\mathrm{PFLL}}$ converges to F_{VR} pointwise and in the sense of Mosco as $e \downarrow 0$ (Theorem 4.18). The long-wavelength (dipole) approximation, ubiquitous in practical QEDFT [13, 44, 50], applies when the system size is small compared to the wavelength of the relevant photon modes, so that the vector potential is effectively uniform across the system. We realize this limit by instead rescaling the system: let $F_{\mathrm{PFL},\varepsilon}$ be the PFL functional of the model in which $\mathfrak{A}(\mathbf{x})$ is replaced by $\mathfrak{A}(\varepsilon\mathbf{x})$, so that $\varepsilon = 1$ is the original model and ε plays the role of the ratio of system size to wavelength. As $\varepsilon \downarrow 0$, these functionals converge in the sense of Mosco to the dipole functional F_{d} (Theorem 4.19), whose current argument

$\mathbf{j}^{\mathrm{c,d}}$ is the combined current density formed with the spatially uniform field $\mathfrak{A}(0)$. In the length gauge, F_{d} is the constrained search for the usual dipole Hamiltonian (Corollary 4.22), and Proposition 4.20 gives $F_{\mathrm{d}} \to F_{\mathrm{VR}}$ as $e \downarrow 0$. For fixed N and form factor, these relations are summarized in the diagram

$$\begin{array}{ccccc}
F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{c}}) = F^{e,\chi}_{\mathrm{PFL}}(\rho,\mathbf{j}^{\mathrm{c}}) & & \xrightarrow{\mathbf{j}^{\mathrm{c}}=0} & & F^{e,\chi}_{\mathrm{PFLL}}(\rho,0) = F^{e,\chi}_{\mathrm{PFL}}(\rho,0) \\
\Big\downarrow \text{dipole, } \varepsilon\downarrow 0 & & & & \\
F_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) & & & & \Big\downarrow e\downarrow 0 \\
\Big\downarrow e\downarrow 0 & & & & \\
F^{0,\chi}_{\mathrm{PFL}}(\rho,\mathbf{j}^{\mathrm{p}}) = F_{\mathrm{VR}}(\rho,\mathbf{j}^{\mathrm{p}}) & & \xrightarrow{\mathbf{j}^{\mathrm{p}}=0} & & F^{0,\chi}_{\mathrm{PFL}}(\rho,0) = F_{\mathrm{L}}(\rho)
\end{array}$$

(The curved arrow $e\downarrow 0$ connects $F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{c}})$ directly to $F^{0,\chi}_{\mathrm{PFL}}(\rho,\mathbf{j}^{\mathrm{p}})$.)

where F_{L} is the Lieb functional [33]. The arrow $\varepsilon \downarrow 0$ denotes Mosco convergence, and the arrows $e \downarrow 0$ denote pointwise convergence, which for the curved arrow also holds in the Mosco sense.

Organization of the paper. Sections 2 and 3 introduce the Fock-space setting and the Pauli–Fierz Hamiltonian. The main results are stated in Section 4 and proved in Section 5. The appendices collect transformation properties of the model (dilations, gauge covariance, Weyl displacements, and the length-gauge transformation, among others) and further technical tools.

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Disclosure of AI use and Lean verification

The authors made substantial use of the large language models Claude Opus 5.5 (Anthropic) and GPT 6 Astra (OpenAI) to edit the text, to generate and refine statements and proofs, to check arguments and find errors, and to write the Lean formalization described below. All output was reviewed and edited by the authors, who take full responsibility for the content.

A Lean 4 formalization in the directory `gpt_lean`[1] verifies all new results except those on the long-wavelength limit (Section 4.8). Standard results not involving the Pauli–Fierz model enter as explicit hypotheses: the canonical commutation relations, Weyl operators, Fock-space factorization and the Wiener–Itô–Segal isomorphism; normal and partial traces and closed quadratic forms; completed tensor powers; Sobolev representatives, a local Sobolev embedding, the Hardy and fractional Hardy inequalities, Rellich compactness for $H^{1/2}$ and density in $\dot{H}^{-1/2}$; and L^p duality and the Fenchel–Moreau theorem.

[1] https://github.com/xyzw/qedft_pf_pub

2. Preliminary notions

2.1. **N-particle spaces and the bosonic Fock space.** Let $d \in \mathbb{N}$ be the number of spatial dimensions, $N \in \mathbb{N}$ the number of particles, and $q \in \mathbb{N}$, $q \geq 1$, the number of internal states (for example, $q = 2$ for spin-1/2 particles or for the two transverse polarizations of a photon). We denote the fermionic (a) or bosonic (s) N-particle spaces by

$$\mathfrak{H}^N_{a/s} = L^2_{a/s}((\mathbb{R}^d \times \{1, \dots, q\})^N),$$

where L^2_a (resp. L^2_s) is the Hilbert space of totally antisymmetric (resp. symmetric) square-integrable complex-valued functions both equipped with the inner product

$$\langle \varphi, \psi \rangle_{\mathfrak{H}^N} = \sum_{\sigma_1, \dots, \sigma_N \in \{1, \dots, q\}} \int_{\mathbb{R}^{dN}} \overline{\varphi(\mathbf{x}_1, \sigma_1, \dots, \mathbf{x}_N, \sigma_N)} \times \psi(\mathbf{x}_1, \sigma_1, \dots, \mathbf{x}_N, \sigma_N) \, \mathrm{d}\mathbf{x}_1 \dots \mathrm{d}\mathbf{x}_N.$$

Total antisymmetry (resp. symmetry) is understood with respect to simultaneous permutations of the spatial and spin variables. In what follows, we will often aggregate the spatial variables as $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N)$, and the spin variables as $\boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_N)$ and the spatial-spin variables as $\mathbf{Z} = (\mathbf{z}_1, \dots, \mathbf{z}_N)$, where $\mathbf{z}_j = (\mathbf{x}_j, \sigma_j)$. By abuse of notation, we write $\psi(\mathbf{X}, \boldsymbol{\sigma}) = \psi(\mathbf{Z})$. Whenever necessary, we distinguish the number of particles N in the aggregate vectors as $\mathbf{X}^{(N)}$, $\boldsymbol{\sigma}^{(N)}$ and $\mathbf{Z}^{(N)}$. We equip $\mathbb{R}^d \times \{1, \dots, q\}$ with the product of Lebesgue and counting measure and use the shorthand

$$\int_{\mathbb{R}^d \times \{1, \dots, q\}} h(\mathbf{z}) \, \mathrm{d}\mathbf{z} := \sum_{\sigma=1}^{q} \int_{\mathbb{R}^d} h(\mathbf{x}, \sigma) \, \mathrm{d}\mathbf{x}.$$

Accordingly, for $\mathbf{z} = (\mathbf{x}, \sigma)$ and $\mathbf{z}' = (\mathbf{x}', \sigma')$,

$$\delta(\mathbf{z} - \mathbf{z}') := \delta(\mathbf{x} - \mathbf{x}')\delta_{\sigma,\sigma'}.$$

Electrons will be described by the antisymmetric space $\mathfrak{H}^N_a$ with fixed N, and photons by the bosonic Fock space built from the symmetric spaces.

The bosonic Fock space is defined as the infinite direct sum

$$\mathcal{F}_s = \mathfrak{H}^0 \oplus \mathfrak{H}^1 \oplus \mathfrak{H}^2_s \oplus \dots, \quad \text{with the convention} \quad \mathfrak{H}^0 \equiv \mathbb{C},$$

consisting of infinite tuples $\Psi = (\psi^0, \psi^1, \psi^2, \dots)$, where $\psi^N \in \mathfrak{H}^N_s$, such that

$$\|\Psi\|^2 = \sum_{N \geq 0} \|\psi^N\|^2 < \infty.$$

This space is separable, since $\mathfrak{H}^1$ is. Equipped with the corresponding inner product, i.e.,

$$\langle \Phi, \Psi \rangle_{\mathcal{F}} = \sum_{N \geq 0} \langle \varphi^N, \psi^N \rangle_{\mathfrak{H}^N},$$

the space $\mathcal{F}_s$ is a Hilbert space. Instead of the tuple notation, $\Psi = \psi^0 \oplus \psi^1 \oplus \psi^2 \oplus \dots$ is used sometimes. The canonically embedded subspaces $\mathfrak{H}^N_s \subset \mathcal{F}_s$ are called the N-particle sectors. For any $N \in \mathbb{N}$, the truncated Fock spaces are given by

$$\mathcal{F}^{\leq N}_s = \mathfrak{H}^0 \oplus \mathfrak{H}^1 \oplus \mathfrak{H}^2_s \oplus \dots \oplus \mathfrak{H}^N_s.$$

Moreover, the finite-particle vectors form the dense subspace

$$\mathcal{F}_s^{\mathrm{fin}} = \bigcup_{N\geq 1} \mathcal{F}_s^{\leq N}.$$

We denote by Ω the canonical vacuum vector $\Omega = 1 \oplus 0 \oplus 0 \oplus \dots$ of $\mathcal{F}_s$.

It is possible to symmetrically compose two elements $\psi_1 \in \mathfrak{H}_s^{N_1}$ and $\psi_2 \in \mathfrak{H}_s^{N_2}$ and obtain an element in $\mathfrak{H}_s^{N_1+N_2}$, namely the symmetric tensor product

$$\psi_1 \vee \psi_2 = (N_1!N_2!(N_1+N_2)!)^{-1/2} \sum_{\tau\in S_{N_1+N_2}} \psi_1(\mathbf{z}_{\tau(1)},\dots,\mathbf{z}_{\tau(N_1)}) \times \psi_2(\mathbf{z}_{\tau(N_1+1)},\dots,\mathbf{z}_{\tau(N_1+N_2)}),$$

where S_N denotes the symmetric group on $\{1,\dots,N\}$.

Next, we define the creation and annihilation operators [7, Section 5.2]. For any $f \in \mathfrak{H} := \mathfrak{H}^1$, define the creation operator $a^\dagger(f) : \mathcal{F}_s^{\mathrm{fin}} \to \mathcal{F}_s^{\mathrm{fin}}$ sectorwise by

$$a^\dagger(f)\psi = f \vee \psi$$

for $\psi \in \mathfrak{H}_s^N$, and extend the definition linearly to $\mathcal{F}_s^{\mathrm{fin}}$. Thus $a^\dagger(f)\mathfrak{H}_s^N \subset \mathfrak{H}_s^{N+1}$.

On the same finite-particle space, define the annihilation operator by

$$(a(f)\psi)(\mathbf{z}_1,\dots,\mathbf{z}_{N-1}) = \sqrt{N}\int_{\mathbb{R}^d\times\{1,\dots,q\}} \overline{f(\mathbf{z})}\psi(\mathbf{z},\mathbf{z}_1,\dots,\mathbf{z}_{N-1})\,\mathrm{d}\mathbf{z}, \qquad \psi\in\mathfrak{H}_s^N,$$

and extend it linearly to $\mathcal{F}_s^{\mathrm{fin}}$. We set $a(f)\Omega = 0$, while $a^\dagger(f)\Omega = f$. Moreover,

$$\langle \Phi, a^\dagger(f)\Psi\rangle_{\mathcal{F}} = \langle a(f)\Phi,\Psi\rangle_{\mathcal{F}}, \qquad \Phi,\Psi\in\mathcal{F}_s^{\mathrm{fin}}.$$

The canonical commutation relations (CCR)

$$[a(g),a^\dagger(f)] = \langle g,f\rangle_{\mathfrak{H}}\mathbb{1}_{\mathcal{F}_s},$$
$$[a(g),a(f)] = [a^\dagger(g),a^\dagger(f)] = 0$$

hold for any $f,g\in\mathfrak{H}$ on $\mathcal{F}_s^{\mathrm{fin}}$. These operators are closable, and we use the same symbols for their closures, which are mutual Hilbert-space adjoints. The Segal field operator

$$\boxed{\Phi(f) = a^\dagger(f) + a(f)}$$

is essentially self-adjoint on $\mathcal{F}_s^{\mathrm{fin}}$, and we denote its closure by the same symbol. The *conjugate* Segal field operator, also called the field-momentum operator, is

$$\boxed{\Pi(f) = \Phi(\mathrm{i}f) = \mathrm{i}\big(a^\dagger(f) - a(f)\big).} \tag{1}$$

It is likewise essentially self-adjoint on $\mathcal{F}_s^{\mathrm{fin}}$, and the same symbol denotes its closure. For the vacuum, $\|\Phi(f)\Omega\| = \|\Pi(f)\Omega\| = \|f\|$. For $f\neq 0$, the creation and annihilation operators are unbounded on $\mathcal{F}_s$, but their restrictions to truncated Fock spaces are bounded. More precisely, for $N\in\mathbb{N}$,

$$a(f) : \mathcal{F}_s^{\leq N} \longrightarrow \mathcal{F}_s^{\leq N-1}, \qquad \|a(f)\Psi\| \leq \sqrt{N}\,\|f\|\|\Psi\|,$$
$$a^\dagger(f) : \mathcal{F}_s^{\leq N} \longrightarrow \mathcal{F}_s^{\leq N+1}, \qquad \|a^\dagger(f)\Psi\| \leq \sqrt{N+1}\,\|f\|\|\Psi\|.$$

In contrast, the symbols $a(\mathbf{z})$ and $a^\dagger(\mathbf{z})$ are operator-valued distributions, not operators defined at each fixed $\mathbf{z}$. If $\psi^N\in\mathfrak{H}_s^N$, then $\mathbf{z}\mapsto a(\mathbf{z})\psi^N$ denotes the $\mathfrak{H}_s^{N-1}$-valued L^2 function defined, for almost every $\mathbf{z}$, by

$$(a(\mathbf{z})\psi^N)(\mathbf{z}_1,\dots,\mathbf{z}_{N-1}) = \sqrt{N}\psi^N(\mathbf{z}_1,\dots,\mathbf{z}_{N-1},\mathbf{z}).$$

In particular,

$$\int_{\mathbb{R}^d\times\{1,\dots,q\}} \|a(\mathbf{z})\psi^N\|^2 \,\mathrm{d}\mathbf{z} = N\|\psi^N\|^2.$$

Then, the creation operator is defined by the weak adjoint relation

$$\langle \Phi, a^\dagger(\mathbf{z})\Psi\rangle_{\mathcal{F}} := \langle a(\mathbf{z})\Phi, \Psi\rangle_{\mathcal{F}}, \qquad \Phi,\Psi\in\mathcal{F}_s^{\mathrm{fin}}.$$

Let $\mathcal{S}_{N+1}$ denote the normalized symmetrization operator,

$$(\mathcal{S}_{N+1}F)(\mathbf{z}_1,\dots,\mathbf{z}_{N+1}) = \frac{1}{(N+1)!}\sum_{\tau\in S_{N+1}} F(\mathbf{z}_{\tau(1)},\dots,\mathbf{z}_{\tau(N+1)}).$$

Then, as an identity of distributions,

$$(a^\dagger(\mathbf{z})\psi^N)(\mathbf{z}_1,\dots,\mathbf{z}_{N+1}) = \sqrt{N+1}\,\mathcal{S}_{N+1}\left[\psi^N(\mathbf{z}_1,\dots,\mathbf{z}_N)\delta(\mathbf{z}_{N+1}-\mathbf{z})\right].$$

The smeared identities

$$a^\dagger(f) = \int_{\mathbb{R}^d\times\{1,\dots,q\}} f(\mathbf{z})a^\dagger(\mathbf{z})\,\mathrm{d}\mathbf{z},$$
$$a(f) = \int_{\mathbb{R}^d\times\{1,\dots,q\}} \overline{f(\mathbf{z})}a(\mathbf{z})\,\mathrm{d}\mathbf{z}$$

hold as quadratic forms on $\mathcal{F}_s^{\mathrm{fin}}$. In the same sense, without smearing, the point-field CCR are

$$[a(\mathbf{z}), a^\dagger(\mathbf{z}')] = \delta(\mathbf{z}-\mathbf{z}')\mathbb{1}_{\mathcal{F}_s},$$
$$[a^\dagger(\mathbf{z}), a^\dagger(\mathbf{z}')] = [a(\mathbf{z}), a(\mathbf{z}')] = 0.$$

Smearing the first identity against $\overline{g(\mathbf{z})}f(\mathbf{z}')$ recovers the first CCR above.

2.2. **Partial traces and reduced states.** Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be separable Hilbert spaces and let $\Gamma\in\mathfrak{S}_1(\mathcal{H}_1\otimes\mathcal{H}_2)$ be trace class. Here, $\mathfrak{S}_p$ is the Banach space of p-Schatten-class operators. The partial trace of Γ over the second factor is the unique trace-class operator $\mathrm{Tr}_2\,\Gamma$ on $\mathcal{H}_1$ characterized by

$$\mathrm{Tr}_{\mathcal{H}_1}\left((\mathrm{Tr}_2\,\Gamma)B\right) = \mathrm{Tr}_{\mathcal{H}_1\otimes\mathcal{H}_2}\left(\Gamma(B\otimes\mathbb{1}_{\mathcal{H}_2})\right), \qquad \text{for all } B\in\mathcal{B}(\mathcal{H}_1). \tag{2}$$

Here $\mathcal{B}(\mathcal{H}_1)$ denotes the bounded operators on $\mathcal{H}_1$. Similarly, $\mathrm{Tr}_1\,\Gamma$ is characterized by testing against $\mathbb{1}_{\mathcal{H}_1}\otimes C$, with $C\in\mathcal{B}(\mathcal{H}_2)$. If $(e_j)_{j\geq1}$ is any orthonormal basis of $\mathcal{H}_2$, then

$$\mathrm{Tr}_2\,\Gamma = \sum_{j\geq1}(\mathbb{1}_{\mathcal{H}_1}\otimes\langle e_j|)\,\Gamma\,(\mathbb{1}_{\mathcal{H}_1}\otimes|e_j\rangle),$$

where $\mathbb{1}_{\mathcal{H}_1}\otimes|e_j\rangle : \mathcal{H}_1\to\mathcal{H}_1\otimes\mathcal{H}_2$ maps φ to $\varphi\otimes e_j$, and $\mathbb{1}_{\mathcal{H}_1}\otimes\langle e_j|$ is its adjoint. The sum converges in trace norm and is independent of the chosen basis. Partial trace preserves positivity and the trace. Thus, if $\Gamma\geq0$ and $\mathrm{Tr}\,\Gamma=1$, then both partial traces are again density matrices.

In the electron–photon system below, $\mathcal{H}_1=\mathfrak{H}_{\mathrm{el}}^N$ and $\mathcal{H}_2=\mathcal{F}_{\mathrm{ph}}$. We denote density matrices on the full composite space by $\mathbf{\Gamma}$, retaining unbolded symbols for reduced density matrices. The states

$$\Gamma_{\mathrm{el}} = \mathrm{Tr}_{\mathrm{ph}}\,\mathbf{\Gamma}, \qquad \Gamma_{\mathrm{ph}} = \mathrm{Tr}_{\mathrm{el}}\,\mathbf{\Gamma}$$

are called the electronic and photon reduced states. When the total state is a wavefunction Ψ, the phrase *trace out the photons* means first forming the rank-one density matrix $|\Psi\rangle\langle\Psi|$ and then taking $\mathrm{Tr}_{\mathrm{ph}}\,|\Psi\rangle\langle\Psi|$.

For a normalized pure state, its Schmidt decomposition has the form

$$\Psi = \sum_{j=1}^{r} \sqrt{p_j}\, \Phi_j \otimes \Xi_j, \qquad p_j > 0, \qquad \sum_{j=1}^{r} p_j = 1, \tag{3}$$

where $r \in \mathbb{N} \cup \{\infty\}$ is the Schmidt rank, with $r \leq \min\{\dim \mathcal{H}_1, \dim \mathcal{H}_2\}$, and $(\Phi_j)_{j=1}^r$ and $(\Xi_j)_{j=1}^r$ are orthonormal families in $\mathcal{H}_1$ and $\mathcal{H}_2$, respectively. The two reduced states are then

$$\operatorname{Tr}_2 |\Psi\rangle\langle\Psi| = \sum_{j=1}^{r} p_j |\Phi_j\rangle\langle\Phi_j|, \qquad \operatorname{Tr}_1 |\Psi\rangle\langle\Psi| = \sum_{j=1}^{r} p_j |\Xi_j\rangle\langle\Xi_j|. \tag{4}$$

Thus they have the same nonzero eigenvalues, and either reduced state is pure exactly when $r = 1$, equivalently when Ψ is a product vector. More precisely, a pure marginal is itself a tensor factor of Ψ: for a unit vector $\Xi \in \mathcal{H}_2$,

$$\operatorname{Tr}_1 |\Psi\rangle\langle\Psi| = |\Xi\rangle\langle\Xi| \quad \Longrightarrow \quad \Psi = \Phi \otimes \Xi \ \text{ for a unit vector } \Phi \in \mathcal{H}_1. \tag{5}$$

Indeed, (4) then forces $r = 1$ and $|\Xi_1\rangle\langle\Xi_1| = |\Xi\rangle\langle\Xi|$, so $\Xi_1 = e^{\mathrm{i}\theta}\Xi$ for some $\theta \in \mathbb{R}$ and $\Psi = \Phi_1 \otimes \Xi_1 = (e^{\mathrm{i}\theta}\Phi_1) \otimes \Xi$.

More generally, a normalized vector $\Psi \in \mathcal{H}_1 \otimes \mathcal{H}_2$ is called a *purification* of a density matrix γ on $\mathcal{H}_1$ if

$$\operatorname{Tr}_2 |\Psi\rangle\langle\Psi| = \gamma.$$

Such a purification in the fixed auxiliary space $\mathcal{H}_2$ exists exactly when $\operatorname{rank}\gamma \leq \dim \mathcal{H}_2$. Indeed, if $\gamma = \sum_{j=1}^{r} p_j |\Phi_j\rangle\langle\Phi_j|$, one may choose an orthonormal family $(\Xi_j)_{j=1}^r$ in $\mathcal{H}_2$ and use (3). Since $\mathcal{F}_{\mathrm{ph}}$ is infinite dimensional, every electronic density matrix admits such an abstract Hilbert-space purification. However, the purification might have infinite photon energy.

For a positive trace-class Γ, the defining identity (2) also applies to positive unbounded observables by monotone approximation. In particular,

$$\operatorname{Tr}\big((A \otimes \mathbb{1}_{\mathcal{H}_2})\Gamma\big) = \operatorname{Tr}\big(A \operatorname{Tr}_2 \Gamma\big), \qquad A \geq 0, \tag{6}$$

where both sides are form traces. In particular, the left-hand side means

$$\operatorname{Tr}\Big((\sqrt{A} \otimes \mathbb{1}_{\mathcal{H}_2})\Gamma(\sqrt{A} \otimes \mathbb{1}_{\mathcal{H}_2})\Big).$$

The analogous identity holds for an observable acting only on $\mathcal{H}_2$. This is the sense in which finite electronic kinetic energy and finite photon energy pass to the corresponding reduced states.

The electronic density and paramagnetic current density used below depend only on Γ_{el}, while the free-field energy depends only on Γ_{ph}. By contrast, the field-induced current density contains a joint electron-position–photon observable and is generally not determined by either reduced state separately. The pair of reduced states retains all expectations of observables acting on only one factor, but does not in general determine the electron–photon correlations needed for the field-induced current density.

2.3. **Second quantization of operators.** We briefly recall the second quantization of one-particle operators and refer to [53, Section 7] for details. Let A be a self-adjoint operator on $\mathfrak{H}$. Its N-particle lift $A^{(N)}$ is the closure of $\sum_{j=1}^{N} A_{\mathbf{z}_j}$, initially defined on the algebraic symmetric tensor product of N copies of $D(A)$,

where $A_{\mathbf{z}_j}$ acts on the jth variable. It is self-adjoint on $\mathfrak{H}_s^N$, and we set $A^{(0)} = 0$. The second quantization of A is the self-adjoint operator

$$\mathrm{d}\Gamma(A) = \bigoplus_{N\geq 0} A^{(N)}$$

on $\mathcal{F}_s$, with domain consisting of all $\Psi = \bigoplus_N \psi^N$ such that $\psi^N \in D(A^{(N)})$ and $\sum_N \|A^{(N)}\psi^N\|^2 < \infty$. If $(f_j)_{j\geq 1} \subset D(A)$ is an orthonormal basis of $\mathfrak{H}$, then

$$\mathrm{d}\Gamma(A) = \sum_{j,k\geq 1} \langle f_j, Af_k\rangle\, a^\dagger(f_j)a(f_k)$$

in the sense of quadratic forms on finite-particle vectors [53, Lemma 7.8]. In particular, the number operator $\mathcal{N} = \mathrm{d}\Gamma(\mathbb{1}_{\mathfrak{H}}) = \sum_{j\geq 1} a^\dagger(f_j)a(f_j)$ acts as multiplication by N on $\mathfrak{H}_s^N$. For a tuple $\boldsymbol{A} = (A_1, \dots, A_m)$ of strongly commuting self-adjoint operators and $\boldsymbol{\alpha} \in \mathbb{R}^m$, we write $\mathrm{d}\Gamma(\boldsymbol{A}) = (\mathrm{d}\Gamma(A_1), \dots, \mathrm{d}\Gamma(A_m))$ and $\boldsymbol{\alpha}\cdot\mathrm{d}\Gamma(\boldsymbol{A}) := \mathrm{d}\Gamma(\boldsymbol{\alpha}\cdot\boldsymbol{A})$.

The multiplicative second quantization of a unitary U on $\mathfrak{H}$ is the unitary operator $\Gamma(U) = \bigoplus_{N\geq 0} U^{\otimes N}|_{\mathfrak{H}_s^N}$ on $\mathcal{F}_s$, with $U^{\otimes 0} = 1$ [53, Remark 7.10]. It satisfies

$$\Gamma(U)a^\#(f)\Gamma(U)^\dagger = a^\#(Uf), \qquad \Gamma(U)\mathrm{d}\Gamma(A)\Gamma(U)^\dagger = \mathrm{d}\Gamma(UAU^\dagger),$$
$$\Gamma(e^{-\mathrm{i}tA}) = e^{-\mathrm{i}t\mathrm{d}\Gamma(A)},$$

where $a^\#$ stands for either $a^\dagger$ or a. When no confusion can arise, we use the same symbol U for $\Gamma(U)$.

3. Nonrelativistic quantum electrodynamics

For the remainder of the paper we take $d = 3$ and $q = 1$ (spinless electrons), and write

$$\mathfrak{H}_{\mathrm{el}}^N := \mathfrak{H}_a^N, \qquad \mathcal{F}_{\mathrm{ph}} := \mathcal{F}_s(\mathfrak{H}_{\mathrm{ph}}), \qquad \mathcal{H}_N := \mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\mathrm{ph}},$$

where the one-photon space $\mathfrak{H}_{\mathrm{ph}}$ is defined in Section 3.1 below. The restriction to spinless electrons is for notational simplicity only, and all results extend to the spinful case with the appropriate modifications. Writing $\mathfrak{H}_{\mathrm{ph}}^{\otimes_s M}$ for the M-photon sector of $\mathcal{F}_{\mathrm{ph}}$, with $\mathfrak{H}_{\mathrm{ph}}^{\otimes_s 0} = \mathbb{C}$ and $\mathfrak{H}_{\mathrm{ph}}^{\otimes_s 1} = \mathfrak{H}_{\mathrm{ph}}$, every $\Psi \in \mathcal{H}_N$ has the unique decomposition into M-photon components

$$\Psi = \bigoplus_{M=0}^{\infty} \psi^{(M)}, \qquad \psi^{(M)} \in \mathfrak{H}_{\mathrm{el}}^N \otimes \mathfrak{H}_{\mathrm{ph}}^{\otimes_s M}, \qquad \sum_{M=0}^{\infty} \|\psi^{(M)}\|^2 < \infty. \tag{7}$$

We often view the elements of $\mathcal{H}_N$ as Fock-space-valued functions of the electronic positions. The canonical unitary identification $L^2(\mathbb{R}^{3N}) \otimes \mathcal{F}_{\mathrm{ph}} \cong L^2(\mathbb{R}^{3N}; \mathcal{F}_{\mathrm{ph}})$ maps $\mathcal{H}_N$ onto the functions $\mathbf{X} \mapsto \Psi(\mathbf{X}) \in \mathcal{F}_{\mathrm{ph}}$ that are antisymmetric under permutations of $\mathbf{x}_1, \dots, \mathbf{x}_N$, and

$$\|\Psi\|^2 = \int_{\mathbb{R}^{3N}} \|\Psi(\mathbf{X})\|_{\mathcal{F}_{\mathrm{ph}}}^2 \mathrm{d}\mathbf{X}.$$

Derivatives in the electronic positions are weak derivatives of such functions. For $\Psi \in L^2(\mathbb{R}^{3N}; \mathcal{F}_{\mathrm{ph}})$, $1 \leq n \leq N$ and $\mu = 1, 2, 3$, we say that $\partial_{x_n^\mu}\Psi \in L^2(\mathbb{R}^{3N}; \mathcal{F}_{\mathrm{ph}})$ if there is an element $\partial_{x_n^\mu}\Psi$ of $L^2(\mathbb{R}^{3N}; \mathcal{F}_{\mathrm{ph}})$ such that

$$\int_{\mathbb{R}^{3N}} \partial_{x_n^\mu}\Phi(\mathbf{X})\, \Psi(\mathbf{X})\mathrm{d}\mathbf{X} = -\int_{\mathbb{R}^{3N}} \Phi(\mathbf{X})\, \partial_{x_n^\mu}\Psi(\mathbf{X})\mathrm{d}\mathbf{X} \qquad \text{for every } \Phi \in C_c^\infty(\mathbb{R}^{3N}),$$

where the integrals are Bochner integrals in $\mathcal{F}_{\rm ph}$. Pairing with a fixed $\Xi \in \mathcal{F}_{\rm ph}$ shows that this holds if and only if, for every $\Xi \in \mathcal{F}_{\rm ph}$, the scalar function $\mathbf{X} \mapsto \langle \Xi, \Psi(\mathbf{X})\rangle_{\mathcal{F}_{\rm ph}}$ has weak derivative $\mathbf{X} \mapsto \langle \Xi, \partial_{x_n^\mu}\Psi(\mathbf{X})\rangle_{\mathcal{F}_{\rm ph}}$. In terms of (7), the M-photon component of $\partial_{x_n^\mu}\Psi$ is the weak partial derivative of $\psi^{(M)}$, viewed as a function of the electronic and photon variables, with respect to x_n^μ. We write $\boldsymbol{\nabla}_{\mathbf{x}_n}\Psi = (\partial_{x_n^1}\Psi, \partial_{x_n^2}\Psi, \partial_{x_n^3}\Psi)$ and $\|\boldsymbol{\nabla}_{\mathbf{x}_n}\Psi\|^2 = \sum_{\mu=1}^3 \|\partial_{x_n^\mu}\Psi\|^2$.

3.1. **One-photon space.** Photons have two physical polarizations. One may either use the polarization representation

$$\mathfrak{H}_{\rm ph} = L^2(\mathbb{R}^3 \times \{1,2\})$$

or, without choosing a polarization frame, the solenoidal representation

$$\mathfrak{H}_{\rm sol} = \{\mathbf{f} \in L^2(\mathbb{R}^3, \mathbb{C}^3) : \mathbf{k}\cdot\mathbf{f}(\mathbf{k}) = 0 \text{ for a.a. } \mathbf{k}\}.$$

Choose measurable, real, orthonormal polarization vectors $\boldsymbol{\varepsilon}_1, \boldsymbol{\varepsilon}_2$ such that $\boldsymbol{\varepsilon}_\lambda(\mathbf{k})\cdot\mathbf{k} = 0$ and use the identity

$$\sum_{\lambda=1}^{2} \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) \otimes \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) = \mathbb{1} - \frac{\mathbf{k}\otimes\mathbf{k}}{|\mathbf{k}|^2} =: P_{\rm sol}(\mathbf{k}) \tag{8}$$

to define the solenoidal projector $P_{\rm sol}$. All identities involving $P_{\rm sol}$ are understood almost everywhere, and its value at $\mathbf{k} = 0$ may be fixed arbitrarily. Pointwise multiplication by $P_{\rm sol}$ is an orthogonal projection on $L^2(\mathbb{R}^3, \mathbb{C}^3)$, and

$$\mathfrak{H}_{\rm sol} = \operatorname{Ran} P_{\rm sol}$$

is therefore closed. Under the inverse Fourier transform it is the space of square-integrable vector fields that are divergence-free in the sense of distributions.

More explicitly, the map

$$\iota_{\boldsymbol{\varepsilon}} : \mathfrak{H}_{\rm ph} \longrightarrow \mathfrak{H}_{\rm sol}, \qquad \iota_{\boldsymbol{\varepsilon}} f = \sum_{\lambda=1}^{2} f_\lambda \boldsymbol{\varepsilon}_\lambda, \qquad (\iota_{\boldsymbol{\varepsilon}}^\dagger \mathbf{f})_\lambda = \boldsymbol{\varepsilon}_\lambda \cdot \mathbf{f},$$

is unitary. If $\boldsymbol{\varepsilon}'$ is another measurable polarization frame, then $\iota_{\boldsymbol{\varepsilon}'}^\dagger \iota_{\boldsymbol{\varepsilon}}$ is unitary on $\mathfrak{H}_{\rm ph}$, and its second quantization satisfies

$$\Gamma(\iota_{\boldsymbol{\varepsilon}'}^\dagger \iota_{\boldsymbol{\varepsilon}})\, a^\#(\iota_{\boldsymbol{\varepsilon}}^\dagger \mathbf{f})\, \Gamma(\iota_{\boldsymbol{\varepsilon}'}^\dagger \iota_{\boldsymbol{\varepsilon}})^\dagger = a^\#(\iota_{\boldsymbol{\varepsilon}'}^\dagger \mathbf{f}), \qquad \mathbf{f} \in \mathfrak{H}_{\rm sol}.$$

Thus the creation and annihilation operators of a solenoidal mode $\mathbf{f}$, and all operators built from them below, are unitarily equivalent in the two frames.

3.2. **The vector potential operator.** The photon *dispersion relation*, or simply the *dispersion*, is $\omega(\mathbf{k}) = |\mathbf{k}|$. The free-field Hamiltonian is $H_{\rm rad} = \mathrm{d}\Gamma(\omega)$, discussed further in Section 3.3. We fix a momentum-space coupling profile, or form factor, $\widehat{\chi}$, incorporating the ultraviolet cutoff, and assume that it satisfies

$$\boxed{\widehat{\chi}(\mathbf{k}) = \overline{\widehat{\chi}(-\mathbf{k})}, \qquad \widehat{\chi} \in L^2(\mathbb{R}^3), \qquad \frac{\widehat{\chi}}{\sqrt{\omega}} \in L^2(\mathbb{R}^3).} \tag{9}$$

Such a form factor is necessary to obtain a well-defined Hamiltonian [36, Chapter 11]. The L^2 condition controls, in particular, the vacuum term in the creation-operator estimate. The weighted condition gives relative bounds with respect to

$\sqrt{H_{\mathrm{rad}}}$ and also imposes an infrared condition at $\mathbf{k} = 0$. The hard ultraviolet cutoff used in the examples is

$$\widehat{\chi}_\Lambda(\mathbf{k}) = \frac{\mathbb{1}_{|\mathbf{k}|\leq\Lambda}(\mathbf{k})}{\sqrt{|\mathbf{k}|}}. \tag{10}$$

For $0 \leq \Lambda < \infty$ this satisfies (9), with the value at $\mathbf{k} = 0$ again irrelevant, and

$$\|\widehat{\chi}_\Lambda\|^2 = 2\pi\Lambda^2, \qquad \left\|\frac{\widehat{\chi}_\Lambda}{\sqrt{\omega}}\right\|^2 = 4\pi\Lambda. \tag{11}$$

The assumptions and representability constructions below apply to a general fixed $\widehat{\chi}$. For $\mu = 1, 2, 3$, define the coupling function

$$G^\mu_{\mathbf{x}}(\mathbf{k}, \lambda) = \frac{\varepsilon^\mu_\lambda(\mathbf{k})\widehat{\chi}(-\mathbf{k})e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{\sqrt{2}} \tag{12}$$

and, equivalently in the solenoidal representation,

$$\mathbf{G}^\mu_{\mathbf{x}}(\mathbf{k}) = \frac{P_{\mathrm{sol}}(\mathbf{k})\mathbf{e}_\mu\widehat{\chi}(-\mathbf{k})e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{\sqrt{2}}, \qquad \iota_{\boldsymbol{\varepsilon}} G^\mu_{\mathbf{x}} = \mathbf{G}^\mu_{\mathbf{x}}, \tag{13}$$

where $\mathbf{e}_\mu$ is the μth coordinate vector. The identity for the solenoidal projector (8) gives the exact, uniform relations

$$\sum_{\mu=1}^{3} \|G^\mu_{\mathbf{x}}\|^2 = \|\widehat{\chi}\|^2, \qquad \sum_{\mu=1}^{3} \left\|\frac{G^\mu_{\mathbf{x}}}{\sqrt{\omega}}\right\|^2 = \left\|\frac{\widehat{\chi}}{\sqrt{\omega}}\right\|^2. \tag{14}$$

Dominated convergence also shows that $\mathbf{x} \mapsto G^\mu_{\mathbf{x}}$ is continuous both in $\mathfrak{H}_{\mathrm{ph}}$ and in the norm $f \mapsto \|f/\sqrt{\omega}\|$.

On the finite-particle core $\mathcal{F}^{\mathrm{fin}}_{\mathrm{ph}}$, define the quantized vector potential, componentwise, by the Segal field

$$\boxed{\mathfrak{A}^\mu(\mathbf{x}) = \Phi(G^\mu_{\mathbf{x}}) = a^\dagger(G^\mu_{\mathbf{x}}) + a(G^\mu_{\mathbf{x}}).} \tag{15}$$

It is symmetric and essentially self-adjoint there, and the same notation will denote its self-adjoint closure. We suppress the dependence of $G^\mu_{\mathbf{x}}$ and $\mathfrak{A}^\mu(\mathbf{x})$ on the fixed form factor $\widehat{\chi}$. A superscript χ on the representability sets and universal functionals records this choice. The field $\mathfrak{A}^\mu(\mathbf{x})$ maps each M-photon sector into the direct sum of the $(M-1)$- and $(M+1)$-photon sectors (with the negative sector omitted when $M = 0$).

In the point-field notation of Section 2.1, with $\mathbf{z} = (\mathbf{k}, \lambda)$, in the weak smeared sense on $\mathcal{F}^{\mathrm{fin}}_{\mathrm{ph}}$,

$$a^\dagger(f) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} f(\mathbf{k}, \lambda) a^\dagger(\mathbf{k}, \lambda) \mathrm{d}\mathbf{k}, \qquad a(f) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} \overline{f(\mathbf{k}, \lambda)} a(\mathbf{k}, \lambda) \mathrm{d}\mathbf{k}.$$

We may write (15) as

$$\boxed{\mathfrak{A}(\mathbf{x}) = \frac{1}{\sqrt{2}} \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) \big[\widehat{\chi}(-\mathbf{k})e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}} a^\dagger(\mathbf{k}, \lambda) + \widehat{\chi}(\mathbf{k})e^{\mathrm{i}\mathbf{k}\cdot\mathbf{x}} a(\mathbf{k}, \lambda)\big] \mathrm{d}\mathbf{k}.} \tag{16}$$

The integral in (16) is an operator-valued distribution. On the electron–photon space the notation $\mathfrak{A}^\mu(\mathbf{x}_n)$ means operator-valued multiplication:

$$(\mathfrak{A}^\mu(\mathbf{x}_n)\Psi)(\mathbf{X}) = \mathfrak{A}^\mu(\mathbf{x}_n)\Psi(\mathbf{X}), \qquad \mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N),$$

initially on the natural finite-particle form core. The continuity and uniform bounds above make this multiplication strongly measurable and extend it to the domain used in the Pauli–Fierz form. In the sense of operator-valued distributions we have the Coulomb gauge

$$\boxed{\operatorname{div}\mathfrak{A} = 0.}$$

More explicitly, for every $\eta \in C_c^\infty(\mathbb{R}^3)$,

$$\sum_{\mu=1}^{3} \int_{\mathbb{R}^3} (\partial_\mu \eta)(\mathbf{x}) \mathfrak{A}^\mu(\mathbf{x}) \mathrm{d}\mathbf{x} = 0. \tag{17}$$

This is first an identity on $\mathcal{F}_{\mathrm{ph}}^{\mathrm{fin}}$ and, by (18) and (19) below, also a form identity on $D(\sqrt{H_{\mathrm{rad}}})$. It follows directly from $\mathbf{k} \cdot \boldsymbol{\varepsilon}_\lambda(\mathbf{k}) = 0$.

3.3. **The free field and field bounds.** The free-field Hamiltonian is the second quantization of the dispersion,

$$H_{\mathrm{rad}} = \mathrm{d}\Gamma(\omega) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} |\mathbf{k}|\, a^\dagger(\mathbf{k}, \lambda) a(\mathbf{k}, \lambda) \mathrm{d}\mathbf{k}.$$

On the M-photon sector, H_{rad} is multiplication by $\sum_{m=1}^{M} |\mathbf{k}_m|$. It is positive and self-adjoint,

$$\sigma(H_{\mathrm{rad}}) = [0, \infty), \qquad \ker H_{\mathrm{rad}} = \operatorname{Span}\{\Omega\},$$

and its restriction to $\Omega^\perp$ has purely absolutely continuous spectrum.

The standard creation–annihilation estimates imply, uniformly in $\mathbf{x}$,

$$\|a(G_{\mathbf{x}}^\mu)\Psi\| \leq \|G_{\mathbf{x}}^\mu/\sqrt{\omega}\|\, \|\sqrt{H_{\mathrm{rad}}}\Psi\|, \tag{18}$$

$$\|a^\dagger(G_{\mathbf{x}}^\mu)\Psi\| \leq \|G_{\mathbf{x}}^\mu/\sqrt{\omega}\|\, \|\sqrt{H_{\mathrm{rad}}}\Psi\| + \|G_{\mathbf{x}}^\mu\|\, \|\Psi\|. \tag{19}$$

The same estimates hold with $G_{\mathbf{x}}^\mu$ replaced by any $f \in \mathfrak{H}_{\mathrm{ph}}$ such that $f/\sqrt{\omega} \in \mathfrak{H}_{\mathrm{ph}}$, for every $\Psi \in D(\sqrt{H_{\mathrm{rad}}})$. Consequently, for a constant $C_\chi < \infty$ depending only on the form factor,

$$\|\mathfrak{A}(\mathbf{x})\Psi\|^2 \leq C_\chi \big(\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 + \|\Psi\|^2 \big). \tag{20}$$

These standard field estimates and the associated Pauli–Fierz form construction are discussed, for example, in [34].

The transverse electric and magnetic fields are

$$\mathfrak{E}_\perp(\mathbf{x}) = -\mathrm{i}[H_{\mathrm{rad}}, \mathfrak{A}(\mathbf{x})], \qquad \mathfrak{B}(\mathbf{x}) = \boldsymbol{\nabla} \times \mathfrak{A}(\mathbf{x}), \tag{21}$$

where the commutator and the curl are understood in the sense of operator-valued distributions, that is, after smearing with test fields as in (17). The subscript records that $\mathfrak{E}_\perp$ is only the divergence-free part of the electric field. In Coulomb gauge the longitudinal part is the instantaneous Coulomb field of the charges, which manifests itself as the Coulomb interaction in the Hamiltonian [54]. More explicitly, let $\mathbf{u} \in C_c^\infty(\mathbb{R}^3; \mathbb{R}^3)$ and $g_{\mathbf{u}} = \sum_{\mu=1}^{3} \int_{\mathbb{R}^3} u^\mu(\mathbf{x}) G_{\mathbf{x}}^\mu \mathrm{d}\mathbf{x}$, so that $\int_{\mathbb{R}^3} \mathbf{u} \cdot \mathfrak{A} = a^\dagger(g_{\mathbf{u}}) + a(g_{\mathbf{u}})$. The Fourier transform of $\mathbf{u}$ decays rapidly, hence $\omega g_{\mathbf{u}} \in \mathfrak{H}_{\mathrm{ph}}$, and

$$\int_{\mathbb{R}^3} \mathbf{u} \cdot \mathfrak{E}_\perp = -\mathrm{i}\big(a^\dagger(\omega g_{\mathbf{u}}) - a(\omega g_{\mathbf{u}})\big), \qquad \int_{\mathbb{R}^3} \mathbf{u} \cdot \mathfrak{B} = \int_{\mathbb{R}^3} (\boldsymbol{\nabla} \times \mathbf{u}) \cdot \mathfrak{A}\, \mathrm{d}\mathbf{x}$$

are self-adjoint Segal fields. For a general form factor the fields need not be defined pointwise. If $\sqrt{\omega}\, \widehat{\chi} \in L^2(\mathbb{R}^3)$, the estimates (18) and (19) define $\mathfrak{E}_\perp(\mathbf{x})$ and $\mathfrak{B}(\mathbf{x})$ as forms on $D(\sqrt{H_{\mathrm{rad}}})$ for every $\mathbf{x}$.

Let us summarize the basic properties of these fields. Identities between fields at points are understood after smearing with test fields $\mathbf{u}, \mathbf{v} \in C_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$, as operator identities on $\mathcal{F}_{\mathrm{ph}}^{\mathrm{fin}}$. Both fields are transverse, $\operatorname{div} \mathfrak{E}_\perp = \operatorname{div} \mathfrak{B} = 0$. In fact, for $\mathfrak{E}_\perp$ the vector $g_{\boldsymbol{\nabla}\eta}$ vanishes for every $\eta \in C_c^\infty(\mathbb{R}^3)$, exactly as in (17), and for $\mathfrak{B}$ this follows from $\boldsymbol{\nabla} \times \boldsymbol{\nabla}\eta = 0$. The components of $\mathfrak{A}$ commute, as do those of $\mathfrak{E}_\perp$, and the two fields form a canonical pair:

$$[\mathfrak{A}^\mu(\mathbf{x}), \mathfrak{A}^\nu(\mathbf{y})] = [\mathfrak{E}_\perp^\mu(\mathbf{x}), \mathfrak{E}_\perp^\nu(\mathbf{y})] = 0,$$
$$[\mathfrak{A}^\mu(\mathbf{x}), \mathfrak{E}_\perp^\nu(\mathbf{y})] = -\mathrm{i}\int_{\mathbb{R}^3} \omega(\mathbf{k})|\widehat{\chi}(\mathbf{k})|^2 P_{\mathrm{sol}}(\mathbf{k})^{\mu\nu} e^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\mathrm{d}\mathbf{k}.$$

Indeed, $[a^\dagger(f) + a(f), a^\dagger(h) + a(h)] = 2\mathrm{i}\,\mathrm{Im}\langle f, h\rangle$. The scalar products $\langle g_{\mathbf{u}}, g_{\mathbf{v}}\rangle$ and $\langle \omega g_{\mathbf{u}}, \omega g_{\mathbf{v}}\rangle$ are real, since $\mathbf{u}, \mathbf{v}$ are real and $|\widehat{\chi}|$, ω and P_{sol} are even in $\mathbf{k}$, while

$$\Big[\int_{\mathbb{R}^3} \mathbf{u}\cdot\mathfrak{A}, \int_{\mathbb{R}^3} \mathbf{v}\cdot\mathfrak{E}_\perp\Big] = -2\mathrm{i}\,\mathrm{Re}\langle g_{\mathbf{u}}, \omega g_{\mathbf{v}}\rangle.$$

Commutators involving $\mathfrak{B}$ follow by taking the curl in the corresponding variable. In particular, the components of $\mathfrak{B}$ commute with those of $\mathfrak{A}$ and with each other. For the hard cutoff (10), $\omega|\widehat{\chi}_\Lambda|^2$ is the indicator function of the ball of radius Λ, so

$$[\mathfrak{A}^\mu(\mathbf{x}), \mathfrak{E}_\perp^\nu(\mathbf{y})] = -\mathrm{i}\int_{|\mathbf{k}|\le\Lambda} P_{\mathrm{sol}}(\mathbf{k})^{\mu\nu} e^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\mathrm{d}\mathbf{k}. \tag{22}$$

The right-hand side is $-\mathrm{i}(2\pi)^3$ times the transverse delta function with momenta cut off at Λ. The factor $(2\pi)^3$ reflects the normalization of $\widehat{\chi}$.

Since $\mathfrak{E}_\perp$ and $\mathfrak{B}$ carry the form factor, H_{rad} is not their field energy. Write $:\cdot:$ for normal ordering, which places all creation operators to the left of all annihilation operators. Inserting (16), the terms with two creation or two annihilation operators cancel between the electric and magnetic parts, and a formal computation gives

$$\frac{1}{2}\int_{\mathbb{R}^3} :|\mathfrak{E}_\perp|^2 + |\mathfrak{B}|^2: = (2\pi)^3 \mathrm{d}\Gamma\big(\omega^2|\widehat{\chi}|^2\big).$$

This equals H_{rad} exactly when $|\widehat{\chi}| = (2\pi)^{-3/2}\omega^{-1/2}$, that is, without cutoff.

3.4. **The Pauli–Fierz Hamiltonian.** We first construct the internal Hamiltonian. Put

$$\mathcal{Q}_{\mathrm{PF}} := \Big\{\Psi \in \mathcal{H}_N : \boldsymbol{\nabla}_{\mathbf{x}_n}\Psi \in L^2(\mathbb{R}^{3N};\mathcal{F}_{\mathrm{ph}})^3 \ (1 \le n \le N), \quad \sqrt{H_{\mathrm{rad}}}\Psi \in \mathcal{H}_N\Big\} \tag{23}$$

and equip it with the reference norm

$$\|\Psi\|_{\mathcal{Q}_{\mathrm{PF}}}^2 := \|\Psi\|^2 + \sum_{n=1}^N \|\boldsymbol{\nabla}_{\mathbf{x}_n}\Psi\|^2 + \|\sqrt{H_{\mathrm{rad}}}\Psi\|^2. \tag{24}$$

Thus $\mathcal{Q}_{\mathrm{PF}}$ is the antisymmetric, Fock-space-valued electronic H^1 space intersected with the form domain of the radiation energy. The algebraic tensor product

$$\mathscr{C}_{\mathrm{PF}} = \big(C_c^\infty(\mathbb{R}^{3N}) \cap \mathfrak{H}_{\mathrm{el}}^N\big) \otimes_{\mathrm{alg}} \mathcal{F}_s^{\mathrm{alg}}\big(C_c^\infty\big((\mathbb{R}^3 \setminus \{0\}) \times \{1,2\}\big)\big) \tag{25}$$

is dense in $\mathcal{Q}_{\mathrm{PF}}$ for $\|\cdot\|_{\mathcal{Q}_{\mathrm{PF}}}$. Here $\mathcal{F}_s^{\mathrm{alg}}(\mathcal{D})$ is the algebraic symmetric Fock space over a space $\mathcal{D}$ of one-photon functions, that is, the finite linear combinations of

the vacuum and of symmetric tensor products of finitely many elements of $\mathcal{D}$. Fix $e \geq 0$[2] and set

$$\boxed{\mathbf{D}_n = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\mathfrak{A}(\mathbf{x}_n).}$$

The internal Pauli–Fierz Hamiltonian is

$$\boxed{H^{0,0} = \frac{1}{2}\sum_{n=1}^{N} \mathbf{D}_n^2 + \sum_{1\leq n<m\leq N} \frac{1}{|\mathbf{x}_n - \mathbf{x}_m|} + H_{\mathrm{rad}}} \tag{26}$$

on $\mathscr{C}_{\mathrm{PF}}$. Expanding the square, the weak Coulomb gauge (17) gives $\mathbf{D}_n^2\Psi = -\Delta_{\mathbf{x}_n}\Psi + 2\mathrm{i}e\mathfrak{A}(\mathbf{x}_n)\cdot\boldsymbol{\nabla}_{\mathbf{x}_n}\Psi + e^2|\mathfrak{A}(\mathbf{x}_n)|^2\Psi$, so (26) is a nonnegative symmetric operator on $\mathscr{C}_{\mathrm{PF}}$. The field bound (20) and $-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} = \mathbf{D}_n + e\mathfrak{A}(\mathbf{x}_n)$ control the ordinary and covariant derivatives in terms of each other, and the Coulomb repulsion is infinitesimally form bounded with respect to the electronic kinetic energy [43, Theorem X.16]. Hence there are constants $0 < c \leq C < \infty$, depending on N, e and the cutoff, such that on $\mathscr{C}_{\mathrm{PF}}$,

$$c\|\Psi\|^2_{\mathcal{Q}_{\mathrm{PF}}} \leq \langle\Psi, (H^{0,0}+1)\Psi\rangle \leq C\|\Psi\|^2_{\mathcal{Q}_{\mathrm{PF}}}. \tag{27}$$

From now on, $H^{0,0}$ denotes the Friedrichs extension [31, Chapter 3] of (26). Since $\mathscr{C}_{\mathrm{PF}}$ is dense in $\mathcal{Q}_{\mathrm{PF}}$, (27) identifies its form domain:

$$Q(H^{0,0}) = \mathcal{Q}_{\mathrm{PF}}. \tag{28}$$

For a semibounded self-adjoint operator H and $\Psi \in Q(H)$, we write $\langle\Psi, H\Psi\rangle$ for the value of its closed form at Ψ, even if $\Psi \notin D(H)$. Operator cores and operator domains are studied in [22, 21, 38], but only the form domain will be of relevance here.

For real external potentials satisfying

$$v \in L^{3/2}(\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3), \qquad \mathbf{A} \in L^3(\mathbb{R}^3,\mathbb{R}^3) + L^{\infty}(\mathbb{R}^3,\mathbb{R}^3), \tag{29}$$

the Hamiltonian is formally

$$\boxed{H^{v,\mathbf{A}} = \sum_{n=1}^{N}\left[\frac{1}{2}\big(\mathbf{D}_n + \mathbf{A}(\mathbf{x}_n)\big)^2 + v(\mathbf{x}_n)\right] + \sum_{1\leq n<m\leq N}\frac{1}{|\mathbf{x}_n - \mathbf{x}_m|} + H_{\mathrm{rad}}.}$$

By the Sobolev inequality, $|\mathbf{A}(\mathbf{x}_n)|^2$ and $v(\mathbf{x}_n)$ are infinitesimally form bounded with respect to $-\Delta_{\mathbf{x}_n}$, hence by (27) also with respect to $H^{0,0}$. Cauchy–Schwarz controls the cross term $\mathrm{Re}\langle\mathbf{D}_n\Psi, \mathbf{A}(\mathbf{x}_n)\Psi\rangle$. The KLMN theorem [43, Theorem X.17] therefore defines $H^{v,\mathbf{A}}$ as a semibounded self-adjoint operator with

$$Q(H^{v,\mathbf{A}}) = \mathcal{Q}_{\mathrm{PF}} \tag{30}$$

and shifted form norm equivalent to $\|\cdot\|_{\mathcal{Q}_{\mathrm{PF}}}$.

The bottom of the spectrum is

$$E(v,\mathbf{A}) = \inf\sigma(H^{v,\mathbf{A}}) = \inf_{\substack{\Psi\in\mathcal{Q}_{\mathrm{PF}}\\ \|\Psi\|=1}} \langle\Psi, H^{v,\mathbf{A}}\Psi\rangle, \tag{31}$$

[2]The photon parity $(-1)^{\mathcal{N}} = \Gamma(-\mathbb{1})$ satisfies $(-1)^{\mathcal{N}}a^{\#}(f)(-1)^{\mathcal{N}} = -a^{\#}(f)$, so it reverses the sign of $\mathfrak{A}(\mathbf{x})$, commutes with H_{rad} and acts trivially on the electrons. It therefore maps the Hamiltonians below at coupling e to those at $-e$ and preserves ρ_Ψ and the combined current density $\mathbf{j}^{\mathrm{c}}_\Psi$ of (36). Hence the representability sets and universal functionals are the same for e and $-e$.

which is greater than $-\infty$ by the KLMN theorem. We call $E(v, \mathbf{A})$ the ground-state energy even when the infimum is not attained. A ground state is a normalized minimizer, equivalently an eigenvector at the bottom of the spectrum.

Mixed states of the electron–photon system are the density matrices on $\mathcal{H}_N$, that is, the operators $\mathbf{\Gamma} \in \mathfrak{S}_1(\mathcal{H}_N)$ with $\mathbf{\Gamma} \geq 0$ and $\operatorname{Tr} \mathbf{\Gamma} = 1$. Among these, the finite-energy ones form the class

$$\mathcal{D} = \left\{ \mathbf{\Gamma} \in \mathfrak{S}_1(\mathcal{H}_N) : \mathbf{\Gamma} \geq 0, \quad \operatorname{Tr} \mathbf{\Gamma} = 1, \quad \operatorname{Tr}\left(H^{0,0}\mathbf{\Gamma}\right) < \infty \right\}. \tag{32}$$

Here the energy trace is understood in the form sense: for a spectral decomposition $\mathbf{\Gamma} = \sum_r p_r |\Psi_r\rangle\langle\Psi_r|$ over the positive eigenvalues we take

$$\operatorname{Tr}\left(H^{0,0}\mathbf{\Gamma}\right) = \sum_r p_r \|\sqrt{H^{0,0}}\Psi_r\|^2 \in [0, \infty],$$

where the rth term is $+\infty$ unless $\Psi_r \in \mathcal{Q}_{\mathrm{PF}}$. In particular, every eigenvector of a $\mathbf{\Gamma} \in \mathcal{D}$ with positive eigenvalue lies in $\mathcal{Q}_{\mathrm{PF}}$. The elements of $\mathcal{D}$ are the finite-energy density matrices, often called ensembles in DFT.

Ground-state existence is a separate compactness and infrared question and does not follow from self-adjointness. For atoms and molecules satisfying appropriate binding conditions, existence with massless photons, arbitrary coupling, and a finite ultraviolet cutoff was established in [19, 34]. Abstract existence criteria for massless Pauli–Fierz Hamiltonians were given in [17]. Conversely, translation-invariant models with nonzero net charge can have no Fock-space ground state [20]. Ionization thresholds and exponential localization below them are analyzed in [18]. For particles bound by external potentials with a spatially cut off interaction, ground states, localization, and resonance phenomena were studied in [1]. Finally, for abstract massless, linearly coupled Pauli–Fierz models, local finiteness of the point spectrum and a limiting absorption principle away from eigenvalues are among the results of [16].

4. Main results

In this section, we present our main results, which are proved in Section 5.

4.1. **The combined current density.** For $\Phi, \Psi \in \mathcal{H}_N$, let $\langle \Phi, \Psi \rangle_{\mathbf{x}}$ denote the partial inner product in every variable (including the photon inner product) except the first electronic position $\mathbf{x} = \mathbf{x}_1$, and $\|\Phi\|_{\mathbf{x}} := \langle \Phi, \Phi \rangle_{\mathbf{x}}^{1/2}$ the corresponding partial norm. For $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, define the *electron density* ρ_Ψ, the *paramagnetic current density* $\mathbf{j}_\Psi^{\mathrm{p}}$, the *field-induced current density* $\mathbf{j}_\Psi^{\mathrm{ph}}$, and the *combined current density* $\mathbf{j}_\Psi^{\mathrm{c}}$ by

$$\rho_\Psi(\mathbf{x}) = N \langle \Psi, \Psi \rangle_{\mathbf{x}}, \tag{33}$$

$$\mathbf{j}_\Psi^{\mathrm{p}}(\mathbf{x}) = N \operatorname{Im} \langle \Psi, \boldsymbol{\nabla}_{\mathbf{x}} \Psi \rangle_{\mathbf{x}}, \tag{34}$$

$$\mathbf{j}_\Psi^{\mathrm{ph}}(\mathbf{x}) = -eN \operatorname{Re} \langle \Psi, \mathfrak{A}(\mathbf{x}) \Psi \rangle_{\mathbf{x}}, \tag{35}$$

$$\mathbf{j}_\Psi^{\mathrm{c}}(\mathbf{x}) = N \operatorname{Re} \langle \Psi, \left(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}} - e\mathfrak{A}(\mathbf{x}) \right) \Psi \rangle_{\mathbf{x}} = \mathbf{j}_\Psi^{\mathrm{p}}(\mathbf{x}) + \mathbf{j}_\Psi^{\mathrm{ph}}(\mathbf{x}). \tag{36}$$

If Ψ is normalized, then $\int_{\mathbb{R}^3} \rho_\Psi = N$. From the quadratic-form identity

$$\frac{1}{2}(\mathbf{D}_n + \mathbf{A})^2 = \frac{1}{2}\mathbf{D}_n^2 + \frac{1}{2}(\mathbf{D}_n \cdot \mathbf{A} + \mathbf{A} \cdot \mathbf{D}_n) + \frac{1}{2}|\mathbf{A}|^2$$

we obtain the decomposition

$$\boxed{\langle \Psi, H^{v,\mathbf{A}}\Psi\rangle = \langle \Psi, H^{0,0}\Psi\rangle + \langle v + \tfrac{1}{2}|\mathbf{A}|^2, \rho_\Psi\rangle + \langle \mathbf{A}, \mathbf{j}^{\mathrm{c}}_\Psi\rangle.} \tag{37}$$

Equation (37) shows that the external potentials couple to the state through the density and combined current density. We therefore choose these as the basic variables of our density-functional formulation.

The following bounds show how finite energy controls the density and current densities and determine the function spaces used below. Recall from Section 3.4 that $\mathbf{D}_n = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\mathfrak{A}(\mathbf{x}_n)$ is the covariant momentum of the nth electron. The constant C_χ is from the field bound (20).

Proposition 4.1 (A priori density–current bounds)**.** *In the following estimates, quotients are defined to be zero wherever the density vanishes. For every normalized $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, we have $\rho_\Psi \geq 0$, $\int_{\mathbb{R}^3} \rho_\Psi = N$, $\sqrt{\rho_\Psi} \in H^1(\mathbb{R}^3)$, and*

$$\int_{\mathbb{R}^3} \left(|\boldsymbol{\nabla}\sqrt{\rho_\Psi}|^2 + \frac{|\mathbf{j}^{\mathrm{c}}_\Psi|^2}{\rho_\Psi} \right) \leq \sum_{n=1}^{N} \|\mathbf{D}_n \Psi\|^2. \tag{38}$$

Moreover,

$$\int_{\mathbb{R}^3} \frac{|\mathbf{j}^{\mathrm{ph}}_\Psi|^2}{\rho_\Psi} \leq e^2 N \|\mathfrak{A}(\mathbf{x}_1)\Psi\|^2 \leq e^2 N C_\chi \big(\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 + 1 \big). \tag{39}$$

In particular, $\rho_\Psi \in L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3)$ and $\mathbf{j}^{\mathrm{c}}_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi, \mathbf{j}^{\mathrm{ph}}_\Psi \in L^1(\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3)$.

The same conclusions hold for every normalized finite-energy density matrix $\boldsymbol{\Gamma} = \sum_r p_r |\Psi_r\rangle\langle\Psi_r| \in \mathcal{D}$, with $\rho_{\boldsymbol{\Gamma}} = \sum_r p_r \rho_{\Psi_r}$ and similarly for all three current densities. Each squared norm on the right-hand sides of the estimates is replaced by the corresponding nonnegative form trace, defined by spectral averaging, e.g., $\mathrm{Tr}\big(\mathbf{D}_n^2 \boldsymbol{\Gamma}\big) = \sum_r p_r \|\mathbf{D}_n \Psi_r\|^2$.

The Coulomb-gauge relation $\operatorname{div} \mathfrak{A} = 0$ does *not* imply that the field-induced current density of an electron-photon entangled state is solenoidal.

Proposition 4.2 (Divergence of the field-induced current density)**.** *For every $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, in the sense of distributions,*

$$\operatorname{div} \mathbf{j}^{\mathrm{ph}}_\Psi(\mathbf{x}) = -2eN \operatorname{Re} \sum_{\mu=1}^{3} \langle \partial_\mu \Psi, \mathfrak{A}^\mu(\mathbf{x})\Psi\rangle_{\mathbf{x}}. \tag{40}$$

The right-hand side is integrable, and

$$\int_{\mathbb{R}^3} \big| \operatorname{div} \mathbf{j}^{\mathrm{ph}}_\Psi \big| \leq 2eN \|\boldsymbol{\nabla}_{\mathbf{x}_1}\Psi\| \, \|\mathfrak{A}(\mathbf{x}_1)\Psi\| < \infty. \tag{41}$$

Neither $\mathbf{j}^{\mathrm{ph}}_\Psi$ nor $\mathbf{j}^{\mathrm{ph}}_\Psi/\rho_\Psi$ is divergence-free in general.

For a concrete one-electron example, let $\varphi_0, \varphi_1 \in H^1(\mathbb{R}^3)$, let $\xi \in D(\sqrt{\omega})$ be normalized, assume $\|\varphi_0\|^2 + \|\varphi_1\|^2 = 1$, and set $\Psi(\mathbf{x}) = \varphi_0(\mathbf{x})\Omega + \varphi_1(\mathbf{x}) a^\dagger(\xi)\Omega$. Then $\rho_\Psi = |\varphi_0|^2 + |\varphi_1|^2$ and with $\mathbf{g}_\xi(\mathbf{x}) = \langle \Omega, \mathfrak{A}(\mathbf{x}) a^\dagger(\xi)\Omega\rangle$ it holds

$$\mathbf{j}^{\mathrm{ph}}_\Psi = -2e \operatorname{Re}(\overline{\varphi_0}\varphi_1 \mathbf{g}_\xi). \tag{42}$$

Although $\operatorname{div} \mathbf{g}_\xi = 0$, the right-hand side of (42) has nonzero divergence in general.

Recall the definition $\mathbf{j}_\Psi = \mathbf{j}^{\mathrm{c}}_\Psi + \rho_\Psi \mathbf{A}$ of the physical current density.

Proposition 4.3 (Fields in a ground state)**.** *Let Ψ be a ground state of $H^{v,\mathbf{A}}$. Then $\mathbf{j}_\Psi \in L^1(\mathbb{R}^3;\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3;\mathbb{R}^3)$, and the following hold.*

(i) The current density is divergence-free: $\operatorname{div} \mathbf{j}_\Psi = 0$ *in the sense of distributions.*
(ii) The transverse electric field vanishes: $\langle \Psi, \mathfrak{E}_\perp(\mathbf{x})\Psi\rangle = 0$.
(iii) The magnetic field satisfies the Ampère law

$$\boldsymbol{\nabla} \times \langle \Psi, \mathfrak{B}(\mathbf{x})\Psi\rangle = e \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \omega(\mathbf{k})|\widehat{\chi}(\mathbf{k})|^2 P_{\mathrm{sol}}(\mathbf{k}) e^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})} \mathbf{j}_\Psi(\mathbf{y}) \mathrm{d}\mathbf{k}\, \mathrm{d}\mathbf{y}.$$

(iv) If $\mathbf{A} = 0$ and the ground state is nondegenerate, then $\mathbf{j}_\Psi = 0$ and $\langle \Psi, \mathfrak{A}(\mathbf{x})\Psi\rangle = \langle \Psi, \mathfrak{B}(\mathbf{x})\Psi\rangle = 0$.

Thus, the ground state carries the static field generated by its own current density. The transverse electric field vanishes, and the magnetic field obeys the magnetostatic Ampère law, with the divergence-free current density $\mathbf{j}_\Psi$ as its source and the kernel of the commutator $[\mathfrak{A}, \mathfrak{E}_\perp]$ in place of the transverse delta function (compare (22)).

Items (i)–(iii) are well known at the formal level. Since time derivatives of expectation values vanish in an eigenstate, they are the stationary forms of the continuity equation and of the Ehrenfest–Maxwell equation for the vector potential, whose source is the current density (see [46, Eq. (49), Sec. IV.A and App. C]). Item (iv) is the usual time-reversal argument. We record Proposition 4.3, with a variational proof under the present hypotheses, for later comparison with the optimizers of the constrained search in Section 4.6.1.

4.2. **N-representability.** A *density–current pair* consists of a density and a current density. The main density variable is the pair $(\rho, \mathbf{j}^{\mathrm{c}})$ formed with the combined current density, rather than a fixed decomposition of $\mathbf{j}^{\mathrm{c}}$ into electronic and photonic pieces. The pure-state N-representability class is then

$$\mathcal{J}_N^{e,\chi} = \{(\rho_\Psi, \mathbf{j}^{\mathrm{c}}_\Psi) : \Psi \in \mathcal{Q}_{\mathrm{PF}},\ \|\Psi\| = 1\}.$$

The photon variables also turn a pure total state into a purification of a mixed electronic state. To make this precise, denote the finite-kinetic-energy electronic mixed-state class by

$$\mathcal{J}^{\mathrm{el}}_{N,\mathrm{mix}} = \left\{(\rho_\Gamma, \mathbf{j}^{\mathrm{p}}_\Gamma) :\ \Gamma \in \mathfrak{S}_1(\mathfrak{H}^N_{\mathrm{el}}),\ \Gamma \geq 0,\ \operatorname{Tr}\Gamma = 1,\ \operatorname{Tr}(-\boldsymbol{\Delta}\Gamma) < \infty\ \right\}. \tag{43}$$

Here $\boldsymbol{\Delta}$ is the Laplacian in all N electronic coordinates. Equivalently, by the mixed-state one-body density-matrix theorem [9] (see [36, Chapter 3] for an elementary proof), a pair $(\rho, \mathbf{j})$ is in $\mathcal{J}^{\mathrm{el}}_{N,\mathrm{mix}}$ if and only if there is a one-particle density matrix γ on $L^2(\mathbb{R}^3)$ such that

$$0 \leq \gamma \leq 1, \qquad \operatorname{Tr}\gamma = N, \qquad \operatorname{Tr}(-\Delta\gamma) < \infty, \qquad (\rho_\gamma, \mathbf{j}^{\mathrm{p}}_\gamma) = (\rho, \mathbf{j}). \tag{44}$$

Equation (44) is an exact operator characterization, although it is not yet an intrinsic characterization solely by elementary conditions on $(\rho, \mathbf{j})$.

Theorem 4.4 (Photon purification and exact electronic projection)**.** *For every $e \geq 0$,*

$$\{(\rho_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi) : \Psi \in \mathcal{Q}_{\mathrm{PF}},\ \|\Psi\| = 1\} = \mathcal{J}^{\mathrm{el}}_{N,\mathrm{mix}}. \tag{45}$$

More sharply, the zero-field-current slice of the pure-state triple class is exactly

$$\left\{(\rho_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi, \mathbf{j}^{\mathrm{ph}}_\Psi) : \Psi \in \mathcal{Q}_{\mathrm{PF}},\ \|\Psi\| = 1,\ \mathbf{j}^{\mathrm{ph}}_\Psi = 0\right\} = \left\{(\rho, \mathbf{j}, 0) : (\rho, \mathbf{j}) \in \mathcal{J}^{\mathrm{el}}_{N,\mathrm{mix}}\right\}. \tag{46}$$

Thus the photon space allows one to purify every finite-energy electronic density matrix.

For the mixed-state statement below, recall the class $\mathcal{D}$ of finite-energy density matrices from (32). For $\mathbf{\Gamma} \in \mathcal{D}$ with spectral decomposition $\mathbf{\Gamma} = \sum_r p_r |\Psi_r\rangle\langle\Psi_r|$ over the positive eigenvalues, set

$$\rho_{\mathbf{\Gamma}} = \sum_r p_r \rho_{\Psi_r}, \qquad \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} = \sum_r p_r \mathbf{j}^{\mathrm{c}}_{\Psi_r}. \tag{47}$$

Theorem 4.5 (Equivalence of pure and mixed N-representability)**.** *Suppose that $\widehat{\chi} = 0$ almost everywhere on a measurable set $S \subset \mathbb{R}^3$ of positive measure. Then pure and mixed N-representability coincide:*

$$\mathcal{J}_N^{e,\chi} = \{(\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}) : \mathbf{\Gamma} \in \mathcal{D}\}. \tag{48}$$

In particular, $\mathcal{J}_N^{e,\chi}$ is convex.

Clearly, for the hard cutoff (10) with $0 \le \Lambda < \infty$, the hypothesis holds.

When an electronic representative can itself be chosen pure, no photon purification is needed. If $(\rho, \rho\mathbf{v})$ is represented in ordinary paramagnetic CDFT by a finite-kinetic-energy state $\Phi \in \mathfrak{H}^N_{\mathrm{el}}$, then $(\rho, \rho\mathbf{v}) \in \mathcal{J}_N^{e,\chi}$ for every $e \ge 0$. Indeed, we can simply take $\Psi = \Phi \otimes \Omega$. Since $\langle \Omega, \mathfrak{A}(\mathbf{x})\Omega\rangle = 0$, one has $\rho_\Psi = \rho$, $\mathbf{j}^{\mathrm{ph}}_\Psi = 0$, and $\mathbf{j}^{\mathrm{c}}_\Psi = \mathbf{j}^{\mathrm{p}}_\Phi = \rho\mathbf{v}$. The field bound implies $\langle \Psi, H^{0,0}\Psi\rangle < \infty$, since the ultraviolet cutoff makes the vacuum fluctuation in $|\mathfrak{A}|^2$ finite.

An intrinsic sufficient condition follows from a coherent displacement that depends on the electronic positions. The resulting conditional field can be nontransverse even though the field operator is transverse.

Theorem 4.6 (Photonic representability)**.** *Let $N \in \mathbb{N}$ and $e \ge 0$, and suppose $\widehat{\chi} \not\equiv 0$. Let*

$$\rho \ge 0, \qquad \int_{\mathbb{R}^3} \rho = N, \qquad \sqrt{\rho} \in H^1(\mathbb{R}^3),$$

and let $\mathbf{a}, \mathbf{b} \in H^1_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R}^3)$ and $S \in H^1_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R})$ satisfy

$$\int_{\mathbb{R}^3} \rho\big(|\mathbf{a}|^2 + |\mathbf{\nabla}\mathbf{a}|^2 + |\mathbf{b}|^2 + |\mathbf{\nabla}\mathbf{b}|^2 + |\mathbf{\nabla}S|^2\big) < \infty,$$

where $\mathbf{\nabla}\mathbf{a}$ and $\mathbf{\nabla}\mathbf{b}$ are weak Jacobians. Then there is a normalized pure state $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ such that

$$\rho_\Psi = \rho, \qquad \mathbf{j}^{\mathrm{p}}_\Psi = \rho(\mathbf{\nabla}S + \mathbf{b}), \qquad \mathbf{j}^{\mathrm{ph}}_\Psi = -e\rho\mathbf{a}, \tag{49}$$

and

$$\begin{aligned} &\sum_{n=1}^N \|\mathbf{\nabla}_{\mathbf{x}_n}\Psi\|^2 + \langle \Psi, H_{\mathrm{rad}}\Psi\rangle \\ &\quad \le C_{N,\chi}\left(1 + \int_{\mathbb{R}^3} |\mathbf{\nabla}\sqrt{\rho}|^2 + \int_{\mathbb{R}^3} \rho\big(|\mathbf{a}|^2 + |\mathbf{\nabla}\mathbf{a}|^2 + |\mathbf{b}|^2 + |\mathbf{\nabla}\mathbf{b}|^2 + |\mathbf{\nabla}S|^2\big)\right), \end{aligned} \tag{50}$$

with a constant independent of ρ, $\mathbf{a}$, $\mathbf{b}$ and S.

In particular, every $\mathbf{a} \in W^{1,\infty}(\mathbb{R}^3; \mathbb{R}^3)$ is allowed for every density in the theorem. The paramagnetic velocity $\mathbf{b}$ is subject only to the same weighted Sobolev condition and need be neither bounded nor curl-free. For instance, the rigid rotation $\mathbf{b} = \boldsymbol{\omega} \times \mathbf{x}$ is allowed whenever $\int \rho|\mathbf{x}|^2 < \infty$. The local Sobolev condition asks for a velocity

defined on the whole space, but no positive lower bound on ρ is required. Form equivalence (27) also bounds the internal energy by the right-hand side of (50), with a constant depending additionally on e.

Corollary 4.7 (A Sobolev class of combined current densities)**.** *Suppose $e > 0$ and $\widehat{\chi} \not\equiv 0$. For every $N \in \mathbb{N}$,*

$$\left\{ (\rho, \rho\mathbf{v}) : \begin{array}{ll} \rho \geq 0, & \int_{\mathbb{R}^3} \rho = N, \quad \sqrt{\rho} \in H^1, \\ \mathbf{v} \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^3), & \displaystyle\int_{\mathbb{R}^3} \rho\big(|\mathbf{v}|^2 + |\boldsymbol{\nabla}\mathbf{v}|^2\big) < \infty \end{array} \right\} \subset \mathcal{J}_N^{e,\chi}.$$

The same conclusion holds for velocities $\boldsymbol{\nabla} S + \mathbf{w}$ with $S \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R})$, $\mathbf{w} \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^3)$, and

$$\int_{\mathbb{R}^3} \rho\big(|\boldsymbol{\nabla} S|^2 + |\mathbf{w}|^2 + |\boldsymbol{\nabla}\mathbf{w}|^2\big) < \infty.$$

Proof. Apply Theorem 4.6 with $\mathbf{a} = -\mathbf{v}/e$, $S = 0$ and $\mathbf{b} = 0$. For the second assertion use $\mathbf{a} = -\mathbf{w}/e$, the given S, and $\mathbf{b} = 0$. Then (36) gives the prescribed combined current density. □

4.3. **Universal density functionals.** By Proposition 4.1, every N-representable pair $(\rho, \mathbf{j}^{\mathrm{c}})$ belongs to the Banach space $X \times Y$, where

$$X = L^1(\mathbb{R}^3) \cap L^3(\mathbb{R}^3), \qquad Y = L^1(\mathbb{R}^3,\mathbb{R}^3) \cap L^{3/2}(\mathbb{R}^3,\mathbb{R}^3), \tag{51}$$

with the max norms $\|\rho\|_X = \max\{\|\rho\|_1, \|\rho\|_3\}$ and $\|\mathbf{j}^{\mathrm{c}}\|_Y = \max\{\|\mathbf{j}^{\mathrm{c}}\|_1, \|\mathbf{j}^{\mathrm{c}}\|_{3/2}\}$. Their duals are $X^* = L^\infty(\mathbb{R}^3) + L^{3/2}(\mathbb{R}^3)$ and $Y^* = L^\infty(\mathbb{R}^3,\mathbb{R}^3) + L^3(\mathbb{R}^3,\mathbb{R}^3)$, with dual norms given by $\|v\|_{X^*} = \inf_{v=v_\infty+v_{3/2}} \big(\|v_\infty\|_\infty + \|v_{3/2}\|_{3/2}\big)$ and $\|\mathbf{A}\|_{Y^*} = \inf_{\mathbf{A}=\mathbf{A}_\infty+\mathbf{A}_3} \big(\|\mathbf{A}_\infty\|_\infty + \|\mathbf{A}_3\|_3\big)$, where the infima run over decompositions in the respective summand spaces. The same spaces were considered for CDFT in [27].

For $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$, define the *Pauli–Fierz Levy–Lieb universal functional*

$$\boxed{F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{c}}) := \inf_{\substack{\Psi\in\mathcal{Q}_{\mathrm{PF}},\,\|\Psi\|=1 \\ \rho_\Psi=\rho \\ \mathbf{j}^{\mathrm{c}}_\Psi=\mathbf{j}^{\mathrm{c}}}} \langle \Psi, H^{0,0}\Psi\rangle}, \tag{52}$$

with value $+\infty$ if the constraint set is empty. The variational principle implies

$$E(v,\mathbf{A}) = \inf_{(\rho,\mathbf{j}^{\mathrm{c}})\in X\times Y} \left[F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{c}}) + \langle v + \tfrac{1}{2}|\mathbf{A}|^2, \rho\rangle + \langle \mathbf{A}, \mathbf{j}^{\mathrm{c}}\rangle\right]. \tag{53}$$

The quadratic diamagnetic term $\frac{1}{2}\langle|\mathbf{A}|^2,\rho\rangle$ means that $E(v,\mathbf{A})$ need not be jointly concave in $(v,\mathbf{A})$. To obtain a jointly concave energy, we follow [56] and absorb this term into the scalar potential by setting $u = v + \frac{1}{2}|\mathbf{A}|^2$, and define

$$\bar{E}(u,\mathbf{A}) = E(u - \frac{1}{2}|\mathbf{A}|^2, \mathbf{A}).$$

For each fixed N-representable pair $(\rho,\mathbf{j}^{\mathrm{c}})$, the expression inside the infimum in (53) is then affine in $(u,\mathbf{A})$. Thus $\bar{E}$ is a pointwise infimum of affine functions and is jointly concave, providing the basis for the following convex-duality construction. The *Pauli–Fierz Lieb universal functional* is then defined as the convex conjugate

$$F^{e,\chi}_{\mathrm{PFL}}(\rho,\mathbf{j}^{\mathrm{c}}) = \sup_{(u,\mathbf{A})\in X^*\times Y^*} \left[\bar{E}(u,\mathbf{A}) - \langle u,\rho\rangle - \langle \mathbf{A},\mathbf{j}^{\mathrm{c}}\rangle\right]. \tag{54}$$

It is thus convex and lower semicontinuous in the norm topology of $X \times Y$, and biconjugation gives

$$F^{e,\chi}_{\mathrm{PFL}} = \overline{\mathrm{conv}} F^{e,\chi}_{\mathrm{PFLL}} \leq F^{e,\chi}_{\mathrm{PFLL}}. \tag{55}$$

Here $\overline{\mathrm{conv}}$ denotes the norm-lower-semicontinuous convex envelope. Equivalently, it is the weak-lower-semicontinuous convex envelope. For comparison, recall the class $\mathcal{D}$ of finite-energy density matrices from (32) and define the mixed-state functional

$$\boxed{\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) = \inf_{\substack{\mathbf{\Gamma} \in \mathcal{D} \\ \rho_{\mathbf{\Gamma}} = \rho \\ \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} = \mathbf{j}^{\mathrm{c}}}} \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big)}. \tag{56}$$

Directly from the variational principle we have

$$F^{e,\chi}_{\mathrm{PFL}} \leq \widetilde{F}^{e,\chi}_{\mathrm{PFL}} \leq F^{e,\chi}_{\mathrm{PFLL}}. \tag{57}$$

As in the case of ordinary DFT and CDFT, equality of the first two functionals requires a separate lower-semicontinuity and compactness argument, supplied by Theorem 4.8 below. A closely related result is attainment of the defining infimum of $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$, also called expectation-valuedness of the functional.

4.4. **Existence and nonexistence of optimizers.** We now establish attainment of the mixed-state constrained search and identify it with the Lieb functional. The main difficulty comes from the possible occurrence of soft photons: an energy bound alone does not control photon number, since a minimizing sequence may contain arbitrarily many photons of arbitrarily small frequency.

Theorem 4.8 (Existence of a PFL optimizer)**.** *Whenever finite, the mixed-state functional $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$ has an optimizer. Every optimizer $\mathbf{\Gamma}$ has finite mean photon number, namely*

$$\mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}) \leq C_{N,e,\chi}\big(1 + \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})\big),$$

with a constant $C_{N,e,\chi}$ depending only on N, e and χ. The functional $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$ is norm lower semicontinuous on $X \times Y$, and

$$\boxed{\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) = F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})} \tag{58}$$

for all $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$.

The proof removes soft photons and restores the combined current density exactly, at a controlled energy cost. The electronic current shift of Appendix C preserves the density, fermionic antisymmetry, and the remaining photon marginal. Applied to a minimizing sequence, it yields a uniform bound on mean photon number. Photon localization and passage to the limit then give a mixed-state minimizer. The same estimates establish norm lower semicontinuity and hence equality with the Lieb functional.

However, pure-state attainment fails in general even for $N = 1$.

Proposition 4.9 (Nonexistence of a PFLL optimizer)**.** *Let $N = 1$ and fix the form factor. For every $e \geq 0$, there is a density–current pair $(\rho_e, \mathbf{j}_e) \in \mathcal{J}^{e,\chi}_1$ such that $F^{e,\chi}_{\mathrm{PFLL}}(\rho_e, \mathbf{j}_e) < \infty$ and its infimum is not attained. The pair may depend on both e and the fixed form factor. In particular, this holds for the standard hard ultraviolet cutoff (10) at every $e \geq 0$ and every finite Λ.*

The density ρ_e is supported in a thin solid torus around a long, narrow ellipse, and the velocity $\mathbf{j}_e/\rho_e$ has circulation π around each loop of the torus, half the circulation quantum. A single orbital cannot carry this velocity, since the phase of a nonvanishing wavefunction winds by a multiple of 2π, but the equal mixture of two orbitals with winding numbers 0 and 1 can. Attaching orthogonal soft-photon states to the two orbitals turns this mixture into a pure state with the same density and combined current density, at an energy cost that can be made arbitrarily small but not zero. To exclude a pure minimizer, we compare a lower bound for pure states with an upper bound from mixed states. As the ellipse is narrow, the field has small circulation around the loops, and the two bounds force a pure minimizer to be almost photon-free. Its vacuum component is then bounded away from zero along some loop, so its phase winds by a multiple of 2π, which contradicts the circulation π.

An obvious sufficient condition for pure-state attainment is the existence of a pure ground state with the prescribed density-current pair (v-representability). In fact, a pure ground state of $H^{v,\mathbf{A}}$, with potentials in (29), minimizes the PFLL constrained search at its own density–current pair: the external terms in (37) are the same for all states with that pair, so lowering the internal energy would contradict the ground-state property. In particular, the PFLL infimum at the density–current pair of a ground-state density matrix is attained whenever the corresponding ground state is non-degenerate, since every ground-state density matrix is then the rank-one projector onto that ground state.

4.5. **Soft-photon purification.** Arbitrarily soft photons allow a mixture to be represented by a pure electron–photon state at arbitrarily small energy cost, while the density and combined current density remain unchanged.

Theorem 4.10 (Soft-photon purification and equality of functionals)**.** *Fix $N \in \mathbb{N}$ and $e \geq 0$. For every $\mathbf{\Gamma} \in \mathcal{D}$ and every $\delta > 0$, there is a normalized $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ with finite mean photon number such that*

$$(\rho_\Psi, \mathbf{j}^{\mathrm{c}}_\Psi) = (\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}), \qquad \langle \Psi, H^{0,0}\Psi\rangle \leq \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \delta. \tag{59}$$

Consequently,

$$\boxed{F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) = F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})} \tag{60}$$

for all $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$. If this value is finite at $(\rho, \mathbf{j}^{\mathrm{c}})$, the pure-state infimum is attained if and only if the total Pauli–Fierz mixed-state minimization has a rank-one minimizer.

This does not contradict Levy's and Lieb's nonconvexity result for the electronic Levy–Lieb functional [29, 33], since a pure electron–photon state can have a mixed electronic marginal and, already at zero coupling, arbitrarily soft photons purify electronic mixed states at arbitrarily small energy cost.

Corollary 4.11 (Convexity, N-representability, and pure minimizing sequences)**.** *For every $N \in \mathbb{N}$ and $e \geq 0$, $F^{e,\chi}_{\mathrm{PFLL}}$ is proper, convex, and norm lower semicontinuous on $X \times Y$. Moreover,*

$$\boxed{\mathcal{J}^{e,\chi}_N = \{(\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}) : \mathbf{\Gamma} \in \mathcal{D}\} = \mathrm{dom}\, F^{e,\chi}_{\mathrm{PFL}}.} \tag{61}$$

In particular, the pure-state N-representability class is convex. Let $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$ with $F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty$, and let $\mathbf{\Gamma}_* \in \mathcal{D}$ be a minimizer in (56), so that $(\rho_{\mathbf{\Gamma}_*}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_*}) =$

$(\rho, \mathbf{j}^{\mathrm{c}})$. *Then there are normalized* $\Psi_j \in \mathcal{Q}_{\mathrm{PF}}$ *with*

$$(\rho_{\Psi_j}, \mathbf{j}^{\mathrm{c}}_{\Psi_j}) = (\rho, \mathbf{j}^{\mathrm{c}}), \qquad \langle \Psi_j, H^{0,0}\Psi_j\rangle \longrightarrow F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}),$$

and

$$\sup_j \langle \Psi_j, \mathcal{N}\Psi_j\rangle \leq 1 + \mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}_*) \leq 1 + C_{N,e,\chi}\big(1 + F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})\big). \tag{62}$$

This result extends Theorem 4.5 to general form factors. Equality of the infima and the bound (62) do not imply pure-state attainment: the soft photons can still prevent the necessary compactness. The construction uses the infinitely many continuum modes of arbitrarily small positive frequency. In contrast to Theorem 4.5, it requires no region on which the coupling vanishes, so it also strengthens the representability conclusion of that previous result.

At zero combined current density, both functionals reduce to searches constrained by the density alone.

Proposition 4.12 (Vanishing combined current density)**.** *For* $\sqrt{\rho} \in H^1(\mathbb{R}^3)$ *with* $\rho \geq 0$ *and* $\int_{\mathbb{R}^3} \rho = N$*, the following relations hold true:*

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho, 0) = \inf_{\substack{\Psi \in \mathcal{Q}_{\mathrm{PF}},\ \|\Psi\|=1 \\ \rho_\Psi = \rho}} \langle \Psi, H^{0,0}\Psi\rangle, \tag{63}$$

$$F^{e,\chi}_{\mathrm{PFL}}(\rho, 0) = \min_{\substack{\mathbf{\Gamma} \in \mathcal{D} \\ \rho_{\mathbf{\Gamma}} = \rho}} \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) \tag{64}$$

$$= \sup_{v \in X^*} \big[E(v, 0) - \langle v, \rho\rangle\big]. \tag{65}$$

Using Theorem 4.10, the above two zero-current functionals coincide. Note that the current constraint can be dropped from both constrained searches.

These functionals still include the quantized field and its coupling to the electrons. At nonzero coupling, their common value generally differs from the purely electronic Lieb functional $F_{\mathrm{L}}(\rho) = F_{\mathrm{VR}}(\rho, 0)$ recalled below in Section 4.7. The difference is a nontrivial variational contribution arising from electronic and photonic relaxation and their correlations at fixed density. The vacuum shift $e^2 N \|\widehat{\chi}\|^2/2$ gives an upper bound on this difference (Theorem 4.18).

4.6. **Properties of optimizers.** By Theorem 4.8, the constrained search has an optimizer whenever its value is finite. In this section we describe such optimizers: their fields, their symmetries and dark modes, and how many soft photons they contain. By dark modes we mean photon modes on which $\widehat{\chi}$ vanishes; these do not couple to the electrons. In each proof we compare an optimizer with other states that have the same density and combined current density, so we never assume that the optimizer is a ground state of some $H^{v,\mathbf{A}}$.

4.6.1. *Fields of constrained optimizers.* We now ask which conclusions of Proposition 4.3 require a ground state, and which follow from constrained minimization alone. Here an optimizer means any $\mathbf{\Gamma} \in \mathcal{D}$ satisfying

$$\rho_{\mathbf{\Gamma}} = \rho, \qquad \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} = \mathbf{j}^{\mathrm{c}}, \qquad \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) = F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty.$$

There need not be supporting external potentials (no v-representability required). In their absence, the prescribed current is $\mathbf{j}^{\mathrm{c}}$, whereas a physical current $\mathbf{j} = \mathbf{j}^{\mathrm{c}} + \rho\mathbf{A}$ requires a specified external vector potential. All traces below are understood in the form sense, with the fields smeared as in Section 3.3.

Proposition 4.13 (Fields of optimizers)**.** *Let $\mathbf{\Gamma}$ be a PFL optimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$. The following properties hold true.*

(i) For real $\mathbf{u}_1, \dots, \mathbf{u}_n \in C_c^\infty(\mathbb{R}^3; \mathbb{R}^3)$ and every real $\varphi \in \mathcal{S}(\mathbb{R}^n)$,

$$\sum_{j=1}^{n} \operatorname{Re} \operatorname{Tr} \Big(\Big[(\partial_j \varphi) \Big(\int_{\mathbb{R}^3} \mathbf{u}_1 \cdot \mathfrak{A}, \dots, \int_{\mathbb{R}^3} \mathbf{u}_n \cdot \mathfrak{A} \Big) \Big] \Big[\int_{\mathbb{R}^3} \mathbf{u}_j \cdot \mathfrak{E}_\perp \Big] \mathbf{\Gamma} \Big) = 0. \tag{66}$$

(ii) In particular, the transverse electric field vanishes, $\operatorname{Tr}(\mathfrak{E}_\perp \mathbf{\Gamma}) = 0$ in the sense of distributions. This means that

$$\operatorname{Tr} \Big(\Big[\int_{\mathbb{R}^3} \mathbf{u} \cdot \mathfrak{E}_\perp \Big] \mathbf{\Gamma} \Big) = 0 \qquad \text{for every } \mathbf{u} \in C_c^\infty(\mathbb{R}^3; \mathbb{R}^3). \tag{67}$$

(iii) If the prescribed current has the form

$$\mathbf{j}^{\mathrm{c}} = \rho \boldsymbol{\nabla} S, \qquad S \in W^{1,1}_{\mathrm{loc}}(\mathbb{R}^3; \mathbb{R}), \qquad \boldsymbol{\nabla} S \in L^3(\mathbb{R}^3; \mathbb{R}^3) + L^\infty(\mathbb{R}^3; \mathbb{R}^3),$$

then every coherent photon amplitude vanishes: $\operatorname{Tr}(a(h)\mathbf{\Gamma}) = 0$ for all $h \in \mathfrak{H}_{\mathrm{ph}}$ with $h/\sqrt{\omega} \in \mathfrak{H}_{\mathrm{ph}}$. In particular, the vector potential vanishes pointwise and the magnetic field vanishes in the sense of distributions:

$$\operatorname{Tr}(\mathfrak{A}(\mathbf{x})\mathbf{\Gamma}) = 0 \quad (\mathbf{x} \in \mathbb{R}^3), \qquad \operatorname{Tr}(\mathfrak{B}\mathbf{\Gamma}) = 0.$$

Item (i) extends (67), its limiting linear case, from the expectation value to all equal-time statistics of the smeared transverse field. The kinetic, Coulomb, and external terms of $H^{v,\mathbf{A}}$ commute with $\varphi(\int \mathbf{u}_1 \cdot \mathfrak{A}, \dots, \int \mathbf{u}_n \cdot \mathfrak{A})$. Formally, the left-hand side of (66) is therefore minus the time derivative at $t = 0$ of $\operatorname{Tr}\big(\varphi(\int \mathbf{u}_1 \cdot \mathfrak{A}, \dots, \int \mathbf{u}_n \cdot \mathfrak{A})\, e^{-\mathrm{i}tH^{v,\mathbf{A}}} \mathbf{\Gamma} e^{\mathrm{i}tH^{v,\mathbf{A}}}\big)$: under the full dynamics, every such expectation value is stationary to first order at an optimizer. In a Schrödinger representation of the field, in which the smeared fields act as coordinates (Appendix D with $\mathfrak{h} = \mathfrak{H}_{\mathrm{ph}}$), (66) says that the probability current in field configuration space is weakly divergence-free. It is thus the field-space counterpart of Proposition 4.3(i).

The field variations in the proof of Proposition 4.13 preserve both constraints on the density and the combined current density. By contrast, an electronic phase changes $\mathbf{j}^{\mathrm{c}}$ by $\rho \boldsymbol{\nabla} S$, and a general photon displacement changes it by $-e\rho \mathbf{c}_f$, with $\mathbf{c}_f$ as in (218). Consequently, the variations proving continuity and the Ampère law for ground states are not generally available at a fixed pair. The next proposition shows that a constrained optimizer can have a combined current density with nonzero divergence at positive coupling. It also shows that even a unique optimizer need not be a ground state for any external potentials in (29).

Proposition 4.14 (Ground-state conclusions that fail for optimizers)**.** *Let $N = 1$, and set*

$$\rho(\mathbf{x}) = \pi^{-3/2} e^{-|\mathbf{x}|^2}, \qquad \mathbf{j}^{\mathrm{c}}(\mathbf{x}) = \rho(\mathbf{x})\mathbf{q}, \qquad 0 \neq \mathbf{q} \in \mathbb{R}^3.$$

(i) Let $e > 0$, and let $\widehat{\chi}$ satisfy (9). The pair $(\rho, \mathbf{j}^{\mathrm{c}})$ has a PFL optimizer, and every such optimizer satisfies

$$\operatorname{Tr}(\mathfrak{A}\mathbf{\Gamma}) = \operatorname{Tr}(\mathfrak{B}\mathbf{\Gamma}) = \operatorname{Tr}(\mathfrak{E}_\perp \mathbf{\Gamma}) = 0, \qquad \operatorname{div} \mathbf{j}^{\mathrm{c}} = -2(\mathbf{q} \cdot \mathbf{x})\rho \neq 0.$$

The vector-potential identity holds pointwise, and the magnetic and electric field expectation values hold in the sense of distributions.

(ii) Let $e = 0$. The unique PFL optimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$ is

$$\begin{gathered}\boldsymbol{\Gamma}_{\mathbf{q}} = |\Psi_{\mathbf{q}}\rangle\langle\Psi_{\mathbf{q}}|, \qquad \Psi_{\mathbf{q}}(\mathbf{x}) = e^{\mathrm{i}\mathbf{q}\cdot\mathbf{x}}\pi^{-3/4}e^{-|\mathbf{x}|^2/2}\Omega, \\ F_{\mathrm{PFL}}^{0,\chi}(\rho, \rho\mathbf{q}) = \frac{3}{4} + \frac{|\mathbf{q}|^2}{2}.\end{gathered} \tag{68}$$

It is not a ground state, or even an eigenstate, of any $H^{v,\mathbf{A}}$ with potentials in (29).

Part (i) shows that continuity and Ampère's law are not consequences of constrained optimality. Indeed, since it involves the physical current $\mathbf{j}^{\mathrm{c}} + \rho\mathbf{A}$, Ampère's law is most natural in a situation where the external potential $\mathbf{A}$ is given. By part (ii), uniqueness of a constrained optimizer cannot replace the ground-state assumptions in Proposition 4.3(iv): the unique constrained optimizer can have nonzero current.

As is made clearer in the proof below (in Section 5.10), the restriction on the potentials in (29) plays an essential role. For example, in the case $e = 0$, the given density-current pair does come from the ground state of an $H^{v,\mathbf{A}}$ with $v(\mathbf{x}) = \frac{1}{2}|\mathbf{x}|^2 \notin L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and $\mathbf{A}(\mathbf{x}) = -\mathbf{q}$.

4.6.2. *Symmetry and dark modes.* For $\mathbf{R} \in \mathrm{O}(3)$, define in the solenoidal representation of the one-photon space the rotation $(\Upsilon_{\mathbf{R}}\mathbf{f})(\mathbf{k}) = \mathbf{R}\mathbf{f}(\mathbf{R}^\top\mathbf{k})$, and put

$$(U_{\mathbf{R}}\Psi)(\mathbf{X}) = \Upsilon_{\mathbf{R}}\Psi(\mathbf{R}^\top\mathbf{x}_1, \dots, \mathbf{R}^\top\mathbf{x}_N)$$

on $\mathcal{H}_N$, as in Proposition A.2. Let Θ be the time reversal (190). For $g = (\mathbf{R}, s) \in \mathrm{O}(3) \times \{1, -1\}$, put

$$V_g = \begin{cases} U_{\mathbf{R}}, & s = 1, \\ U_{\mathbf{R}}\Theta, & s = -1. \end{cases}$$

Proposition 4.15 (Symmetry and dark modes of optimizers)**.** *Let $F_{\mathrm{PFL}}^{e,\chi}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty$.*

(i) Use the hard cutoff (10), and let $G \subset \mathrm{O}(3) \times \{1, -1\}$ be a closed subgroup such that

$$\rho(\mathbf{R}^\top\mathbf{x}) = \rho(\mathbf{x}), \qquad s\mathbf{R}\mathbf{j}^{\mathrm{c}}(\mathbf{R}^\top\mathbf{x}) = \mathbf{j}^{\mathrm{c}}(\mathbf{x}) \qquad ((\mathbf{R}, s) \in G).$$

Then $\boldsymbol{\Gamma} \mapsto V_g\boldsymbol{\Gamma}V_g^{-1}$, $g \in G$, maps the set of PFL optimizers at $(\rho, \mathbf{j}^{\mathrm{c}})$ onto itself, and this set contains a G-invariant optimizer.

(ii) Suppose that $\widehat{\chi} = 0$ almost everywhere on a measurable set $S \subset \mathbb{R}^3$. Let $\mathfrak{H}_S \subset \mathfrak{H}_{\mathrm{ph}}$ consist of the one-photon states supported in S, and factor $\mathcal{F}_{\mathrm{ph}} \simeq \mathcal{F}_s(\mathfrak{H}_S^\perp) \otimes \mathcal{F}_s(\mathfrak{H}_S)$. Then every PFL optimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$ has the form $\boldsymbol{\Gamma}' \otimes |\Omega_S\rangle\langle\Omega_S|$, where Ω_S is the vacuum of the second factor.

For instance, if ρ is radial and $\mathbf{j}^{\mathrm{c}} = 0$, part (i) with $G = \mathrm{O}(3) \times \{1, -1\}$ gives an optimizer invariant under all rotations, reflections, and time reversal. The group $G = \{(\mathbb{1}, \pm 1)\}$ requires only $\mathbf{j}^{\mathrm{c}} = 0$, with no symmetry of ρ. Its Haar average is $\frac{1}{2}(\boldsymbol{\Gamma} + \Theta\boldsymbol{\Gamma}\Theta^{-1})$, so every optimizer $\boldsymbol{\Gamma}$ at $(\rho, 0)$ yields a time-reversal-invariant one. If ρ and $\mathbf{j}^{\mathrm{c}}$ are invariant under rotations about an axis, as for a circulating current, there is an optimizer invariant under these rotations even though time reversal is broken. For the hard cutoff, part (ii) applies with $S = \{|\mathbf{k}| > \Lambda\}$: optimizers carry no photons above the cutoff.

4.6.3. *Soft-photon energy distributions and infrared laws.* We describe photon energy distributions of constrained optimizers and their infrared behavior. Here photon energy and frequency are identified by $\omega(\mathbf{k}) = |\mathbf{k}|$, in the units $\hbar = c = 1$ used above.

Fix a density–current pair $(\rho, \mathbf{j}^{\mathrm{c}})$ with $F_{\mathrm{PFL}}^{e,\chi}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty$, and let $\mathbf{\Gamma}_*$ be any mixed-state optimizer supplied by Theorem 4.8. For a Borel set $B \subset (0, \infty)$, define the photon-number and photon-energy measures

$$\nu_*(B) = \mathrm{Tr}\big(\mathrm{d}\Gamma(\mathbb{1}_{\{|\mathbf{k}|\in B\}})\mathbf{\Gamma}_*\big)\,,$$
$$\mu_*(B) = \mathrm{Tr}\big(\mathrm{d}\Gamma(|\mathbf{k}|\mathbb{1}_{\{|\mathbf{k}|\in B\}})\mathbf{\Gamma}_*\big) = \int_B \varepsilon\,\nu_*(\mathrm{d}\varepsilon).$$

Both are finite. They describe expected photon counts and expected energy in frequency bands, but neither is a probability measure in general. The total mass of μ_* is the expected total radiation energy, $\mu_*((0,\infty)) = \mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}_*)$. By contrast, $\mathrm{Tr}(\mathbb{1}_B(H_{\mathrm{rad}})\mathbf{\Gamma}_*)$ is the probability that the *total photon energy* lies in B.

There is also a density formula. Let $\gamma_*^{(1)}$ be the one-photon reduced density operator, characterized by

$$\mathrm{Tr}\Big(T\gamma_*^{(1)}\Big) = \mathrm{Tr}(\mathrm{d}\Gamma(T)\mathbf{\Gamma}_*)$$

for bounded one-photon operators T. It is positive semidefinite and since its trace gives the mean photon number, it is also trace class. Write $\gamma_*^{(1)} = \sum_j s_j |f_j\rangle\langle f_j|$, with $s_j \geq 0$ and (f_j) orthonormal. The momentum-space photon-number density is defined almost everywhere by

$$n_*(\mathbf{k}, \lambda) = \sum_j s_j |f_j(\mathbf{k}, \lambda)|^2.$$

Polar coordinates give absolutely continuous measures

$$\nu_*(\mathrm{d}\varepsilon) = \mathcal{N}_*(\varepsilon)\mathrm{d}\varepsilon, \quad \mathcal{N}_*(\varepsilon) = \varepsilon^2 \sum_{\lambda=1}^{2} \int_{|\boldsymbol{\theta}|=1} n_*(\varepsilon\boldsymbol{\theta}, \lambda)\mathrm{d}\boldsymbol{\theta},$$
$$\mu_*(\mathrm{d}\varepsilon) = \mathcal{U}_*(\varepsilon)\mathrm{d}\varepsilon, \quad \mathcal{U}_*(\varepsilon) = \varepsilon\mathcal{N}_*(\varepsilon).$$

Summing over polarizations makes these distributions independent of the polarization frame.

Proposition 4.16 (Infrared distribution bounds for optimizers)**.** *There are $C < \infty$ and $0 < \kappa_0 \leq 1$, depending only on N, e, χ, such that every PFL optimizer satisfies, for $0 < \kappa \leq \kappa_0$,*

$$E_*(\kappa) := \int_0^\kappa \mathcal{U}_*(\varepsilon)\mathrm{d}\varepsilon \leq C(\kappa^2 + b_\kappa^2), \tag{69}$$
$$N_*(\kappa) := \int_0^\kappa \mathcal{N}_*(\varepsilon)\mathrm{d}\varepsilon \leq C(\kappa + a_\kappa^2), \tag{70}$$

where

$$a_\kappa = \left\| \frac{\mathbb{1}_{\{|\mathbf{k}|<\kappa\}}\widehat{\chi}}{\sqrt{|\mathbf{k}|}} \right\|, \qquad b_\kappa = \|\mathbb{1}_{\{|\mathbf{k}|<\kappa\}}\widehat{\chi}\|. \tag{71}$$

For the hard cutoff (10), with $\Lambda > 0$ and $\kappa \leq \min\{\kappa_0, \Lambda\}$, these reduce to

$$E_*(\kappa) \leq C\kappa^2, \qquad N_*(\kappa) \leq C\kappa. \tag{72}$$

By evaluating the constants a_κ and b_κ explicitly, the hard cutoff gives the frequency-bin estimates

$$\frac{2}{\kappa}\int_{\kappa/2}^{\kappa}\mathcal{U}_*(\varepsilon)\mathrm{d}\varepsilon \le C\kappa, \qquad \frac{2}{\kappa}\int_{\kappa/2}^{\kappa}\mathcal{N}_*(\varepsilon)\mathrm{d}\varepsilon \le C.$$

One cannot differentiate (72) to deduce the corresponding pointwise inequalities, so these must be seen as cumulative bounds, not as an assured soft-photon spectrum or a proved leading asymptotic. In particular, neither a Planck law nor a temperature follows only from these estimates. If $P^{\mathrm{vac}}_{<\kappa}$ is the projection onto the vacuum in the soft Fock factor, tensored with the identity on the other factors, then

$$\mathrm{Tr}((\mathbb{1}-P^{\mathrm{vac}}_{<\kappa})\mathbf{\Gamma}_*) \le N_*(\kappa) \longrightarrow 0.$$

Thus the probability of any photon below κ tends to zero in an exact optimizer, with rate $O(\kappa)$ for the hard cutoff.

4.7. **Zero coupling and soft-photon relaxation.** At $e = 0$, the combined current density reduces to the paramagnetic current density and the internal Pauli–Fierz Hamiltonian separates into electronic and photon parts:

$$\begin{aligned}\mathbf{j}^{\mathrm{c}}_{\Psi} &= \mathbf{j}^{\mathrm{p}}_{\Psi},\\ H^{0,0}\big|_{e=0} &= H^0_{\mathrm{el}}\otimes\mathbb{1}_{\mathcal{F}_{\mathrm{ph}}} + \mathbb{1}_{\mathfrak{H}^N_{\mathrm{el}}}\otimes H_{\mathrm{rad}},\\ H^0_{\mathrm{el}} &:= \frac{1}{2}\sum_{n=1}^{N}(-\Delta_{\mathbf{x}_n}) + \sum_{1\le n<m\le N}\frac{1}{|\mathbf{x}_n-\mathbf{x}_m|}.\end{aligned}$$

Thus the density and current constraints depend only on the electronic reduced state. However, the photon factor can be used to purify a mixed electronic state, and the massless dispersion permits the orthogonal photon states in that purification to have arbitrarily small, though nonzero, energy.

We define the mixed-state Vignale–Rasolt functional of CDFT by

$$F_{\mathrm{VR}}(\rho,\mathbf{j}^{\mathrm{p}}) := \inf_{\substack{\Gamma\in\mathfrak{S}_1(\mathfrak{H}^N_{\mathrm{el}})\\ \Gamma\ge 0,\ \mathrm{Tr}\,\Gamma=1\\ \rho_\Gamma=\rho\\ \mathbf{j}^{\mathrm{p}}_\Gamma=\mathbf{j}^{\mathrm{p}}}} \mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma\big),$$

with the value $+\infty$ when the constraint set is empty. As elsewhere, the trace involving H^0_{el} is a form trace.

Theorem 4.17 (Soft-photon relaxation at zero coupling)**.** *For every* $(\rho,\mathbf{j}^{\mathrm{p}}) \in \mathcal{J}^{\mathrm{el}}_{N,\mathrm{mix}}$,

$$\boxed{F^{0,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{p}}) = F^{0,\chi}_{\mathrm{PFL}}(\rho,\mathbf{j}^{\mathrm{p}}) = F_{\mathrm{VR}}(\rho,\mathbf{j}^{\mathrm{p}}).} \tag{73}$$

The infimum defining $F^{0,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}^{\mathrm{p}})$ *is attained if and only if the electronic mixed-state minimization has a rank-one minimizer. Equivalently, attainment holds if and only if there is a normalized* $\Phi \in Q(H^0_{\mathrm{el}})$ *such that*

$$(\rho_\Phi,\mathbf{j}^{\mathrm{p}}_\Phi) = (\rho,\mathbf{j}^{\mathrm{p}}), \qquad \langle\Phi,H^0_{\mathrm{el}}\Phi\rangle = F_{\mathrm{VR}}(\rho,\mathbf{j}^{\mathrm{p}}).$$

The proof purifies a fixed mixed electronic state using orthogonal one-photon states whose energies tend to zero. These purifications have no strongly convergent subsequence: any limit would be a product with the photon vacuum and therefore have a pure electronic reduced state, contradicting the fixed mixed one.

The next theorem treats the limit $e \downarrow 0$ at fixed form factor.[3]

Theorem 4.18 (Zero-coupling limit)**.** *As extended-real functionals on $X \times Y$, the pure Pauli–Fierz universal functionals have the following sequential limit as $e \downarrow 0$.*

(i) If $e_k > 0$, $e_k \to 0$, and $(\rho_k, \mathbf{j}_k) \rightharpoonup (\rho, \mathbf{j})$ weakly in $X \times Y$, then

$$F_{\mathrm{VR}}(\rho, \mathbf{j}) \leq \liminf_{k\to\infty} F^{e_k,\chi}_{\mathrm{PFLL}}(\rho_k, \mathbf{j}_k).$$

(ii) If $F_{\mathrm{VR}}(\rho, \mathbf{j}) < \infty$, then the constant sequence of constraints is a recovery sequence. More precisely,

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}) \leq F_{\mathrm{VR}}(\rho, \mathbf{j}) + \frac{N}{2}\|\widehat{\chi}\|^2 e^2, \qquad e \geq 0.$$

Moreover, $(\rho, \mathbf{j}) \in \mathcal{J}^{e,\chi}_N$ for every $e \geq 0$.

Consequently, for every $(\rho, \mathbf{j}) \in X \times Y$,

$$\lim_{e\downarrow 0} F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}) = F^{0,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}) = F_{\mathrm{VR}}(\rho, \mathbf{j}).$$

In particular, the convergence holds in the sequential Mosco sense on $X \times Y$, hence also in the norm-Gamma sense, and every point in the effective domain has a constant recovery sequence.

Part (i) holds along arbitrary weakly convergent constraints, while part (ii) uses only the constant recovery sequence, which suffices for Mosco convergence. An upper bound along every norm-convergent sequence $(\rho_k, \mathbf{j}_k) \to (\rho, \mathbf{j})$ would fail in general, since norm convergence in $X \times Y$ does not control $\int_{\mathbb{R}^3} |\mathbf{j}_k|^2/\rho_k$.

4.8. **The long-wavelength (dipole) limit.** We next keep N, e, the form factor, and the photon dispersion fixed. For $0 \leq \varepsilon \leq 1$, introduce a parameter in the spatial dependence of the quantized field:

$$\mathfrak{A}^{\mu}(\varepsilon\mathbf{x}) = \Phi(G^{\mu}_{\varepsilon\mathbf{x}}), \qquad \mathbf{D}_{n,\varepsilon} := -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\mathfrak{A}(\varepsilon\mathbf{x}_n).$$

The original model corresponds to $\varepsilon = 1$. At $\varepsilon = 0$, the field is the spatially uniform operator $\mathfrak{A}(0)$, giving the velocity-gauge dipole approximation.

A photon dilation shows that $\varepsilon \downarrow 0$ is a long-wavelength limit at fixed system size: rescaling $\mathbf{x} \mapsto \varepsilon\mathbf{x}$ is equivalent to keeping the electrons fixed while stretching the relevant photon wavelengths by a factor $1/\varepsilon$. For $\varepsilon > 0$, the scaling $\varepsilon^{-3/2}\mathbf{f}(\cdot/\varepsilon)$ is unitary on $\mathfrak{H}_{\mathrm{sol}}$. As in Proposition A.3, conjugation by its second quantization maps $\mathfrak{A}(\varepsilon\mathbf{x})$ to the field at $\mathbf{x}$ built with $\varepsilon^{-3/2}\widehat{\chi}(\cdot/\varepsilon)$ in place of $\widehat{\chi}$, and maps H_{rad} to $\varepsilon^{-1}H_{\mathrm{rad}}$. The model at ε is therefore unitarily equivalent to one with photon dispersion $|\mathbf{k}|/\varepsilon$, that is, with the *speed of light* formally set to $1/\varepsilon$ while the system size is kept fixed. In that picture the frequencies and $\|\widehat{\chi}\|^2$, the vacuum expectation of $|\mathfrak{A}(0)|^2$, are unchanged, while for the hard cutoff the coupled wave numbers satisfy $|\mathbf{k}| \leq \varepsilon\Lambda$, so all coupled wavelengths diverge as $\varepsilon \downarrow 0$, becoming large compared to any fixed system size. Correspondingly, with the fields (21), the electrons in the

[3]Let $F_k, F\colon V \to (-\infty, \infty]$ be functionals on a Banach space V. A *recovery sequence* for $u \in V$ is a sequence $u_k \to u$ in norm with $\limsup_{k\to\infty} F_k(u_k) \leq F(u)$. The F_k converge to F in the *norm-Gamma* sense if $F(u) \leq \liminf_{k\to\infty} F_k(u_k)$ whenever $u_k \to u$ in norm, and every $u \in V$ has a recovery sequence. They converge in the *Mosco* sense if, in addition, this lim inf inequality holds whenever $u_k \rightharpoonup u$ weakly. Mosco convergence therefore implies norm-Gamma convergence. We use the sequential versions of these notions, and a limit $e \downarrow 0$ means convergence along every sequence $e_k \downarrow 0$.

model at ε feel the transverse electric field $-\mathrm{i}[H_{\mathrm{rad}}, \mathfrak{A}(\varepsilon\mathbf{x})] = \mathfrak{E}_\perp(\varepsilon\mathbf{x})$ at unchanged strength, whereas the magnetic field $\boldsymbol{\nabla}_{\mathbf{x}} \times \mathfrak{A}(\varepsilon\mathbf{x}) = \varepsilon\mathfrak{B}(\varepsilon\mathbf{x})$ carries a factor ε.

Let $H_\varepsilon^{0,0}$ be the internal Hamiltonian obtained from $H^{0,0}$ by replacing $\mathbf{D}_n$ with $\mathbf{D}_{n,\varepsilon}$. As in Section 3.4, $\langle\Psi, H_\varepsilon^{0,0}\Psi\rangle$ denotes its form value for $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, and energies of density matrices are written as $\mathrm{Tr}\big(H_\varepsilon^{0,0}\boldsymbol{\Gamma}\big)$ in the form sense. The combined current density changes with the field:

$$\mathbf{j}_\Psi^{\mathrm{c},\varepsilon}(\mathbf{x}) := N\,\mathrm{Re}\langle\Psi, \mathbf{D}_{1,\varepsilon}\Psi\rangle_{\mathbf{x}} = \mathbf{j}_\Psi^{\mathrm{p}}(\mathbf{x}) - eN\,\mathrm{Re}\langle\Psi, \mathfrak{A}(\varepsilon\mathbf{x})\Psi\rangle_{\mathbf{x}}.$$

The mixed-state current density is defined by affine extension. The bounds in Proposition 4.1 hold uniformly in ε on sets of bounded form energy.

Using the same spaces $X \times Y$ and external potentials as in (51), set

$$\bar{E}_\varepsilon(u, \mathbf{A}) := \inf_{\substack{\Psi\in\mathcal{Q}_{\mathrm{PF}}\\ \|\Psi\|=1}} \big[\langle\Psi, H_\varepsilon^{0,0}\Psi\rangle + \langle u, \rho_\Psi\rangle + \langle\mathbf{A}, \mathbf{j}_\Psi^{\mathrm{c},\varepsilon}\rangle\big],$$

$$F_{\mathrm{PFL},\varepsilon}(\rho, \mathbf{j}^{\mathrm{c}}) := \sup_{(u,\mathbf{A})\in X^*\times Y^*} \big[\bar{E}_\varepsilon(u, \mathbf{A}) - \langle u, \rho\rangle - \langle\mathbf{A}, \mathbf{j}^{\mathrm{c}}\rangle\big].$$

Let $F_{\mathrm{PFLL},\varepsilon}$ be the pure-state constrained search for $H_\varepsilon^{0,0}$, with $(\rho_\Psi, \mathbf{j}_\Psi^{\mathrm{c},\varepsilon}) = (\rho, \mathbf{j}^{\mathrm{c}})$. As in (55),

$$F_{\mathrm{PFL},\varepsilon} = \overline{\mathrm{conv}} F_{\mathrm{PFLL},\varepsilon}. \tag{74}$$

The fixed parameters N, e, χ are suppressed in this notation. We use the label d for the endpoint $\varepsilon = 0$ throughout, keeping the coupling e fixed, and write $F_{\mathrm{d}} := F_{\mathrm{PFL},\varepsilon}|_{\varepsilon=0}$ and $\mathbf{j}_\Psi^{\mathrm{c,d}} := \mathbf{j}_\Psi^{\mathrm{c},\varepsilon}|_{\varepsilon=0}$. The external classical vector potential $\mathbf{A}(\mathbf{x})$ is unchanged.

Theorem 4.19 (Dipole limit of the PFL functional)**.** *Fix $N \in \mathbb{N}$, $e \geq 0$, and the form factor. The functionals $F_{\mathrm{PFL},\varepsilon}$ converge to F_{d} in the sequential Mosco sense on $X \times Y$:*

(i) If $\varepsilon_k > 0$, $\varepsilon_k \to 0$, and $(\rho_k, \mathbf{j}_k^{\mathrm{c}}) \rightharpoonup (\rho, \mathbf{j}^{\mathrm{c}})$ weakly in $X \times Y$, then

$$F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}) \leq \liminf_{k\to\infty} F_{\mathrm{PFL},\varepsilon_k}(\rho_k, \mathbf{j}_k^{\mathrm{c}}). \tag{75}$$

(ii) For every $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$, there are pairs $(\rho_\varepsilon, \mathbf{j}_\varepsilon^{\mathrm{c}}) \to (\rho, \mathbf{j}^{\mathrm{c}})$ in the norm of $X \times Y$ such that

$$\limsup_{\varepsilon\downarrow 0} F_{\mathrm{PFL},\varepsilon}(\rho_\varepsilon, \mathbf{j}_\varepsilon^{\mathrm{c}}) \leq F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}). \tag{76}$$

The dipole functional can be compared directly with the electronic mixed-state functional defined above. In this comparison, the same current density $\mathbf{j}^{\mathrm{c,d}}$ is used as the paramagnetic-current argument of F_{VR}.

Proposition 4.20 (Electronic comparison for the dipole functional)**.** *For every $N \in \mathbb{N}$, $e \geq 0$, and $(\rho, \mathbf{j}^{\mathrm{c,d}}) \in X \times Y$,*

$$F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{c,d}}) \leq F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c,d}}) \leq F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{c,d}}) + \frac{Ne^2}{2}\|\widehat{\chi}\|^2. \tag{77}$$

Consequently,

$$\mathrm{dom}\, F_{\mathrm{d}} = \mathrm{dom}\, F_{\mathrm{VR}}. \tag{78}$$

For the standard hard cutoff (10), the upper correction in (77) is $N\pi e^2\Lambda^2$.

At the dipole endpoint $\varepsilon = 0$, with e fixed, the internal Hamiltonian is

$$H_{\mathrm{d}} = \frac{1}{2}\sum_{n=1}^{N}\big(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\boldsymbol{\mathfrak{A}}(0)\big)^2 + \sum_{1\le n<m\le N}\frac{1}{|\mathbf{x}_n-\mathbf{x}_m|} + H_{\mathrm{rad}}, \tag{79}$$

understood as the positive self-adjoint operator associated with the corresponding closed form on $\mathcal{Q}_{\mathrm{PF}}$. The *dipole PFLL functional* is its pure-state constrained search, that is, $F_{\mathrm{PFLL,d}} := F_{\mathrm{PFLL},\varepsilon}|_{\varepsilon=0}$,

$$F_{\mathrm{PFLL,d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) := \inf_{\substack{\Psi\in\mathcal{Q}_{\mathrm{PF}},\,\|\Psi\|=1\\ \rho_\Psi=\rho\\ \mathbf{j}^{\mathrm{c,d}}_\Psi=\mathbf{j}^{\mathrm{c,d}}}}\langle\Psi, H_{\mathrm{d}}\Psi\rangle, \tag{80}$$

and its mixed-state constrained search is

$$\widetilde{F}_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) := \inf_{\substack{\boldsymbol{\Gamma}\in\mathfrak{S}_1(\mathcal{H}_N),\ \boldsymbol{\Gamma}\ge 0,\ \mathrm{Tr}\,\boldsymbol{\Gamma}=1\\ \mathrm{Tr}(H_{\mathrm{d}}\boldsymbol{\Gamma})<\infty\\ \rho_{\boldsymbol{\Gamma}}=\rho,\ \mathbf{j}^{\mathrm{c,d}}_{\boldsymbol{\Gamma}}=\mathbf{j}^{\mathrm{c,d}}}}\mathrm{Tr}(H_{\mathrm{d}}\boldsymbol{\Gamma}). \tag{81}$$

The expectation and the trace are taken in the form sense, and an empty admissible set has infimum $+\infty$. The following theorem consistently identifies the pure-state and mixed-state searches with the dipole PFL functional for every finite N.

Theorem 4.21 (Equality of dipole functionals)**.** *We have*

$$\boxed{F_{\mathrm{PFLL,d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) = \widetilde{F}_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) = F_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}})} \tag{82}$$

for all $(\rho,\mathbf{j}^{\mathrm{c,d}}) \in X\times Y$. Every finite mixed-state infimum is attained by a density matrix of finite mean photon number.

As a preparation for passing to the length gauge, put $\mathbf{R} = \sum_{n=1}^{N}\mathbf{x}_n$, so that $e\mathbf{R}$ is the dipole moment of the electrons. If $\sqrt{\omega}\,\widehat{\chi}\in L^2$, define the real symmetric positive semidefinite 3×3 matrix $\mathbf{M} = (M^{\mu\nu})_{\mu,\nu=1}^{3}$ by

$$M^{\mu\nu} = \mathrm{Re}\langle\sqrt{\omega}\,G_0^\mu, \sqrt{\omega}\,G_0^\nu\rangle = \frac{1}{2}\int_{\mathbb{R}^3}\omega(\mathbf{k})|\widehat{\chi}(\mathbf{k})|^2 P_{\mathrm{sol}}(\mathbf{k})^{\mu\nu}\mathrm{d}\mathbf{k}; \tag{83}$$

for the hard cutoff (10), $\mathbf{M} = \frac{4\pi\Lambda^3}{9}\mathbb{1}$ (Appendix A.6). Under the same assumption, the transverse electric field (21) at the origin is a form on $D(\sqrt{H_{\mathrm{rad}}})$ (Section 3.3), namely

$$\boldsymbol{\mathfrak{E}}_\perp^\mu(0) = -\Pi(\omega G_0^\mu), \tag{84}$$

where $\omega G_0^\mu/\sqrt{\omega}\in\mathfrak{H}_{\mathrm{ph}}$ and Π is the extension of the conjugate Segal field (1) to such arguments (Proposition A.10(iv)).

Corollary 4.22 (Length-gauge form of the dipole functional)**.** *Suppose that $\sqrt{\omega}\,\widehat{\chi}\in L^2$. For all $(\rho,\mathbf{j}^{\mathrm{c,d}})\in X\times Y$ with $\int_{\mathbb{R}^3}|\mathbf{x}|^2\rho<\infty$,*

$$\boxed{F_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}}) = \inf_{\substack{\boldsymbol{\Gamma}\in\mathcal{D}\\ \rho_{\boldsymbol{\Gamma}}=\rho,\ \mathbf{j}^{\mathrm{p}}_{\boldsymbol{\Gamma}}=\mathbf{j}^{\mathrm{c,d}}}}\mathrm{Tr}\Big(H_{\mathrm{el}}^0 + H_{\mathrm{rad}} - e\mathbf{R}\cdot\boldsymbol{\mathfrak{E}}_\perp(0) + e^2\mathbf{R}^\top\mathbf{M}\mathbf{R}\Big)\boldsymbol{\Gamma}.} \tag{85}$$

Here $\mathcal{D}$ is the class (32) of finite-energy density matrices, the trace is taken in the form sense and converges absolutely, and every finite infimum is attained.

This is the mixed-state constrained search for the usual length-gauge dipole Hamiltonian [44]. By (82), the same identity holds for the pure-state search over normalized $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, but that infimum need not be attained: at $e = 0$, where the dipole model coincides with the Pauli–Fierz model, Proposition 4.9 provides an example. The constant field has disappeared from the kinetic energy and from the constraint, which becomes the paramagnetic current density as in F_{VR}. It enters only through the last three terms, which add up to the radiation energy $\mathrm{Tr}\Big(H_{\mathrm{rad}} U_{\mathrm{d}} \mathbf{\Gamma} U_{\mathrm{d}}^{\dagger}\Big) \geq 0$ of the transformed density matrix, with U_{d} the unitary (228). Dropping them gives the lower bound in (77).

5. Proofs

The rest of the paper is devoted to proofs.

5.1. **A priori bounds.**

Proof of Proposition 4.1. For $\mu = 1, 2, 3$, write ∂_μ for differentiation with respect to the μth component of $\mathbf{x} = \mathbf{x}_1$, and D_1^μ for the corresponding component of $\mathbf{D}_1$. By (28), the state Ψ has square-integrable weak electronic derivatives and finite photon form energy. The field bound (20) also shows that $\|\mathfrak{A}(\mathbf{x}_n)\Psi\|$ and $\|\mathbf{D}_n\Psi\|$ are finite for every n. We may therefore regard $\mathbf{x} \mapsto \Psi(\mathbf{x}, \cdot)$ as an H^1 function taking values in the Hilbert space of the remaining electronic and photon variables. In terms of the partial norm $\|\cdot\|_{\mathbf{x}}$, the definition of the density gives

$$\|\Psi\|_{\mathbf{x}} = \sqrt{\rho_\Psi(\mathbf{x})/N}.$$

In particular, $\rho_\Psi \geq 0$, and Fubini's theorem and normalization give

$$\int_{\mathbb{R}^3} \rho_\Psi(\mathbf{x}) \mathrm{d}\mathbf{x} = N\|\Psi\|^2 = N.$$

We next prove the joint density–current bound (38). The Sobolev chain rule for the Hilbert-space norm gives $\sqrt{\rho_\Psi} \in H^1$ and, almost everywhere on $\{\rho_\Psi > 0\}$,

$$\partial_\mu \sqrt{\rho_\Psi} = \frac{N \operatorname{Re}\langle \Psi, \partial_\mu \Psi\rangle_{\mathbf{x}}}{\sqrt{\rho_\Psi}}.$$

One can obtain this formula by first differentiating $(\|\Psi\|_{\mathbf{x}}^2 + \varepsilon^2)^{1/2} - \varepsilon$ and then letting $\varepsilon \downarrow 0$. The derivatives are dominated by $\|\partial_\mu \Psi\|_{\mathbf{x}}$. On $\{\rho_\Psi = 0\}$, the weak gradient of $\sqrt{\rho_\Psi}$ vanishes almost everywhere. Since $\mathfrak{A}^\mu(\mathbf{x})$ is self-adjoint, the partial inner product $\langle \Psi, \mathfrak{A}^\mu(\mathbf{x})\Psi\rangle_{\mathbf{x}}$ is real. Set $\zeta^\mu(\mathbf{x}) := \langle \Psi, D_1^\mu \Psi\rangle_{\mathbf{x}}$. The identity $\partial_\mu \Psi = \mathrm{i} D_1^\mu \Psi + \mathrm{i} e \mathfrak{A}^\mu(\mathbf{x})\Psi$ and the definition of the combined current density then give

$$\operatorname{Im} \zeta^\mu = -\frac{\sqrt{\rho_\Psi}\, \partial_\mu \sqrt{\rho_\Psi}}{N}, \qquad \operatorname{Re} \zeta^\mu = \frac{(\mathbf{j}_\Psi^{\mathrm{c}})^\mu}{N}.$$

These identities express the gradient of $\sqrt{\rho_\Psi}$ and the combined current through the imaginary and real parts of the same partial inner product. Cauchy–Schwarz in the remaining variables gives, on $\{\rho_\Psi > 0\}$,

$$\begin{aligned} |\boldsymbol{\nabla}\sqrt{\rho_\Psi}|^2 + \frac{|\mathbf{j}_\Psi^{\mathrm{c}}|^2}{\rho_\Psi} &= \frac{N^2}{\rho_\Psi} \sum_{\mu=1}^{3} \left(|\operatorname{Im} \zeta^\mu|^2 + |\operatorname{Re} \zeta^\mu|^2 \right) \\ &= \frac{N^2}{\rho_\Psi} \sum_{\mu=1}^{3} |\zeta^\mu|^2 \leq N \|\mathbf{D}_1 \Psi\|_{\mathbf{x}}^2. \end{aligned}$$

On $\{\rho_\Psi = 0\}$ we have $\|\Psi\|_{\mathbf{x}} = 0$, so all three current densities vanish there. With the stated convention for the quotient, both terms on the left vanish almost everywhere on this set, and the inequality holds there as well. Exchanging electronic coordinates sends $\mathbf{D}_1$ to the corresponding $\mathbf{D}_n$, and the sign from antisymmetry disappears upon taking squared norms. Consequently,

$$N\|\mathbf{D}_1 \Psi\|^2 = \sum_{n=1}^{N} \|\mathbf{D}_n \Psi\|^2.$$

Integrating the pointwise joint bound proves (38).

We now prove the bound (39) on the field-induced current density. Applying conditional Cauchy–Schwarz to the definition of $\mathbf{j}_\Psi^{\mathrm{ph}}$ and then integrating gives

$$|\mathbf{j}_\Psi^{\mathrm{ph}}(\mathbf{x})|^2 \le e^2 N \rho_\Psi(\mathbf{x}) \|\mathfrak{A}(\mathbf{x})\Psi\|_{\mathbf{x}}^2, \qquad \int_{\mathbb{R}^3} \frac{|\mathbf{j}_\Psi^{\mathrm{ph}}|^2}{\rho_\Psi} \le e^2 N \|\mathfrak{A}(\mathbf{x}_1)\Psi\|^2.$$

For almost every electronic configuration $\mathbf{X}$, apply (20) to the Fock-space vector $\Psi(\mathbf{X})$ at the position $\mathbf{x}_1$. Its constant is independent of that position, so integration in $\mathbf{X}$ gives

$$\|\mathfrak{A}(\mathbf{x}_1)\Psi\|^2 \le C_\chi\big(\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 + \|\Psi\|^2\big) = C_\chi\big(\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 + 1\big).$$

This proves (39).

It remains to prove the integrability of the density and the current densities. The following integrability argument extends the estimates for electronic paramagnetic currents in [25, 27] to the combined and field-induced current densities, using the bounds established above. Since $\sqrt{\rho_\Psi} \in H^1(\mathbb{R}^3)$, the Sobolev embedding gives $\sqrt{\rho_\Psi} \in L^2 \cap L^6$, hence $\rho_\Psi \in L^1 \cap L^3$. For either $\mathbf{j} = \mathbf{j}_\Psi^{\mathrm{c}}$ or $\mathbf{j} = \mathbf{j}_\Psi^{\mathrm{ph}}$, the bounds just proved show that $\mathbf{j}/\sqrt{\rho_\Psi} \in L^2$, with value zero where the density vanishes. Factoring $\mathbf{j} = \sqrt{\rho_\Psi}\,(\mathbf{j}/\sqrt{\rho_\Psi})$ and applying Hölder's inequality gives

$$\|\mathbf{j}\|_{L^1} \le \|\sqrt{\rho_\Psi}\|_{L^2} \left\| \frac{\mathbf{j}}{\sqrt{\rho_\Psi}} \right\|_{L^2}, \qquad \|\mathbf{j}\|_{L^{3/2}} \le \|\sqrt{\rho_\Psi}\|_{L^6} \left\| \frac{\mathbf{j}}{\sqrt{\rho_\Psi}} \right\|_{L^2}.$$

Finally, $\mathbf{j}_\Psi^{\mathrm{p}} = \mathbf{j}_\Psi^{\mathrm{c}} - \mathbf{j}_\Psi^{\mathrm{ph}}$ belongs to the same two spaces.

For a density matrix $\mathbf{\Gamma} = \sum_r p_r |\Psi_r\rangle\langle\Psi_r| \in \mathcal{D}$, apply the preceding argument to the auxiliary vector $(\sqrt{p_r}\Psi_r)_r$, taking the Hilbert direct sum over r as part of the space of remaining variables. This vector is normalized and has finite form energy. Its partial density and currents are the ensemble averages, and the operators act componentwise in r. Their squared norms are therefore the corresponding form traces, which proves the mixed-state extension. □

Proof of Proposition 4.2. Let $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, write ∂_μ for the derivative with respect to the μth component of $\mathbf{x} = \mathbf{x}_1$, and denote the right-hand side of (40) by

$$f_\Psi(\mathbf{x}) := -2eN \operatorname{Re} \sum_{\mu=1}^{3} \langle \partial_\mu \Psi, \mathfrak{A}^\mu(\mathbf{x})\Psi\rangle_{\mathbf{x}}.$$

Let $\|\cdot\|_{\mathcal{Q}_{\mathrm{PF}}}$ be the reference norm (24). As in the proof of Proposition 4.1, applying (20) to $\Phi(\mathbf{X})$ for almost every $\mathbf{X}$ gives

$$\|\mathfrak{A}(\mathbf{x}_1)\Phi\| \le C_\chi^{1/2} \|\Phi\|_{\mathcal{Q}_{\mathrm{PF}}}, \qquad \Phi \in \mathcal{Q}_{\mathrm{PF}}. \tag{86}$$

We first show that f_Ψ is integrable. The conditional Cauchy–Schwarz inequality $|\langle \partial_\mu \Psi, \mathfrak{A}^\mu(\mathbf{x})\Psi\rangle_{\mathbf{x}}| \le \|\partial_\mu \Psi\|_{\mathbf{x}} \|\mathfrak{A}^\mu(\mathbf{x})\Psi\|_{\mathbf{x}}$, followed by Cauchy–Schwarz in $\mathbf{x}$ and in μ, gives

$$\int_{\mathbb{R}^3} |f_\Psi| \le 2eN \sum_{\mu=1}^{3} \|\partial_\mu \Psi\| \, \|\mathfrak{A}^\mu(\mathbf{x}_1)\Psi\| \le 2eN \|\nabla_{\mathbf{x}_1}\Psi\| \, \|\mathfrak{A}(\mathbf{x}_1)\Psi\|. \tag{87}$$

Both factors are finite by (23) and (86).

We now prove (40) in the sense of distributions. Let $v \in C_c^\infty(\mathbb{R}^3)$ be real. For $\Phi, \Phi' \in \mathcal{Q}_{\mathrm{PF}}$ put

$$s_v(\Phi,\Phi') := \sum_{\mu=1}^{3} \Big(\langle \Phi, (\partial_\mu v)(\mathbf{x}_1)\mathfrak{A}^\mu(\mathbf{x}_1)\Phi'\rangle + \langle \partial_\mu\Phi, v(\mathbf{x}_1)\mathfrak{A}^\mu(\mathbf{x}_1)\Phi'\rangle + \langle v(\mathbf{x}_1)\mathfrak{A}^\mu(\mathbf{x}_1)\Phi, \partial_\mu\Phi'\rangle \Big).$$

Since $\langle \Psi, \mathfrak{A}^\mu(\mathbf{x})\Psi\rangle_{\mathbf{x}}$ is real, Fubini's theorem and the definitions give

$$\sum_{\mu=1}^{3} \int_{\mathbb{R}^3} (\partial_\mu v)(\mathbf{j}_\Psi^{\mathrm{ph}})^\mu + \int_{\mathbb{R}^3} v f_\Psi = -eN s_v(\Psi,\Psi),$$

so (40) holds in the sense of distributions once $s_v(\Psi,\Psi) = 0$. The form s_v is sesquilinear, and Cauchy–Schwarz together with (86) gives

$$|s_v(\Phi,\Phi')| \le C_\chi^{1/2}\big(\sqrt{3}\|\boldsymbol{\nabla} v\|_\infty + 2\|v\|_\infty\big)\|\Phi\|_{\mathcal{Q}_{\mathrm{PF}}}\|\Phi'\|_{\mathcal{Q}_{\mathrm{PF}}}.$$

By (27) and (28), the algebraic core $\mathscr{C}_{\mathrm{PF}}$ of (25) is dense in $\mathcal{Q}_{\mathrm{PF}}$ for $\|\cdot\|_{\mathcal{Q}_{\mathrm{PF}}}$. It therefore suffices to show $s_v(\Phi,\Phi') = 0$ for the product vectors $\Phi = \varphi \otimes \Sigma$ and $\Phi' = \varphi' \otimes \Sigma'$ spanning $\mathscr{C}_{\mathrm{PF}}$, where $\varphi, \varphi' \in C_c^\infty(\mathbb{R}^{3N}) \cap \mathfrak{H}_{\mathrm{el}}^N$ and Σ, Σ' are finite-particle vectors in $D(\sqrt{H_{\mathrm{rad}}})$. Since $\mathfrak{A}^\mu(\mathbf{x})$ is symmetric on $D(\sqrt{H_{\mathrm{rad}}})$, the three terms of s_v combine by the product rule into

$$s_v(\Phi,\Phi') = \sum_{\mu=1}^{3} \int_{\mathbb{R}^{3N}} \partial_\mu\big(v(\mathbf{x}_1)\,\overline{\varphi(\mathbf{X})}\,\varphi'(\mathbf{X})\big)\,\langle \Sigma, \mathfrak{A}^\mu(\mathbf{x}_1)\Sigma'\rangle \mathrm{d}\mathbf{X}.$$

The function $\mathbf{x} \mapsto \langle \Sigma, \mathfrak{A}^\mu(\mathbf{x})\Sigma'\rangle$ is bounded and continuous by (20) and the continuity of $\mathbf{x} \mapsto G_{\mathbf{x}}^\mu$. For fixed $\mathbf{x}_2, \dots, \mathbf{x}_N$, the function $\mathbf{x}_1 \mapsto v(\mathbf{x}_1)\overline{\varphi(\mathbf{X})}\varphi'(\mathbf{X})$ lies in $C_c^\infty(\mathbb{R}^3)$. By Fubini's theorem we may first integrate in $\mathbf{x}_1$, and that integral vanishes by the weak Coulomb gauge (17), applied to the real and imaginary parts of this test function. Hence $s_v = 0$ on $\mathcal{Q}_{\mathrm{PF}}$, which proves (40). Now $\operatorname{div} \mathbf{j}_\Psi^{\mathrm{ph}} = f_\Psi$, and (87) is (41).

Finally, the right-hand side of (40) contains no derivative of the field and need not vanish. In the one-electron example following Proposition 4.2, with $\mathbf{j}_\Psi^{\mathrm{ph}}$ given by (42), it equals $-2e \operatorname{Re}\big(\mathbf{g}_\xi \cdot \boldsymbol{\nabla}(\overline{\varphi_0}\varphi_1)\big)$, which is nonzero for $e > 0$ and generic φ_0, φ_1. Choosing φ_0, φ_1 such that $\rho_\Psi = |\varphi_0|^2 + |\varphi_1|^2$ is constant on an open set where this expression does not vanish shows that $\mathbf{j}_\Psi^{\mathrm{ph}}/\rho_\Psi$ is not divergence-free either. □

5.2. **Proof of Proposition 4.3.** Let Ψ be a ground state of $H^{v,\mathbf{A}}$. Items (i)–(iii) are first-order conditions of the variational principle (31): a one-parameter family of trial states through Ψ has energy at least $E(v,\mathbf{A})$, with equality at $t = 0$. Item (iv) follows from time-reversal symmetry. By Proposition 4.1, $\mathbf{j}_\Psi^{\mathrm{c}} \in L^1 \cap L^{3/2}$ and $\rho_\Psi \in L^1 \cap L^3$, so Hölder's inequality gives $\rho_\Psi \mathbf{A} \in L^1 \cap L^{3/2}$ for $\mathbf{A} \in L^3 + L^\infty$.

We first prove (i). For real $\varphi \in C_c^\infty(\mathbb{R}^3)$ and $t \in \mathbb{R}$, the gauge unitary $U_{t\varphi}$ of (195) preserves $\mathcal{Q}_{\mathrm{PF}}$, and by (37) and (196)

$$\langle U_{t\varphi}\Psi, H^{v,\mathbf{A}} U_{t\varphi}\Psi\rangle = E(v,\mathbf{A}) + t\int_{\mathbb{R}^3} \boldsymbol{\nabla}\varphi \cdot \mathbf{j}_\Psi + \frac{t^2}{2}\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\varphi|^2 \rho_\Psi.$$

The minimum at $t = 0$ gives $\int \boldsymbol{\nabla}\varphi \cdot \mathbf{j}_\Psi = 0$, which is (i).

We next derive an identity for the mean photon amplitude, with

$$g_{\mathbf{j}_\Psi} = \sum_{\mu=1}^{3} \int_{\mathbb{R}^3} j_\Psi^\mu(\mathbf{x}) G_{\mathbf{x}}^\mu \mathrm{d}\mathbf{x}.$$

Let $f \in D(\omega)$. By Corollary A.8, applied to $\mathbf{\Gamma} = |\Psi\rangle\langle\Psi|$, $W(tf)$ preserves $\mathcal{Q}_{\mathrm{PF}}$, and the energy of $W(tf)\Psi$ is the quadratic polynomial (220) in t. Its linear coefficient is

$$2\,\mathrm{Re}\langle\Psi, a(\omega f)\Psi\rangle - e\int \mathbf{c}_f \cdot \mathbf{j}_\Psi = 2\,\mathrm{Re}\langle\Psi, a(\omega f)\Psi\rangle - 2e\,\mathrm{Re}\langle f, g_{\mathbf{j}_\Psi}\rangle,$$

with $\mathbf{c}_f$ as in (218). This coefficient vanishes, and applying this also to $\mathrm{i}f$ in place of f gives

$$\langle\Psi, a(\omega f)\Psi\rangle = e\langle f, g_{\mathbf{j}_\Psi}\rangle \qquad \text{for all } f \in D(\omega).$$

We next prove (ii) and (iii). For test fields $\mathbf{u}, \mathbf{v} \in C_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$, the kernels of $\int \mathbf{u}\cdot\mathfrak{E}_\perp$ and of $\int(\boldsymbol{\nabla}\times\mathbf{v})\cdot\mathfrak{B} = \int(\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{v})\cdot\mathfrak{A}$ are $-\mathrm{i}\omega g_{\mathbf{u}}$ and $g_{-\Delta\mathbf{v}} = \omega^2 g_{\mathbf{v}}$, since $\boldsymbol{\nabla}\times\boldsymbol{\nabla}\times\mathbf{v} = -\Delta\mathbf{v} + \boldsymbol{\nabla}\,\mathrm{div}\,\mathbf{v}$ and gradients have zero kernel. The choices $f = g_{\mathbf{u}}$ and $f = \omega g_{\mathbf{v}}$ in this identity therefore give

$$\Big\langle\Psi, \Big(\int \mathbf{u}\cdot\mathfrak{E}_\perp\Big)\Psi\Big\rangle = -2e\,\mathrm{Im}\langle g_{\mathbf{u}}, g_{\mathbf{j}_\Psi}\rangle = 0,$$
$$\Big\langle\Psi, \Big(\int(\boldsymbol{\nabla}\times\mathbf{v})\cdot\mathfrak{B}\Big)\Psi\Big\rangle = 2e\,\mathrm{Re}\langle\omega g_{\mathbf{v}}, g_{\mathbf{j}_\Psi}\rangle.$$

The first scalar product is real as in Section 3.3, which proves (ii). Since

$$2\,\mathrm{Re}\langle\omega G_{\mathbf{x}}^\mu, G_{\mathbf{y}}^\nu\rangle = \int_{\mathbb{R}^3} \omega(\mathbf{k})|\widehat{\chi}(\mathbf{k})|^2 P_{\mathrm{sol}}(\mathbf{k})^{\mu\nu} e^{\mathrm{i}\mathbf{k}\cdot(\mathbf{x}-\mathbf{y})}\mathrm{d}\mathbf{k},$$

the second identity is (iii) paired with $\mathbf{v}$.

We finally prove (iv). By Proposition A.4, the time reversal Θ of (190) reverses $\mathfrak{A}$, $\mathfrak{B}$, and $\mathbf{D}_n$ and commutes with $H^{v,0}$. Hence $\Theta\Psi$ is a ground state, and by nondegeneracy a multiple of Ψ. On the other hand, $\mathbf{j}^{\mathrm{c}}_{\Theta\Psi} = -\mathbf{j}^{\mathrm{c}}_{\Psi}$ and $\langle\Theta\Psi, \mathfrak{A}\Theta\Psi\rangle = -\langle\Psi, \mathfrak{A}\Psi\rangle$, and likewise for $\mathfrak{B}$. All three quantities therefore vanish.

5.3. **Representability results.**

Proof of Theorem 4.4. Let $\Gamma = \sum_{j\geq1} p_j|\Phi_j\rangle\langle\Phi_j|$ be an electronic mixed state in (43), written in its spectral decomposition. For $\varepsilon > 0$, choose an orthonormal family

$$f_j \in L^2(\{0 < |\mathbf{k}| < \varepsilon\} \times \{1,2\})$$

and put $\Xi_j = a^\dagger(f_j)\Omega$. All Ξ_j are normalized and lie in the one-photon sector. The vector

$$\Psi_\varepsilon = \sum_{j\geq1} \sqrt{p_j}\,\Phi_j \otimes \Xi_j \tag{88}$$

is normalized and $\mathrm{Tr}_{\mathrm{ph}}\,|\Psi_\varepsilon\rangle\langle\Psi_\varepsilon| = \Gamma$. It therefore has density ρ_Γ and paramagnetic current density $\mathbf{j}^{\mathrm{p}}_\Gamma$. Moreover, $\mathfrak{A}(\mathbf{x})$ changes photon number by exactly one, whence

$$\langle\Xi_j, \mathfrak{A}(\mathbf{x})\Xi_k\rangle = 0 \quad \text{for all } j,k,$$

and consequently $\mathbf{j}^{\mathrm{ph}}_{\Psi_\varepsilon} = 0$.

It remains to check that $\Psi_\varepsilon \in \mathcal{Q}_{\mathrm{PF}}$. Orthonormality of the photon vectors Ξ_j eliminates the cross terms in the electronic kinetic energy, so

$$\sum_{n=1}^{N} \|\boldsymbol{\nabla}_{\mathbf{x}_n} \Psi_\varepsilon\|^2 = \sum_j p_j \sum_{n=1}^{N} \|\boldsymbol{\nabla}_{\mathbf{x}_n} \Phi_j\|^2 = \mathrm{Tr}(-\boldsymbol{\Delta}\Gamma) < \infty.$$

Likewise, orthonormality of the electronic vectors Φ_j eliminates the cross terms in the photon energy, and H_{rad} acts as multiplication by $\omega(\mathbf{k}) = |\mathbf{k}|$ on the one-photon sector. Hence

$$\begin{aligned}\langle \Psi_\varepsilon, H_{\mathrm{rad}} \Psi_\varepsilon \rangle &= \sum_j p_j \langle \Xi_j, H_{\mathrm{rad}} \Xi_j \rangle \\ &= \sum_j p_j \|\sqrt{\omega} f_j\|^2 \leq \varepsilon \sum_j p_j \|f_j\|^2 = \varepsilon,\end{aligned}$$

where the inequality uses the support condition $|\mathbf{k}| < \varepsilon$, and the last equality uses $\|f_j\| = 1$ and $\sum_j p_j = 1$. Thus $\Psi_\varepsilon \in \mathcal{Q}_{\mathrm{PF}}$, proving the reverse inclusion in (45) as well as the reverse inclusion in (46).

Conversely, let $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ be normalized and define its electronic reduced state by

$$\Gamma := \mathrm{Tr}_{\mathrm{ph}} |\Psi\rangle\langle\Psi|.$$

Partial trace preserves positivity and the trace, so $\Gamma \geq 0$ and $\mathrm{Tr}\,\Gamma = 1$. We must check that this electronic density matrix has finite kinetic energy and reproduces the pair $(\rho_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi)$.

The positive-observable partial-trace identity (6) gives, in the quadratic-form sense,

$$\begin{aligned}\mathrm{Tr}(-\boldsymbol{\Delta}\Gamma) &= \sum_{n=1}^{N} \|\boldsymbol{\nabla}_{\mathbf{x}_n} \Psi\|^2 \\ &\leq 2 \sum_{n=1}^{N} \|\mathbf{D}_n \Psi\|^2 + 2e^2 \sum_{n=1}^{N} \|\mathfrak{A}(\mathbf{x}_n)\Psi\|^2 < \infty.\end{aligned}$$

The equality follows by applying the definition (2) of the partial trace first to bounded spectral truncations of $-\boldsymbol{\Delta}$ and then using monotone convergence. The inequality uses $-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} \Psi = \mathbf{D}_n \Psi + e\mathfrak{A}(\mathbf{x}_n)\Psi$. Both sums are finite by (20) and (28). Thus Γ satisfies all the state conditions in (43).

To see explicitly why the electronic density and paramagnetic current density are preserved, we use a Schmidt decomposition as in (3) and (4),

$$\Psi = \sum_j \sqrt{p_j}\, \Phi_j \otimes \Xi_j, \qquad \Gamma = \sum_j p_j |\Phi_j\rangle\langle\Phi_j|, \qquad \sum_j p_j = 1.$$

The electronic vectors Φ_j and the photon vectors Ξ_j form orthonormal families. The finite kinetic trace implies that each Φ_j with $p_j > 0$ has finite kinetic energy and that the Schmidt series also converges in the electronic H^1 norm. Inserting this series into (33) and (34), the photon inner products $\langle \Xi_j, \Xi_k \rangle = \delta_{jk}$ remove all cross terms, giving

$$\rho_\Psi = \sum_j p_j \rho_{\Phi_j} = \rho_\Gamma, \qquad \mathbf{j}^{\mathrm{p}}_\Psi = \sum_j p_j \mathbf{j}^{\mathrm{p}}_{\Phi_j} = \mathbf{j}^{\mathrm{p}}_\Gamma.$$

The density series converges in L^1 by normalization, and the current series by Cauchy–Schwarz and the finite kinetic trace. These identities therefore hold almost everywhere, and prove the forward inclusion in (45).

If the original state additionally satisfies $\mathbf{j}_\Psi^{\mathrm{ph}} = 0$, its triple is $(\rho_\Gamma, \mathbf{j}_\Gamma^{\mathrm{p}}, 0)$ with $(\rho_\Gamma, \mathbf{j}_\Gamma^{\mathrm{p}}) \in \mathcal{J}_{N,\mathrm{mix}}^{\mathrm{el}}$. This proves the forward inclusion in (46). The reverse inclusion was supplied by the one-photon purification above. □

Proof of Theorem 4.5. **Step 1. Splitting off the uncoupled photon modes.** Replacing S by $S \cap B_r$ for sufficiently large r, we may assume that S is bounded. By the symmetry $\widehat{\chi}(\mathbf{k}) = \overline{\widehat{\chi}(-\mathbf{k})}$ in (9), $\widehat{\chi}(-\mathbf{k}) = 0$ for almost every $\mathbf{k} \in S$, so by (12) every $G_{\mathbf{x}}^\mu$ vanishes almost everywhere on $S \times \{1,2\}$. The orthogonal decomposition

$$\mathfrak{H}_{\mathrm{ph}} = \mathfrak{h}_R \oplus \mathfrak{h}_S, \qquad \mathfrak{h}_R = L^2(S^c \times \{1,2\}), \qquad \mathfrak{h}_S = L^2(S \times \{1,2\}),$$

induces the canonical factorization $\mathcal{F}_s(\mathfrak{H}_{\mathrm{ph}}) \simeq \mathcal{F}_s(\mathfrak{h}_R) \otimes \mathcal{F}_s(\mathfrak{h}_S)$, and hence

$$\mathcal{H}_N \simeq \mathcal{K}_R \otimes \mathcal{F}_S, \qquad \mathcal{K}_R := \mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_s(\mathfrak{h}_R), \qquad \mathcal{F}_S := \mathcal{F}_s(\mathfrak{h}_S).$$

Under this identification $\mathfrak{A}(\mathbf{x}) = \mathfrak{A}_R(\mathbf{x}) \otimes \mathbb{1}_{\mathcal{F}_S}$, where $\mathfrak{A}_R$ is the field on $\mathcal{F}_s(\mathfrak{h}_R)$ with the same kernels $G_{\mathbf{x}}^\mu$, and $H_{\mathrm{rad}} = H_{\mathrm{rad},R} \otimes \mathbb{1}_{\mathcal{F}_S} + \mathbb{1} \otimes H_{\mathrm{rad},S}$, where $H_{\mathrm{rad},R}$ and $H_{\mathrm{rad},S}$ are the second quantizations of the restrictions of ω to S^c and S. For real $v \in C_c^\infty(\mathbb{R}^3)$ and $\mathbf{A} \in C_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$, let $H_R^{v,\mathbf{A}}$ be the Hamiltonian on $\mathcal{K}_R$ defined like $H^{v,\mathbf{A}}$, with $\mathfrak{A}_R$ and $H_{\mathrm{rad},R}$ in place of $\mathfrak{A}$ and H_{rad}. Then, as closed forms,

$$H^{v,\mathbf{A}} = H_R^{v,\mathbf{A}} \otimes \mathbb{1}_{\mathcal{F}_S} + \mathbb{1}_{\mathcal{K}_R} \otimes H_{\mathrm{rad},S}, \tag{89}$$

and in particular $Q(H^{0,0}) = Q(H_R^{0,0} \otimes \mathbb{1}_{\mathcal{F}_S}) \cap Q(\mathbb{1}_{\mathcal{K}_R} \otimes H_{\mathrm{rad},S})$.

Step 2. The density and current density depend only on the coupled marginal. Let $\mathbf{\Gamma} \in \mathcal{D}$, and put $\Gamma_R = \mathrm{Tr}_{\mathcal{F}_S} \mathbf{\Gamma}$ and $\Gamma_S = \mathrm{Tr}_{\mathcal{K}_R} \mathbf{\Gamma}$. Both terms in (89) are nonnegative after $N\|v\|_\infty$ is added to the first. The positive-observable identity (6) therefore gives

$$\mathrm{Tr}\big(H^{v,\mathbf{A}}\mathbf{\Gamma}\big) = \mathrm{Tr}\Big(H_R^{v,\mathbf{A}}\Gamma_R\Big) + \mathrm{Tr}(H_{\mathrm{rad},S}\Gamma_S), \tag{90}$$

where all terms are finite by (30). Subtracting the case $v = 0$, $\mathbf{A} = 0$ removes the last term. Applying (37) to the spectral decomposition of $\mathbf{\Gamma}$, we obtain

$$\int_{\mathbb{R}^3} \big(v + \tfrac{1}{2}|\mathbf{A}|^2\big)\rho_{\mathbf{\Gamma}} + \int_{\mathbb{R}^3} \mathbf{A} \cdot \mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c}} = \mathrm{Tr}\Big(H_R^{v,\mathbf{A}}\Gamma_R\Big) - \mathrm{Tr}\Big(H_R^{0,0}\Gamma_R\Big).$$

The right-hand side depends on $\mathbf{\Gamma}$ only through Γ_R. Taking first $\mathbf{A} = 0$ and then general $\mathbf{A}$ shows that two density matrices in $\mathcal{D}$ with the same marginal on $\mathcal{K}_R$ have the same density and the same combined current density.

Step 3. Purification by uncoupled one-photon states. Fix $\mathbf{\Gamma} \in \mathcal{D}$ and write $\Gamma_R = \sum_r p_r |\Phi_r\rangle\langle\Phi_r|$ with $p_r > 0$ and orthonormal Φ_r, the index r ranging over a finite or countable set. Since S has positive measure, $\mathfrak{h}_S$ is infinite dimensional and contains an orthonormal family (f_r) indexed by the same set. Put $\Xi_r = a_S^\dagger(f_r)\Omega_S$ and $R_S = \operatorname{ess\,sup}_{\mathbf{k}\in S} |\mathbf{k}| < \infty$. The Ξ_r are orthonormal, so by (3) and (4) the unit vector

$$\Psi = \sum_r \sqrt{p_r}\, \Phi_r \otimes \Xi_r$$

satisfies

$$\mathrm{Tr}_{\mathcal{F}_S} |\Psi\rangle\langle\Psi| = \Gamma_R, \qquad \mathrm{Tr}_{\mathcal{K}_R} |\Psi\rangle\langle\Psi| = \sum_r p_r |\Xi_r\rangle\langle\Xi_r|.$$

Applying (6) to the two terms of (89) with $v = 0$ and $\mathbf{A} = 0$, and using (90) for $\mathbf{\Gamma}$, we get

$$\|(H_R^{0,0} \otimes \mathbb{1}_{\mathcal{F}_S})^{1/2}\Psi\|^2 = \mathrm{Tr}\Big(H_R^{0,0}\Gamma_R\Big) \leq \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big),$$
$$\|(\mathbb{1}_{\mathcal{K}_R} \otimes H_{\mathrm{rad},S})^{1/2}\Psi\|^2 = \sum_r p_r \langle f_r, \omega f_r\rangle \leq R_S.$$

Thus $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, and $|\Psi\rangle\langle\Psi| \in \mathcal{D}$ has the same marginal Γ_R on $\mathcal{K}_R$ as $\mathbf{\Gamma}$. By Step 2, $(\rho_\Psi, \mathbf{j}^{\mathrm{c}}_\Psi) = (\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}})$. This proves that the right-hand side of (48) is contained in the left-hand side.

Conversely, if $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ is normalized, then $|\Psi\rangle\langle\Psi| \in \mathcal{D}$, which proves the reverse inclusion. Finally, $\mathcal{D}$ is convex, its form energy is affine, and the map $\mathbf{\Gamma} \mapsto (\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}})$ is affine by the weak trace interpretation of (47). Its image is therefore convex, and the equality (48) proves the last assertion. □

5.4. **Proof of Theorem 4.6.** The idea is to distribute the electrons independently, with the real amplitude $\prod_{n=1}^N \sqrt{\rho(\mathbf{x}_n)/N}$, and to let the photon state depend on their positions. The electronic amplitude gives density ρ and no paramagnetic current density, but it is symmetric, so antisymmetry is supplied by a real unit vector built from the pair directions $\mathbf{x}_i - \mathbf{x}_j$ and placed in a few auxiliary photon modes. This factor contributes neither current density nor field expectation. The field-induced current density comes from a coherent state in a separate band of modes, displaced along the coupling functions at the electron positions with weights $\mathbf{u}(\mathbf{x}_n)$. Its conditional field expectation at $\mathbf{x}$ is $(\mathbf{Tu})(\mathbf{x})$ for a positive operator $\mathbf{T}$, and solving $\mathbf{Tu} = \mathbf{a}$ gives $\mathbf{j}^{\mathrm{ph}}_\Psi = -e\rho\mathbf{a}$. All photon factors are real, so no paramagnetic current density is created. The paramagnetic current density $\rho(\boldsymbol{\nabla} S + \mathbf{b})$ is produced by a further factor in the tag: a phase times a coherent state whose Berry connection is $\boldsymbol{\nabla} S + \mathbf{b}$ (Lemma C.3), made permutation invariant by the lift of Lemma B.2.

Step 1. An antisymmetric unit vector. Let $m = N(N-1)/2$ and let $V = \bigvee^m \mathbb{R}^3$ be the mth symmetric power of $\mathbb{R}^3$, with its Hilbert tensor norm and dimension $d = \binom{m+2}{2}$. If $N = 1$, then $V = \mathbb{R}$ and we take $\eta = 1$. For $N > 1$, let

$$\mathcal{O}_N := \big\{\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in \mathbb{R}^{3N} : \mathbf{x}_i \neq \mathbf{x}_j \text{ for all } i \neq j\big\}$$

be the complement of the collision diagonals, and define $\tau, \eta : \mathcal{O}_N \to V$ by

$$\tau(\mathbf{X}) = \bigvee_{i<j} \boldsymbol{\varepsilon}_{ij}(\mathbf{X}), \qquad \eta(\mathbf{X}) = \frac{\tau(\mathbf{X})}{\|\tau(\mathbf{X})\|_V}, \qquad \boldsymbol{\varepsilon}_{ij}(\mathbf{X}) = \frac{\mathbf{x}_i - \mathbf{x}_j}{|\mathbf{x}_i - \mathbf{x}_j|} \in S^2,$$

where $\vee$ denotes the symmetric tensor product. For $v_1, \dots, v_m \in S^2$ the product $v_1 \vee \cdots \vee v_m$ is nonzero: its pairing with $y^{\otimes m}$ is a positive multiple of $\prod_k (v_k \cdot y)$, which does not vanish for $y \in \mathbb{R}^3$ outside the finitely many planes $v_k^\perp$. By continuity and compactness of $(S^2)^m$, $\|\tau\|_V \geq c_N > 0$ on $\mathcal{O}_N$, so η is well defined. Since $\boldsymbol{\nabla}\eta = \|\tau\|_V^{-1}(1 - |\eta\rangle\langle\eta|)\boldsymbol{\nabla}\tau$, τ is multilinear in the $\boldsymbol{\varepsilon}_{ij}$, and $|\boldsymbol{\nabla}_{\mathbf{x}_n}\boldsymbol{\varepsilon}_{ij}| \leq C|\mathbf{x}_i - \mathbf{x}_j|^{-1}$ for $n \in \{i, j\}$, we obtain

$$\|\eta(\mathbf{X})\|_V = 1, \qquad \sum_{n=1}^N \|\boldsymbol{\nabla}_{\mathbf{x}_n}\eta(\mathbf{X})\|_V^2 \leq C_N \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^2}. \tag{91}$$

Permuting the electronic positions permutes the unordered pair factors and reverses their orientations once for every inversion. Thus $\eta(\pi\mathbf{X}) = \operatorname{sgn}(\pi)\eta(\mathbf{X})$. Its coordinates in a real orthonormal basis of V are real antisymmetric functions.[4]

The singularities in (91) are locally integrable in three relative dimensions, and it is easy to see that $\eta \in H^1_{\mathrm{loc}}(\mathbb{R}^{3N}; V)$.

Step 2. Photon modes and their real structure. Work in the solenoidal one-photon representation (13), using the unitary identification with the original Fock space. Define the conjugation by $(J\mathbf{f})(\mathbf{k}) = \overline{\mathbf{f}(-\mathbf{k})}$. A vector $\mathbf{f}$ is called J-real if $J\mathbf{f} = \mathbf{f}$. Every coupling function satisfies $J\mathbf{G}^\mu_{\mathbf{x}} = \mathbf{G}^\mu_{\mathbf{x}}$ for all $\mathbf{x}$ and μ. Indeed, $P_{\mathrm{sol}}(-\mathbf{k}) = P_{\mathrm{sol}}(\mathbf{k})$ is real and $\overline{\widehat{\chi}(\mathbf{k})} = \widehat{\chi}(-\mathbf{k})$ by (9), so

$$(J\mathbf{G}^\mu_{\mathbf{x}})(\mathbf{k}) = \frac{P_{\mathrm{sol}}(\mathbf{k})\mathbf{e}_\mu \overline{\widehat{\chi}(\mathbf{k})} e^{-\mathrm{i}\mathbf{k}\cdot\mathbf{x}}}{\sqrt{2}} = \mathbf{G}^\mu_{\mathbf{x}}(\mathbf{k}).$$

Since the form factor is nonzero, there is a bounded annulus $A = \{\mathbf{k} : r < |\mathbf{k}| < R\}$, with $0 < r < R < \infty$, such that $\int_A |\widehat{\chi}|^2 > 0$. Define the translation-invariant matrix kernel $\mathbf{K} = (K^{\mu\nu})_{\mu,\nu=1}^3$ by

$$K^{\mu\nu}(\mathbf{x},\mathbf{y}) = 2\,\mathrm{Re}\langle \mathbb{1}_A \mathbf{G}^\mu_{\mathbf{x}}, \mathbb{1}_A \mathbf{G}^\nu_{\mathbf{y}}\rangle, \qquad \mathbf{M} = \mathbf{K}(\mathbf{x},\mathbf{x}).$$

The function $\mathbb{1}_A \mathbf{G}^\mu_{\mathbf{x}}$ is J-real. All its spatial derivatives are uniformly bounded both in the one-photon norm and after multiplication by $\sqrt{\omega}$, since their momentum supports are bounded. The real matrix $\mathbf{M}$ is independent of $\mathbf{x}$, and

$$\mathbf{c}^{\mathsf{T}}\mathbf{M}\mathbf{c} = \int_A |\widehat{\chi}(\mathbf{k})|^2 |P_{\mathrm{sol}}(\mathbf{k})\mathbf{c}|^2 \mathrm{d}\mathbf{k} > 0 \qquad (\mathbf{c} \in \mathbb{R}^3 \setminus \{0\}).$$

Indeed, $P_{\mathrm{sol}}(\mathbf{k})\mathbf{c} = 0$ only when $\mathbf{k}$ is parallel to $\mathbf{c}$, which has measure zero. Thus $\mathbf{M}$ is positive definite. The kernel $\mathbf{K}$ is smooth with bounded derivatives and $\mathbf{K}(\mathbf{y},\mathbf{x}) = \mathbf{K}(\mathbf{x},\mathbf{y})^{\mathsf{T}}$.

Write $\mathfrak{H}_A = \mathbb{1}_A \mathfrak{H}_{\mathrm{sol}}$ and $\mathfrak{H}_{\mathbb{R}^3\setminus A} = \mathbb{1}_{\mathbb{R}^3\setminus A}\mathfrak{H}_{\mathrm{sol}}$. Under the Fock factorization

$$\mathcal{F}_s(\mathfrak{H}_{\mathrm{sol}}) \simeq \mathcal{F}_s(\mathfrak{H}_A) \otimes \mathcal{F}_s(\mathfrak{H}_{\mathbb{R}^3\setminus A}),$$

choose orthonormal $\xi_1, \dots, \xi_d \in \mathfrak{H}_{\mathbb{R}^3\setminus A}$, supported in the annulus $\{\mathbf{k} : r/2 < |\mathbf{k}| < r\}$, which is disjoint from A, and put $\Xi_\alpha = a^\dagger(\xi_\alpha)\Omega_{\mathbb{R}^3\setminus A}$, where $\Omega_{\mathbb{R}^3\setminus A}$ is the vacuum of the second factor. The free photon energy is bounded on the span of the Ξ_α. Writing η_α for the coordinates of η in a real orthonormal basis of V, set

$$\zeta(\mathbf{X}) = \sum_{\alpha=1}^d \eta_\alpha(\mathbf{X})\Xi_\alpha = a^\dagger\Big(\sum_{\alpha=1}^d \eta_\alpha(\mathbf{X})\xi_\alpha\Big)\Omega_{\mathbb{R}^3\setminus A}.$$

This is a unit antisymmetric vector and, for $n = 1, \dots, N$,

$$\langle \zeta, \boldsymbol{\nabla}_{\mathbf{x}_n}\zeta\rangle = 0, \qquad \langle \zeta, \mathfrak{A}_{\mathbb{R}^3\setminus A}(\mathbf{x})\zeta\rangle = 0. \tag{92}$$

The first equality follows from $\sum_\alpha \eta_\alpha \boldsymbol{\nabla}_{\mathbf{x}_n}\eta_\alpha = \frac{1}{2}\boldsymbol{\nabla}_{\mathbf{x}_n}\|\eta\|_V^2 = 0$, and the second because all Ξ_α have the same photon number and the field changes photon number by one. Here $\mathfrak{A}_{\mathbb{R}^3\setminus A}$ denotes the field with coupling functions projected onto $\mathfrak{H}_{\mathbb{R}^3\setminus A}$. The auxiliary modes need not be decoupled from the electrons, since $\widehat{\chi}$ may

[4] A vector-valued tag is necessary. For $N \geq 2$ the configuration space of distinct points in $\mathbb{R}^3$ is connected, so a continuous real antisymmetric function must vanish somewhere. Rotating a pair $\mathbf{x}_i, \mathbf{x}_j$ about its midpoint traces a sphere of directions $\boldsymbol{\varepsilon}_{ij}$ on which the transposition (ij) acts antipodally, so by the Borsuk–Ulam theorem a complex-valued one must vanish as well. For $N = 2$, the tag $\eta = \boldsymbol{\varepsilon}_{12}$ with $\dim V = 3$ is therefore of minimal dimension.

be nonzero on their support; the second identity ensures that they nevertheless contribute nothing to the field expectation.

Step 3. The displacement profile. On the real Hilbert space $L^2(\rho\,\mathrm{d}\mathbf{x};\mathbb{R}^3)$ (weighted L^2 space), define

$$(\mathbf{K}_\rho\mathbf{u})(\mathbf{x}) = \int_{\mathbb{R}^3} \mathbf{K}(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{y})\rho(\mathbf{y})\mathrm{d}\mathbf{y}, \qquad \mathbf{T} = \mathbf{M} + \frac{N-1}{N}\mathbf{K}_\rho.$$

The integral operator $\mathbf{K}_\rho$ is bounded and self-adjoint. It is positive, since

$$\langle \mathbf{u}, \mathbf{K}_\rho\mathbf{u}\rangle_{L^2(\rho\,\mathrm{d}\mathbf{x};\mathbb{R}^3)} = 2\left\| \int_{\mathbb{R}^3} \rho(\mathbf{y}) \sum_{\mu=1}^{3} u^\mu(\mathbf{y}) \mathbb{1}_A(\cdot)\mathbf{G}^\mu_{\mathbf{y}}(\cdot)\mathrm{d}\mathbf{y}\right\|^2 \geq 0,$$

where the norm is that of the one-photon space $\mathfrak{H}_{\mathrm{sol}}$. If $\lambda > 0$ is the smallest eigenvalue of $\mathbf{M}$, then $\mathbf{T} \geq \lambda\mathbb{1}$. Hence for $\mathbf{u} = \mathbf{T}^{-1}\mathbf{a}$,

$$\|\sqrt{\rho}\,\mathbf{u}\| \leq \lambda^{-1}\|\sqrt{\rho}\,\mathbf{a}\|. \tag{93}$$

Because $\mathbf{K}$ has bounded derivatives and $\int_{\mathbb{R}^3}\rho|\mathbf{u}| \leq \sqrt{N}\|\sqrt{\rho}\,\mathbf{u}\|$, the function $\mathbf{K}_\rho\mathbf{u}$ is smooth with bounded derivatives. The solution $\mathbf{u}$ is determined only ρ-almost everywhere. The equation $\mathbf{T}\mathbf{u} = \mathbf{a}$ is equivalent to $\mathbf{M}\mathbf{u} = \mathbf{a} - \frac{N-1}{N}\mathbf{K}_\rho\mathbf{u}$ ρ-almost everywhere, and the right-hand side is defined almost everywhere on $\mathbb{R}^3$, we fix $\mathbf{u}$ on all of $\mathbb{R}^3$ by

$$\mathbf{u}(\mathbf{x}) = \mathbf{M}^{-1}\Big(\mathbf{a}(\mathbf{x}) - \frac{N-1}{N}(\mathbf{K}_\rho\mathbf{u})(\mathbf{x})\Big).$$

Then $\mathbf{u}$ is in H^1_{loc} and satisfies

$$\int_{\mathbb{R}^3} \rho\big(|\mathbf{u}|^2 + |\boldsymbol{\nabla}\mathbf{u}|^2\big) \leq C_{N,\chi}\int_{\mathbb{R}^3}\rho\big(|\mathbf{a}|^2 + |\boldsymbol{\nabla}\mathbf{a}|^2\big). \tag{94}$$

Indeed, the zeroth-order part is (93). For the gradient, Cauchy–Schwarz with $\int_{\mathbb{R}^3}\rho = N$ gives

$$\sup_{\mathbf{x}} |\boldsymbol{\nabla}(\mathbf{K}_\rho\mathbf{u})(\mathbf{x})| \leq \|\boldsymbol{\nabla}\mathbf{K}\|_\infty \int_{\mathbb{R}^3}\rho|\mathbf{u}| \leq \sqrt{N}\lambda^{-1}\|\boldsymbol{\nabla}\mathbf{K}\|_\infty\|\sqrt{\rho}\,\mathbf{a}\|,$$

and $\boldsymbol{\nabla}\mathbf{u} = \mathbf{M}^{-1}(\boldsymbol{\nabla}\mathbf{a} - \frac{N-1}{N}\boldsymbol{\nabla}\mathbf{K}_\rho\mathbf{u})$. Only the bounded first derivatives of $\mathbf{K}$ are used here, and no derivative of the density is taken.

Step 4. The representing vector and its energy. Let $W(\mathbf{f})$ be the Weyl operator (200) on $\mathcal{F}_s(\mathfrak{H}_A)$, and let Ω_A be the vacuum of this factor. Let $B(\mathbf{X}) = \prod_{n=1}^N \sqrt{\rho(\mathbf{x}_n)/N}$ be the electronic amplitude. It has norm one and $\sum_n \|\boldsymbol{\nabla}_{\mathbf{x}_n}B\|^2 = \|\boldsymbol{\nabla}\sqrt{\rho}\|^2$. Define the displacement

$$\mathbf{f}_{\mathbf{X}} = \sum_{n=1}^{N}\sum_{\mu=1}^{3} u^\mu(\mathbf{x}_n)\mathbb{1}_A\mathbf{G}^\mu_{\mathbf{x}_n}$$

and the state

$$\boxed{\Psi(\mathbf{X}) = B(\mathbf{X})W(\mathbf{f}_{\mathbf{X}})\Omega_A \otimes \zeta(\mathbf{X}).} \tag{95}$$

The displacement $\mathbf{f}_{\mathbf{X}}$ is symmetric in the electronic positions and J-real. Thus Ψ is antisymmetric and

$$\|\Psi(\mathbf{X})\|^2 = B(\mathbf{X})^2 = \prod_{n=1}^{N}\frac{\rho(\mathbf{x}_n)}{N}.$$

Here $\|\Psi(\mathbf{X})\|$ is the norm in the photon Fock space. The state Ψ is normalized and has density ρ. Since $\mathbf{X} \mapsto \mathbf{f}_{\mathbf{X}}$ is J-real and lies in $H^1_{\mathrm{loc}}(\mathbb{R}^{3N}; \mathfrak{H}_A)$, Proposition A.9(iv) shows that $W(\mathbf{f}_{\mathbf{X}})\Omega_A$ is a unit H^1_{loc} vector and gives, for $n = 1, \dots, N$,

$$\begin{aligned} &\langle W(\mathbf{f}_{\mathbf{X}})\Omega_A, \boldsymbol{\nabla}_{\mathbf{x}_n}\big(W(\mathbf{f}_{\mathbf{X}})\Omega_A\big)\rangle = 0, \\ &\|\boldsymbol{\nabla}_{\mathbf{x}_n}\big(W(\mathbf{f}_{\mathbf{X}})\Omega_A\big)\|^2 = \|\boldsymbol{\nabla}_{\mathbf{x}_n}\mathbf{f}_{\mathbf{X}}\|^2. \end{aligned} \tag{96}$$

Together with (92), these identities make the three terms obtained by differentiating (95) pairwise orthogonal. Hence

$$\begin{aligned} \sum_n \|\boldsymbol{\nabla}_{\mathbf{x}_n}\Psi\|^2 &= \sum_n \|\boldsymbol{\nabla}_{\mathbf{x}_n}B\|^2 + \int_{\mathbb{R}^{3N}} B(\mathbf{X})^2 \sum_n \|\boldsymbol{\nabla}_{\mathbf{x}_n}\zeta\|^2 \mathrm{d}\mathbf{X} \\ &\quad + \int_{\mathbb{R}^{3N}} B(\mathbf{X})^2 \sum_n \|\boldsymbol{\nabla}_{\mathbf{x}_n}\mathbf{f}_{\mathbf{X}}\|^2 \mathrm{d}\mathbf{X} \\ &\le C_N \|\boldsymbol{\nabla}\sqrt{\rho}\|^2 + C_{N,\chi}\int_{\mathbb{R}^3} \rho\big(|\mathbf{a}|^2 + |\boldsymbol{\nabla}\mathbf{a}|^2\big). \end{aligned}$$

To justify the last inequality, first consider the term involving $\boldsymbol{\nabla}_{\mathbf{x}_n}\zeta$. The identity $\|\boldsymbol{\nabla}_{\mathbf{x}_n}\zeta\| = \|\boldsymbol{\nabla}_{\mathbf{x}_n}\eta\|_V$ and (91) reduce it to $C_N \int B^2 \sum_{i<j} |\mathbf{x}_i - \mathbf{x}_j|^{-2}$. For each pair, integrating out the other positions and applying Hardy's inequality

$$\int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})}{|\mathbf{x}-\mathbf{y}|^2}\,\mathrm{d}\mathbf{x} \le 4\|\boldsymbol{\nabla}\sqrt{\rho}\|^2, \qquad \mathbf{y} \in \mathbb{R}^3,$$

gives

$$\int_{\mathbb{R}^{3N}} \frac{B(\mathbf{X})^2}{|\mathbf{x}_i - \mathbf{x}_j|^2}\mathrm{d}\mathbf{X} = \frac{1}{N^2}\int_{\mathbb{R}^3}\int_{\mathbb{R}^3} \frac{\rho(\mathbf{x})\rho(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^2}\mathrm{d}\mathbf{x}\mathrm{d}\mathbf{y} \le \frac{4}{N}\|\boldsymbol{\nabla}\sqrt{\rho}\|^2. \tag{97}$$

For the last term, differentiation in $\mathbf{x}_n$ acts only on the nth summand of $\mathbf{f}_{\mathbf{X}}$, so the uniform bounds on $\mathbb{1}_A\mathbf{G}^\mu_{\mathbf{x}}$ and its derivatives and (94) apply.

The auxiliary modes ξ_α in Step 2 are supported where $|\mathbf{k}| < r < R$. On the one-photon sector the free photon energy acts as multiplication by $\omega(\mathbf{k}) = |\mathbf{k}|$, so

$$\langle \zeta(\mathbf{X}), H_{\mathrm{rad},\mathbb{R}^3\setminus A}\zeta(\mathbf{X})\rangle = \left\| \sqrt{\omega}\sum_{\alpha=1}^d \eta_\alpha(\mathbf{X})\xi_\alpha \right\|^2 \le R\sum_{\alpha=1}^d |\eta_\alpha(\mathbf{X})|^2 = R.$$

Here we used orthonormality of the ξ_α and $\|\eta(\mathbf{X})\|_V = 1$. Since $\int_{\mathbb{R}^{3N}} B(\mathbf{X})^2\mathrm{d}\mathbf{X} = 1$, the integrated contribution of this term is also at most R. The factorization (208) and the coherent-vector energy (216) give

$$\begin{aligned} \|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 &= \int_{\mathbb{R}^{3N}} B(\mathbf{X})^2 \left(\|\sqrt{\omega}\mathbf{f}_{\mathbf{X}}\|^2 + \langle\zeta(\mathbf{X}), H_{\mathrm{rad},\mathbb{R}^3\setminus A}\zeta(\mathbf{X})\rangle\right)\mathrm{d}\mathbf{X} \\ &\le N\int_{\mathbb{R}^3} \rho(\mathbf{x}) \left\| \sqrt{\omega}\sum_{\mu=1}^3 u^\mu(\mathbf{x})\mathbb{1}_A\mathbf{G}^\mu_{\mathbf{x}} \right\|^2 \mathrm{d}\mathbf{x} + R \\ &\le C_{N,\chi}\int_{\mathbb{R}^3} \rho|\mathbf{u}|^2 + R \\ &\le C_{N,\chi}\lambda^{-2}\int_{\mathbb{R}^3} \rho|\mathbf{a}|^2 + R \\ &\le C_{N,\chi}\int_{\mathbb{R}^3} \rho|\mathbf{a}|^2 + C_{N,\chi}. \end{aligned}$$

The first inequality uses $\|\sum_n g_n\|^2 \le N\sum_n \|g_n\|^2$, the one-particle marginal ρ/N of $B(\mathbf{X})^2$, and the photon energy bound above. The second uses the uniform bounds on $\sqrt{\omega}\mathbb{1}_A\mathbf{G}^\mu_{\mathbf{x}}$, and the third is (93) squared. Fixing A once for the given form factor allows λ^{-2} and R to be absorbed into $C_{N,\chi}$ in the last inequality, independently of ρ and $\mathbf{a}$. This proves (50) for $S=0$ and $\mathbf{b}=0$. By (28), Ψ lies in the Pauli–Fierz form domain, including the Coulomb form.

For completeness, these derivative computations are valid for the stated weak regularity. Since $W(\mathbf{f}_{\mathbf{X}})\Omega_A$ is a unit H^1_{loc} vector, so is

$$U(\mathbf{X}) = W(\mathbf{f}_{\mathbf{X}})\Omega_A \otimes \zeta(\mathbf{X}).$$

The estimates above give $B\boldsymbol{\nabla}U \in L^2$. Truncating B at height L, applying the local Sobolev product rule, and passing to the limit proves $\boldsymbol{\nabla}(BU) = (\boldsymbol{\nabla}B)U + B\boldsymbol{\nabla}U$ in L^2. No boundedness or strict positivity of ρ is required.

Step 5. The prescribed current densities. By (92) and (96), the photon scalar product satisfies $\langle U(\mathbf{X}), \boldsymbol{\nabla}_{\mathbf{x}_n} U(\mathbf{X})\rangle = 0$ for almost every electronic configuration $\mathbf{X}$. Hence $\langle \Psi(\mathbf{X}), \boldsymbol{\nabla}_{\mathbf{x}_n}\Psi(\mathbf{X})\rangle = B(\mathbf{X})\boldsymbol{\nabla}_{\mathbf{x}_n}B(\mathbf{X})$, which is real, so $\mathbf{j}^{\mathrm{p}}_\Psi = 0$.

To compute the field-induced current density, we first evaluate the field expectation in the photon state $U(\mathbf{X})$ at fixed electronic configuration $\mathbf{X}$. By (205), the μth component of the field expectation in the coherent state $W(\mathbf{f}_{\mathbf{X}})\Omega_A$ of the first photon factor is $2\,\mathrm{Re}\langle \mathbf{G}^\mu_{\mathbf{x}}, \mathbf{f}_{\mathbf{X}}\rangle$, and the second factor contributes zero. Expanding $\mathbf{f}_{\mathbf{X}} \in \mathfrak{H}_A$ and using the definition of $\mathbf{K}$ therefore gives

$$\langle U(\mathbf{X}), \mathfrak{A}(\mathbf{x})U(\mathbf{X})\rangle = \sum_{n=1}^{N} \mathbf{K}(\mathbf{x},\mathbf{x}_n)\mathbf{u}(\mathbf{x}_n).$$

For $\mathbf{x}_1 = \mathbf{x}$, the $n=1$ term in this field expectation is $\mathbf{K}(\mathbf{x},\mathbf{x})\mathbf{u}(\mathbf{x}) = \mathbf{M}\mathbf{u}(\mathbf{x})$. Moreover, for ρ-almost every $\mathbf{x}$,

$$\frac{NB(\mathbf{x},\mathbf{x}_2,\dots,\mathbf{x}_N)^2}{\rho(\mathbf{x})} = \prod_{n=2}^{N}\frac{\rho(\mathbf{x}_n)}{N}.$$

Thus, conditional on $\mathbf{x}_1 = \mathbf{x}$, the other positions have independent density ρ/N. Averaging leaves the $n=1$ contribution unchanged, while each of the remaining $N-1$ contributions gives the same integral. Consequently,

$$\begin{aligned}\frac{N\,\mathrm{Re}\langle\Psi, \mathfrak{A}(\mathbf{x})\Psi\rangle_{\mathbf{x}}}{\rho(\mathbf{x})} &= \mathbf{M}\mathbf{u}(\mathbf{x}) + \frac{N-1}{N}\int_{\mathbb{R}^3}\mathbf{K}(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{y})\rho(\mathbf{y})\mathrm{d}\mathbf{y}\\ &= (\mathbf{T}\mathbf{u})(\mathbf{x}) = \mathbf{a}(\mathbf{x}),\end{aligned}$$

and (35) gives $\mathbf{j}^{\mathrm{ph}}_\Psi = -e\rho\mathbf{a}$. Both current densities vanish on $\{\rho=0\}$, which proves (49) for $S=0$ and $\mathbf{b}=0$.

Step 6. The paramagnetic current density. Let t be the tag of Lemma C.3 with $\mathbf{w}=\mathbf{b}$ and $\lambda=1$, with values in $\mathcal{F}_s(\mathbb{C}^3)$. Thus $\|t\|=1$, $\mathrm{Im}\langle t, \boldsymbol{\nabla}t\rangle = \boldsymbol{\nabla}S + \mathbf{b}$, and

$$\|\boldsymbol{\nabla}t\|^2 = |\boldsymbol{\nabla}S + \mathbf{b}|^2 + \frac{1}{2}|\boldsymbol{\nabla}\mathbf{b}|^2 + \frac{3}{2}.$$

Let L be its symmetric lift from Lemma B.2, fix an orthonormal basis (e_β) of the separable Hilbert space $\mathcal{K}_N$ in which L takes its values, and put $L_\beta = \langle e_\beta, L\rangle$. By

(237) and (238),

$$\sum_\beta |L_\beta|^2 = 1, \qquad \sum_\beta \overline{L}_\beta \boldsymbol{\nabla}_{\mathbf{x}_n} L_\beta = \mathrm{i}(\boldsymbol{\nabla} S + \mathbf{b})(\mathbf{x}_n),$$
$$\sum_{n,\beta} |\boldsymbol{\nabla}_{\mathbf{x}_n} L_\beta|^2 \le \sum_n \|\boldsymbol{\nabla} t(\mathbf{x}_n)\|^2 + b_N \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^2}.$$

Choose orthonormal $\xi_{\alpha\beta} \in \mathfrak{H}_{\mathbb{R}^3\setminus A}$, $1 \le \alpha \le d$, $\beta \ge 1$, supported in the annulus of Step 2, and replace ζ by

$$\tilde\zeta(\mathbf{X}) = \sum_{\alpha,\beta} \eta_\alpha(\mathbf{X}) L_\beta(\mathbf{X})\, a^\dagger(\xi_{\alpha\beta})\Omega_{\mathbb{R}^3\setminus A}.$$

By orthonormality of the $\xi_{\alpha\beta}$, $\tilde\zeta(\mathbf{X})$ has unit norm,

$$\|\tilde\zeta(\mathbf{X})\|^2 = \sum_{\alpha,\beta} |\eta_\alpha(\mathbf{X})|^2 |L_\beta(\mathbf{X})|^2 = 1.$$

It is again an antisymmetric one-photon vector, so $\langle\tilde\zeta, \mathfrak{A}_{\mathbb{R}^3\setminus A}(\mathbf{x})\tilde\zeta\rangle = 0$, and its photon energy is bounded as before. Since $\sum_\alpha \eta_\alpha \boldsymbol{\nabla}\eta_\alpha = \frac12 \boldsymbol{\nabla}\|\eta\|_V^2 = 0$,

$$\langle\tilde\zeta, \boldsymbol{\nabla}_{\mathbf{x}_n}\tilde\zeta\rangle = \mathrm{i}(\boldsymbol{\nabla} S + \mathbf{b})(\mathbf{x}_n), \qquad \|\boldsymbol{\nabla}_{\mathbf{x}_n}\tilde\zeta\|^2 = \|\boldsymbol{\nabla}_{\mathbf{x}_n}\eta\|_V^2 + \sum_\beta |\boldsymbol{\nabla}_{\mathbf{x}_n} L_\beta|^2.$$

In Step 4, each new cross term contains either the real factor $B\boldsymbol{\nabla}_{\mathbf{x}_n} B$ or the vanishing coherent-state pairing in (96), so it does not contribute. Under B^2 each $\mathbf{x}_n$ has density ρ/N, so by (97) the kinetic energy increases by at most

$$\int_{\mathbb{R}^3} \rho\|\boldsymbol{\nabla} t\|^2 + 2(N-1)b_N\|\boldsymbol{\nabla}\sqrt{\rho}\|^2$$
$$\le \int_{\mathbb{R}^3} \rho\Big(2|\boldsymbol{\nabla} S|^2 + 2|\mathbf{b}|^2 + \frac12|\boldsymbol{\nabla}\mathbf{b}|^2\Big) + \frac32 N + 2(N-1)b_N\|\boldsymbol{\nabla}\sqrt{\rho}\|^2.$$

Since $L \in H^1_{\mathrm{loc}}$, the regularity argument of Step 4 applies verbatim. Step 5 now gives $\mathbf{j}_\Psi^{\mathrm{p}} = \rho(\boldsymbol{\nabla} S + \mathbf{b})$ and still $\mathbf{j}_\Psi^{\mathrm{ph}} = -e\rho\mathbf{a}$. This proves (49) and (50).

5.5. **Proof of Proposition 4.9.** Fix $e \ge 0$ and the form factor. On thin elliptic loops we prescribe a velocity with circulation π, half the circulation quantum of a pure electronic state. A pure minimizer has few soft photons by Proposition 4.16 and, by matching energy bounds, few hard photons. The phase of its vacuum component would then wind by π around a loop, which is impossible.

Step 1. The pairs $(\rho_n, \mathbf{j}_n)$. Let $0 < a_n < b_n$ and $0 < r_n < a_n^2/b_n$ be scales to be chosen later. Let $\boldsymbol{\gamma}_n : \mathbb{R}/L_n\mathbb{Z} \to \mathbb{R}^3$ parametrize the ellipse $\{x_1^2/a_n^2 + x_2^2/b_n^2 = 1,\ x_3 = 0\}$ by arclength, with inward unit normal $\boldsymbol{\nu}_n$ and curvature κ_n. Then $4b_n \le L_n \le 2\pi b_n$, $\kappa_n \le \tilde\kappa_n = b_n/a_n^2$, and $\int_0^{L_n} \kappa_n \mathrm{d}s = 2\pi$. The coordinates

$$\mathbf{X}_n(s, \mathbf{t}) = \boldsymbol{\gamma}_n(s) + t_1\boldsymbol{\nu}_n(s) + t_2\mathbf{e}_3, \qquad \mathbf{t} \in (-r_n, r_n)^2,$$

parametrize an open solid torus $\mathcal{T}_n$ (Fig. 1), since the ellipse is convex and $r_n < 1/\tilde\kappa_n$. By the Frenet equations, $\partial_s \mathbf{X}_n = J_n\dot{\boldsymbol{\gamma}}_n$ with $J_n = 1 - \kappa_n t_1$, and $(\dot{\boldsymbol{\gamma}}_n, \boldsymbol{\nu}_n, \mathbf{e}_3)$ is orthonormal. Hence $\mathrm{d}\mathbf{x} = J_n \mathrm{d}s\mathrm{d}\mathbf{t}$, $\boldsymbol{\nabla} s = J_n^{-1}\dot{\boldsymbol{\gamma}}_n$, and

$$|J_n - 1| \le \varepsilon_n := r_n\tilde\kappa_n < 1.$$

With $w(\mathbf{z}) = \cos^2(\pi z_1/2)\cos^2(\pi z_2/2)$ on $(-1,1)^2$, define, on $\mathcal{T}_n$ and by zero outside,

$$\rho_n(\mathbf{X}_n(s,\mathbf{t})) = \frac{w(\mathbf{t}/r_n)}{L_n r_n^2 J_n(s,\mathbf{t})}, \qquad \mathbf{j}_n = \frac{\pi}{L_n}\rho_n \boldsymbol{\nabla} s. \tag{98}$$

In the variables $\theta = s/L_n \in \mathbb{T} := \mathbb{R}/\mathbb{Z}$ and $\mathbf{z} = \mathbf{t}/r_n \in (-1,1)^2$,

$$\rho_n \mathrm{d}\mathbf{x} = w(\mathbf{z})\mathrm{d}\theta\mathrm{d}\mathbf{z}. \tag{99}$$

Hence $\int \rho_n = 1$, and $\sqrt{\rho_n}$ is Lipschitz with compact support, as $\sqrt{w}$ is Lipschitz and vanishes on the boundary of $(-1,1)^2$. The equal mixture of the normalized orbitals $\varphi_{n,0} = \sqrt{\rho_n}$ and $\varphi_{n,1} = \sqrt{\rho_n}\, e^{2\pi \mathrm{i} s/L_n}$ in $H^1(\mathbb{R}^3)$ has density ρ_n and paramagnetic current density $\mathbf{j}_n$. A single orbital cannot do the same, because its velocity has quantized circulation.

Claim. Let $\psi \in H^1(\mathbb{R}^3)$ with $|\psi|^2 = \rho_n$. Then, for almost every $\mathbf{t} \in (-r_n, r_n)^2$, the velocity $\mathrm{Im}(\overline{\psi}\boldsymbol{\nabla}\psi)/|\psi|^2$ has circulation

$$\oint_{\mathcal{C}_{n,\mathbf{t}}} \frac{\mathrm{Im}(\overline{\psi}\boldsymbol{\nabla}\psi)}{|\psi|^2} \cdot \mathrm{d}\boldsymbol{\ell} = \int_0^{L_n} \frac{\mathrm{Im}(\overline{\psi}\boldsymbol{\nabla}\psi)}{\rho_n}\big(\mathbf{X}_n(s,\mathbf{t})\big) \cdot \partial_s \mathbf{X}_n(s,\mathbf{t})\mathrm{d}s \in 2\pi\mathbb{Z}$$

around the loop $\mathcal{C}_{n,\mathbf{t}}$ parametrized by $s \mapsto \mathbf{X}_n(s,\mathbf{t})$.

Proof of the claim. On $\mathcal{T}_n$, where ρ_n is smooth and positive, $u = \psi/\sqrt{\rho_n} \in H^1_{\mathrm{loc}}(\mathcal{T}_n)$ satisfies $|u| = 1$. As $\overline{\psi}\boldsymbol{\nabla}\psi = \sqrt{\rho_n}\boldsymbol{\nabla}\sqrt{\rho_n} + \rho_n \overline{u}\boldsymbol{\nabla}u$, the velocity is $\mathrm{Im}(\overline{u}\boldsymbol{\nabla}u)$. For almost every $\mathbf{t}$, the function $u_{\mathbf{t}}(s) = u(\mathbf{X}_n(s,\mathbf{t}))$ is absolutely continuous on $\mathbb{R}/L_n\mathbb{Z}$ with values in the unit circle. Hence $u_{\mathbf{t}} = e^{\mathrm{i}\vartheta}$ for an absolutely continuous $\vartheta : [0, L_n] \to \mathbb{R}$ with $\vartheta(L_n) - \vartheta(0) \in 2\pi\mathbb{Z}$. The integrand above equals $\mathrm{Im}(\overline{u_{\mathbf{t}}}\,\partial_s u_{\mathbf{t}}) = \partial_s\vartheta$, so the circulation is $\vartheta(L_n) - \vartheta(0)$. This proves the claim.

Since $\boldsymbol{\nabla}s \cdot \partial_s \mathbf{X}_n = 1$, the velocity $\mathbf{j}_n/\rho_n = (\pi/L_n)\boldsymbol{\nabla}s$ has circulation

$$\oint_{\mathcal{C}_{n,\mathbf{t}}} \frac{\mathbf{j}_n}{\rho_n} \cdot \mathrm{d}\boldsymbol{\ell} = \frac{\pi}{L_n}\int_0^{L_n} \boldsymbol{\nabla}s \cdot \partial_s \mathbf{X}_n \mathrm{d}s = \pi$$

around every loop $\mathcal{C}_{n,\mathbf{t}}$, half the circulation quantum 2π. Hence no $\psi \in H^1(\mathbb{R}^3)$ satisfies $|\psi|^2 = \rho_n$ and $\mathrm{Im}(\overline{\psi}\boldsymbol{\nabla}\psi) = \mathbf{j}_n$. Consequently, for every $e \geq 0$, no photon-free state $\psi \otimes \Omega$ has the pair $(\rho_n, \mathbf{j}_n)$, since $\langle \Omega, \mathfrak{A}(\mathbf{x})\Omega\rangle = 0$ makes its combined current density equal to $\mathrm{Im}(\overline{\psi}\boldsymbol{\nabla}\psi)$.

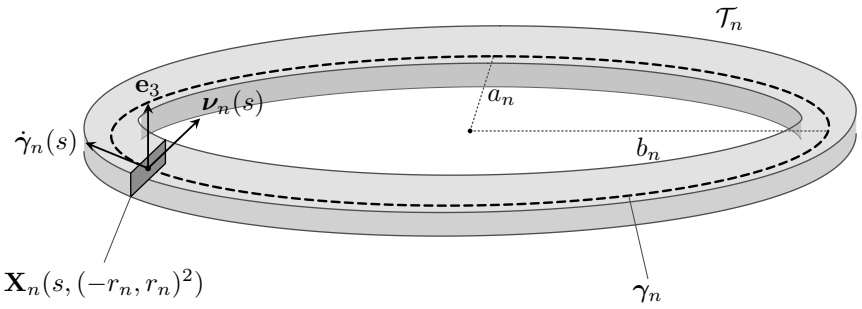


FIGURE 1. The solid torus $\mathcal{T}_n$ around the ellipse $\boldsymbol{\gamma}_n$ (dashed), with the orthonormal frame $(\dot{\boldsymbol{\gamma}}_n, \boldsymbol{\nu}_n, \mathbf{e}_3)$ and the square cross-section $\mathbf{X}_n(s,(-r_n,r_n)^2)$ at $\boldsymbol{\gamma}_n(s)$. Not to scale: in the proof, $a_n \leq b_n^3$ and $r_n = a_n^2 b_n^3/10$.

The claim does not yet prove the proposition, because a minimizer need not be photon-free. Photons can carry the missing half quantum: by Theorem 4.10, there are pure states with the pair $(\rho_n, \mathbf{j}_n)$ whose energies approach the infimum. For $e > 0$, the field also enters the combined current, and its circulation around a loop could make up the difference. The remaining steps rule this out for a minimizer. Step 2 shows that the field has small circulation around thin loops. Steps 3 and 4 give matching lower and upper energy bounds, from which Step 5 deduces that a pure minimizer is almost photon-free. Step 6 then applies the winding argument of the claim to its vacuum component.

Step 2. The flux through the loops. For $\mathbf{t} \in (-r_n, r_n)^2$, let

$$g_{n,s,\mathbf{t}} = \sum_{\mu=1}^{3} G^{\mu}_{\mathbf{X}_n(s,\mathbf{t})}\, \partial_s X^{\mu}_n(s,\mathbf{t}), \qquad \mathcal{F}_{n,\mathbf{t}} = \int_0^{L_n} g_{n,s,\mathbf{t}} \mathrm{d}s.$$

Thus $\Phi(g_{n,s,\mathbf{t}}) = \mathfrak{A}(\mathbf{X}_n) \cdot \partial_s \mathbf{X}_n$, and $\Phi(\mathcal{F}_{n,\mathbf{t}})$ is the circulation of the field around the loop $s \mapsto \mathbf{X}_n(s,\mathbf{t})$.

For $\nu = 0, 1$, put $M_\nu = \|\omega^{-\nu/2}\widehat{\chi}\|$ and $d_\nu(\ell) = \|\min\{1, \ell\omega\}\,\omega^{-\nu/2}\widehat{\chi}\|$, with the norm of $L^2(\mathbb{R}^3)$. By (9), $M_\nu < \infty$ and $d_\nu(\ell) \downarrow 0$ as $\ell \downarrow 0$. By (14) and $|e^{\mathrm{i}t} - 1| \le 2\min\{1, |t|\}$,

$$\sum_{\mu=1}^{3} \|\omega^{-\nu/2} G^{\mu}_{\mathbf{x}}\|^2 = M_\nu^2, \qquad \sum_{\mu=1}^{3} \|\omega^{-\nu/2}(G^{\mu}_{\mathbf{x}} - G^{\mu}_{\mathbf{y}})\|^2 \le 4 d_\nu(|\mathbf{x}-\mathbf{y}|)^2. \tag{100}$$

We now choose a_n. As $d_\nu(\ell) \downarrow 0$, we may take a_n so small that

$$a_n \le b_n^3, \qquad d_0(2a_n) + d_1(2a_n) \le b_n^2. \tag{101}$$

We claim that, with C depending only on the form factor,

$$\sup_{\mathbf{t} \in (-r_n, r_n)^2} \|\omega^{-\nu/2} \mathcal{F}_{n,\mathbf{t}}\| \le C b_n L_n^2, \qquad \nu = 0, 1. \tag{102}$$

All norms in this step are $\|\omega^{-\nu/2} \cdot\|$ on $\mathfrak{H}_{\mathrm{ph}}$. Parametrize the central ellipse by $\varphi \mapsto (a_n \cos\varphi, b_n \sin\varphi, 0)$. Since x_1 has total variation $4a_n$, the $\mu = 1$ part of $\mathcal{F}_{n,0}$ is at most $4a_n M_\nu$. In the $\mu = 2$ part, $\varphi \mapsto \pi - \varphi$ pairs points with equal x_2, opposite orientation, and distance at most $2a_n$, so (100) bounds it by $4b_n d_\nu(2a_n)$. Off the central ellipse, $\partial_s \mathbf{X}_n = (1 - \kappa_n t_1)\dot{\boldsymbol{\gamma}}_n$ with $|\kappa_n t_1| \le \kappa_n r_n$, and $|\mathbf{X}_n(s,\mathbf{t}) - \boldsymbol{\gamma}_n(s)| \le \sqrt{2} r_n$. Since $\int_0^{L_n} \kappa_n \mathrm{d}s = 2\pi$, this gives $\|\mathcal{F}_{n,\mathbf{t}} - \mathcal{F}_{n,0}\| \le 2L_n d_\nu(2r_n) + 2\pi r_n M_\nu$. By (101) and $r_n < a_n^2/b_n < a_n$, all four terms are at most $C(1 + M_\nu) b_n^3 \le C(1 + M_\nu) b_n L_n^2$.

Step 3. A lower bound for pure representatives. Let $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ be normalized with $(\rho_\Psi, \mathbf{j}^{\mathrm{c}}_\Psi) = (\rho_n, \mathbf{j}_n)$. For $N = 1$, $\rho_\Psi(\mathbf{x}) = \|\Psi(\mathbf{x})\|^2$ in the norm of $\mathcal{F}_{\mathrm{ph}}$. Hence $\Psi = 0$ outside $\mathcal{T}_n$. On $\mathcal{T}_n$, where ρ_n is smooth and positive, $\Psi = \sqrt{\rho_n}\, u$ with $u \in H^1_{\mathrm{loc}}(\mathcal{T}_n; \mathcal{F}_{\mathrm{ph}})$, $\|u\| = 1$, and $u(\mathbf{x}) \in D(\sqrt{H_{\mathrm{rad}}})$ for almost every $\mathbf{x}$. Since $\mathrm{Re}\langle u, \boldsymbol{\nabla} u\rangle = \frac{1}{2}\boldsymbol{\nabla}\|u\|^2 = 0$ and $\langle u, \mathfrak{A}^\mu u\rangle$ is real, differentiating $\sqrt{\rho_n}$ produces no cross terms, and

$$\mathbf{j}^{\mathrm{c}}_\Psi = \rho_n\, \mathrm{Re}\langle u, (-\mathrm{i}\boldsymbol{\nabla} - e\mathfrak{A}) u\rangle,$$

$$\langle \Psi, H^{0,0}\Psi\rangle = \frac{1}{2}\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\sqrt{\rho_n}|^2 + \frac{1}{2}\int_{\mathcal{T}_n} \rho_n \|(-\mathrm{i}\boldsymbol{\nabla} - e\mathfrak{A})u\|^2 \mathrm{d}\mathbf{x} + \langle \Psi, H_{\mathrm{rad}}\Psi\rangle.$$

In the coordinates $(s, \mathbf{t})$ of Step 1, put $\mathcal{A}_n = \Phi(g_{n,s,\mathbf{t}}) = \mathfrak{A}(\mathbf{X}_n) \cdot \partial_s \mathbf{X}_n$ and $D_s = -\mathrm{i}\partial_s - e\mathcal{A}_n$. By the chain rule, $(-\mathrm{i}\boldsymbol{\nabla} - e\mathfrak{A})u \cdot \partial_s \mathbf{X}_n = D_s u$. Taking the dot product

of $\mathbf{j}^{\mathrm{c}}_\Psi = \mathbf{j}_n$ with $\partial_s \mathbf{X}_n$ and using $\boldsymbol{\nabla} s \cdot \partial_s \mathbf{X}_n = 1$, we get

$$\rho_n \operatorname{Re}\langle u, D_s u\rangle = \mathbf{j}^{\mathrm{c}}_\Psi \cdot \partial_s \mathbf{X}_n = \mathbf{j}_n \cdot \partial_s \mathbf{X}_n = \frac{\pi}{L_n}\rho_n \,\boldsymbol{\nabla} s \cdot \partial_s \mathbf{X}_n = \frac{\pi}{L_n}\rho_n.$$

Dividing by $\rho_n > 0$ gives

$$\operatorname{Re}\langle u, D_s u\rangle = \frac{\pi}{L_n} \qquad \text{almost everywhere on } \mathcal{T}_n. \tag{103}$$

As $\|u\| = 1$, this gives $\|D_s u\|^2 = \|(D_s - \pi/L_n)u\|^2 + \pi^2/L_n^2$. Keeping only the $\dot{\boldsymbol{\gamma}}_n$-component of the covariant gradient and using $J_n \le 1 + \varepsilon_n$, we obtain

$$\begin{aligned} &\langle \Psi, H^{0,0}\Psi\rangle - \frac{1}{2}\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\sqrt{\rho_n}|^2 \\ &\qquad \ge \frac{1}{2(1+\varepsilon_n)^2}\left[\frac{\pi^2}{L_n^2} + \int_{\mathcal{T}_n} \rho_n \|(D_s - \pi/L_n)u\|^2 \mathrm{d}\mathbf{x}\right] + \langle \Psi, H_{\mathrm{rad}}\Psi\rangle. \end{aligned} \tag{104}$$

To bound the last integral, we represent $\mathcal{F}_{\mathrm{ph}}$ by the Wiener–Itô–Segal isomorphism of Appendix D with $\mathfrak{h} = \mathfrak{H}_{\mathrm{ph}}$. Then $\mathcal{A}_n$ becomes multiplication by a real function $\mathcal{A}_n(s, \mathbf{t}; q)$ of the Gaussian point q, square integrable in s for almost every q, and $\Phi(\mathcal{F}_{n,\mathbf{t}})$ becomes multiplication by its integral over s. On $\mathbb{R}/L\mathbb{Z}$, a real potential $\beta \in L^2$ is gauge equivalent to its mean, so Fourier series give $(-\mathrm{i}\partial_s + \beta)^2 \ge L^{-2}\operatorname{dist}(\int_0^L \beta, 2\pi\mathbb{Z})^2$ as forms on $H^1(\mathbb{R}/L\mathbb{Z})$. For almost every $\mathbf{t}$, the map $s \mapsto u(\mathbf{X}_n(s,\mathbf{t}))$ lies in $H^1(\mathbb{R}/L_n\mathbb{Z}; \mathcal{F}_{\mathrm{ph}})$. For such $\mathbf{t}$ and almost every q, apply this with $\beta = -\pi/L_n - e\mathcal{A}_n(\cdot, \mathbf{t}; q)$, and use $\operatorname{dist}(\pi + x, 2\pi\mathbb{Z})^2 \ge \pi^2 - 2\pi|x|$. Integrating over q, and then over $\mathbf{t}$ by (99), gives

$$\int_{\mathcal{T}_n} \rho_n \|(D_s - \pi/L_n)u\|^2 \mathrm{d}\mathbf{x} \ge \frac{\pi^2}{L_n^2} - \frac{2\pi e}{L_n^2}\int_{\mathcal{T}_n} \rho_n \langle u, |\Phi(\mathcal{F}_{n,\mathbf{t}})|u\rangle \mathrm{d}\mathbf{x}.$$

By (18) and (19), $\langle u, |\Phi(\mathcal{F}_{n,\mathbf{t}})|u\rangle \le \|\Phi(\mathcal{F}_{n,\mathbf{t}})u\| \le 2\|\mathcal{F}_{n,\mathbf{t}}/\sqrt{\omega}\|\,\|\sqrt{H_{\mathrm{rad}}}u\| + \|\mathcal{F}_{n,\mathbf{t}}\|$, and $\int \rho_n \|\sqrt{H_{\mathrm{rad}}}u\| \le \|\sqrt{H_{\mathrm{rad}}}\Psi\|$. Inserting these bounds and (102) into (104) proves

$$\begin{aligned} &\langle \Psi, H^{0,0}\Psi\rangle - \frac{1}{2}\int_{\mathbb{R}^3} |\boldsymbol{\nabla}\sqrt{\rho_n}|^2 \\ &\qquad \ge \frac{\pi^2}{(1+\varepsilon_n)^2 L_n^2} + \langle \Psi, H_{\mathrm{rad}}\Psi\rangle - \delta_n\big(1 + \|\sqrt{H_{\mathrm{rad}}}\Psi\|\big), \end{aligned} \tag{105}$$

where $\delta_n = 2\pi e C b_n$.

Step 4. A mixed-state upper bound. For $K > 0$, let $\mathfrak{A}_{<K}$ be the field with coupling functions $\mathbb{1}_{\{\omega<K\}}G^\mu_{\mathbf{x}}$, and put

$$U_K(\mathbf{x}) = e^{\mathrm{i}e\mathbf{x}\cdot\mathfrak{A}_{<K}(0)} = W(\mathrm{i}f_{\mathbf{x}}), \qquad f_{\mathbf{x}} = e\sum_{\mu=1}^{3} x^\mu \mathbb{1}_{\{\omega<K\}}G^\mu_0,$$

where W is the Weyl displacement operator (200) of Appendix A.5. By the symmetry of the form factor in (9), all scalar products among the coupling functions $G^\mu_{\mathbf{x}}$ and $\mathbb{1}_{\{\omega<K\}}G^\nu_0$, for $\mathbf{x} \in \mathbb{R}^3$ and $\mu, \nu = 1, 2, 3$, are real. By Proposition A.6(iii), the field components $\mathfrak{A}^\mu(\mathbf{x})$ and $\mathfrak{A}^\nu_{<K}(0)$ therefore strongly commute with each other. Hence, for $\varphi = \varphi_{n,0}, \varphi_{n,1}$,

$$(-\mathrm{i}\boldsymbol{\nabla} - e\mathfrak{A}(\mathbf{x}))U_K(\varphi \otimes \Omega) = U_K\big[(-\mathrm{i}\boldsymbol{\nabla}\varphi)\,\Omega - e\varphi\,(\mathfrak{A}(\mathbf{x}) - \mathfrak{A}_{<K}(0))\Omega\big].$$

In the bracket, a zero-photon vector is added to a one-photon vector, since $(\mathfrak{A}^\mu(\mathbf{x}) - \mathfrak{A}^\mu_{<K}(0))\Omega = a^\dagger(G^\mu_{\mathbf{x}} - \mathbb{1}_{\{\omega<K\}}G^\mu_0)\Omega$. Hence the equal mixture $\boldsymbol{\Gamma}_{n,K}$ of the two states

$U_K(\varphi\otimes\Omega)$ has the pair $(\rho_n,\mathbf{j}_n)$. By $|\boldsymbol{\nabla}s|=J_n^{-1}$ and the coherent-state radiation energy (216),

$$\mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}_{n,K}\big)-\frac12\int_{\mathbb{R}^3}|\boldsymbol{\nabla}\sqrt{\rho_n}|^2=\frac{\pi^2}{L_n^2}\int\frac{\rho_n}{J_n^2}\mathrm{d}\mathbf{x}+\int\rho_n(\mathbf{x})\|\sqrt{\omega}f_{\mathbf{x}}\|^2\mathrm{d}\mathbf{x}$$
$$+\frac{e^2}{2}\int\rho_n(\mathbf{x})\sum_{\mu=1}^{3}\|G^\mu_{\mathbf{x}}-\mathbb{1}_{\{\omega<K\}}G^\mu_0\|^2\mathrm{d}\mathbf{x}.$$

Take $K=b_n^{-1}$. Since $|\mathbf{x}|\le b_n+\sqrt{2}r_n<3b_n$ on $\operatorname{supp}\rho_n$ and $\|\sqrt{\omega}f_{\mathbf{x}}\|^2\le e^2K|\mathbf{x}|^2\|\widehat{\chi}\|^2$, (100) bounds the last two integrals by

$$\tau_n=e^2\big(4d_0(3b_n)^2+\|\mathbb{1}_{\{\omega\ge b_n^{-1}\}}\widehat{\chi}\|^2+9b_n\|\widehat{\chi}\|^2\big).$$

By Theorems 4.8 and 4.10, $F^{e,\chi}_{\mathrm{PFLL}}=\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$. Together with $J_n\ge1-\varepsilon_n$, this proves

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho_n,\mathbf{j}_n)-\frac12\int_{\mathbb{R}^3}|\boldsymbol{\nabla}\sqrt{\rho_n}|^2\le\frac{\pi^2}{(1-\varepsilon_n)^2L_n^2}+\tau_n. \tag{106}$$

In particular, $F^{e,\chi}_{\mathrm{PFLL}}(\rho_n,\mathbf{j}_n)<\infty$, so $(\rho_n,\mathbf{j}_n)\in\mathcal{J}_1^{e,\chi}$.

Step 5. Pure minimizers are almost photon-free. We now choose the remaining scales. Let $b_n\downarrow0$ with $b_n<1$, and take $r_n=a_n^2b_n^3/10$, so that $r_n<a_n^2/b_n$ as required in Step 1. Then $\varepsilon_n=b_n^4/10$, and $L_n\ge4b_n$ gives $\varepsilon_n/L_n^2\le b_n^2/160$. Since moreover $d_0(\ell)\downarrow0$ as $\ell\downarrow0$ and $\widehat{\chi}\in L^2(\mathbb{R}^3)$,

$$\frac{\varepsilon_n}{L_n^2}\longrightarrow0,\qquad\delta_n\longrightarrow0,\qquad\tau_n\longrightarrow0. \tag{107}$$

Suppose, for contradiction, that pure minimizers Ψ_n exist for infinitely many n. Pass to that subsequence, and let u_n be as in Step 3. By (105) to (107),

$$\|\sqrt{H_{\mathrm{rad}}}\Psi_n\|^2-\delta_n(1+\|\sqrt{H_{\mathrm{rad}}}\Psi_n\|)\le\frac{\pi^2}{L_n^2}\big((1-\varepsilon_n)^{-2}-(1+\varepsilon_n)^{-2}\big)+\tau_n\longrightarrow0,$$

so $\|\sqrt{H_{\mathrm{rad}}}\Psi_n\|\to0$. By Theorems 4.8 and 4.10, $|\Psi_n\rangle\langle\Psi_n|$ is a mixed-state optimizer. For $0<\kappa\le\kappa_0$, Proposition 4.16 therefore bounds its mean number of photons of frequency below κ by the right-hand side c_κ of (70), independently of n. The mean number of photons of frequency at least κ is at most $\kappa^{-1}\langle\Psi_n,H_{\mathrm{rad}}\Psi_n\rangle$. With $P_\Omega=|\Omega\rangle\langle\Omega|$ on $\mathcal{F}_{\mathrm{ph}}$ and $\mathbb{1}-P_\Omega\le\mathcal{N}$,

$$\int_{\mathcal{T}_n}\rho_n\|(\mathbb{1}-P_\Omega)u_n\|^2\mathrm{d}\mathbf{x}=\|(\mathbb{1}-P_\Omega)\Psi_n\|^2\le\langle\Psi_n,\mathcal{N}\Psi_n\rangle\le c_\kappa+\frac{\langle\Psi_n,H_{\mathrm{rad}}\Psi_n\rangle}{\kappa}.$$

Since $c_\kappa\to0$ as $\kappa\downarrow0$, letting $n\to\infty$ and then $\kappa\downarrow0$ proves

$$\int_{\mathcal{T}_n}\rho_n\|(\mathbb{1}-P_\Omega)u_n\|^2\mathrm{d}\mathbf{x}\longrightarrow0. \tag{108}$$

Moreover, $\|\mathcal{A}_nu\|\le J_n\|\mathfrak{A}(\mathbf{X}_n)u\|$ with $J_n\le2$, so (20) gives $\int\rho_n\|\mathcal{A}_nu_n\|^2\le4C_\chi(\langle\Psi_n,H_{\mathrm{rad}}\Psi_n\rangle+1)$, while (104) and (106) bound $\int\rho_n\|(D_s-\pi/L_n)u_n\|^2$ by C/L_n^2. Writing $\partial_su_n=\mathrm{i}(D_s-\pi/L_n)u_n+\mathrm{i}(\pi/L_n)u_n+\mathrm{i}e\mathcal{A}_nu_n$, we obtain

$$\int_{\mathcal{T}_n}\rho_n\|\partial_su_n\|^2\mathrm{d}\mathbf{x}\le\frac{C}{L_n^2},\qquad eL_n\int_{\mathcal{T}_n}\rho_n\|\mathcal{A}_nu_n\|\mathrm{d}\mathbf{x}\longrightarrow0. \tag{109}$$

Step 6. A pure minimizer cannot carry circulation π. We keep the assumption of Step 5 and the notation introduced there. For $\mathbf{z}\in(-1,1)^2$, let

$u_{\mathbf{z}}(\theta) = u_n(\mathbf{X}_n(L_n\theta, r_n\mathbf{z}))$ on $\mathbb{T}$. Let $\|\cdot\|$ be the norm of $\mathcal{F}_{\mathrm{ph}}$ and $\|\cdot\|_{L^2}$ that of $L^2(\mathbb{T};\mathcal{F}_{\mathrm{ph}})$, and put

$$k_n(\mathbf{z}) = \|\partial_\theta u_{\mathbf{z}}\|_{L^2}^2, \qquad p_n(\mathbf{z}) = \|(\mathbb{1} - P_\Omega)u_{\mathbf{z}}\|_{L^2}^2 + eL_n \int_{\mathbb{T}} \|\mathcal{A}_n u_{\mathbf{z}}\| \mathrm{d}\theta.$$

By (99), (108) and (109) give $\int_{(-1,1)^2} wk_n \le C$ and $\bar{p}_n := \int_{(-1,1)^2} wp_n \to 0$. Since $w\mathrm{d}\mathbf{z}$ is a probability measure, Markov's inequality gives a $\mathbf{z}$ with $k_n(\mathbf{z}) \le 3C$ and $p_n(\mathbf{z}) \le 3\bar{p}_n$ for which $u = u_{\mathbf{z}} \in H^1(\mathbb{T};\mathcal{F}_{\mathrm{ph}})$, $\|u\| = 1$, and (103) holds along u. Multiplying (103) by L_n and integrating over $\mathbb{T}$ gives

$$\Big| \int_{\mathbb{T}} \mathrm{Im}\langle u, \partial_\theta u\rangle \mathrm{d}\theta - \pi \Big| = eL_n \Big| \int_{\mathbb{T}} \langle u, \mathcal{A}_n u\rangle \mathrm{d}\theta \Big| \le 3\bar{p}_n.$$

Let $\alpha = \langle \Omega, u\rangle$ and $u_\perp = (\mathbb{1} - P_\Omega)u$. Since $\|\partial_\theta u_\perp\| \le \|\partial_\theta u\|$, the one-dimensional Sobolev inequality gives

$$\sup_{\mathbb{T}} \big(1 - |\alpha|^2\big) = \sup_{\mathbb{T}} \|u_\perp\|^2 \le \|u_\perp\|_{L^2}^2 + 2\|u_\perp\|_{L^2}\|\partial_\theta u\|_{L^2} \le 3\bar{p}_n + 6\sqrt{C\bar{p}_n}.$$

For large n the right-hand side is at most $\frac{1}{2}$. Then $|\alpha|^2 \ge \frac{1}{2}$ on $\mathbb{T}$, and the winding number $m = (2\pi)^{-1} \int_{\mathbb{T}} \mathrm{Im}(\partial_\theta \alpha/\alpha)\mathrm{d}\theta$ is an integer. As $u_\perp$ and $\partial_\theta u_\perp$ are orthogonal to Ω,

$$\mathrm{Im}\langle u, \partial_\theta u\rangle = |\alpha|^2 \,\mathrm{Im}(\partial_\theta \alpha/\alpha) + \mathrm{Im}\langle u_\perp, \partial_\theta u_\perp\rangle.$$

Integrating over $\mathbb{T}$ and using $|\partial_\theta \alpha| \le \|\partial_\theta u\|$ and the two preceding bounds, we find that $\int_{\mathbb{T}} \mathrm{Im}\langle u, \partial_\theta u\rangle \mathrm{d}\theta$ differs from $2\pi m$ by at most

$$\sqrt{2} \sup_{\mathbb{T}} \big(1 - |\alpha|^2\big)\|\partial_\theta u\|_{L^2} + \|u_\perp\|_{L^2}\|\partial_\theta u\|_{L^2} \longrightarrow 0,$$

and from π by at most $3\bar{p}_n \to 0$. This contradicts $|\pi - 2\pi m| \ge \pi$ for large n, so the assumption of Step 5 is false. Hence pure minimizers exist for at most finitely many n, and any larger n in (98) gives the asserted pair at the fixed coupling and cutoff.

5.6. **Lower semicontinuity with photon loss.** The pure-state infimum need not be attained, as the explicit one-electron examples above show. Along a minimizing sequence, photons may escape to infinity, so a limit state must be allowed to lose photons. We implement photon loss by localizing the photons at a scale R and tracing out the rest. For every R, localization followed by partial trace preserves the normalization and the electronic reduced state exactly, and hence also the electron density and the paramagnetic current density. It does not preserve the combined current density at fixed R, because the field-induced current density depends on the field expectation, which loses the contribution of the traced-out photons. The combined current density is preserved only in the limit $R \to \infty$: the proof of Lemma 5.7 bounds the change in $\int \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}$, for each smooth compactly supported $\boldsymbol{\zeta}$, by a constant depending on the internal energy times a factor that vanishes as $R \to \infty$. The partial trace can also turn a pure state into a mixed state, which motivates the mixed-state compactness arguments here. We first record an abstract trace-norm bound and its compactness consequence. We then prove lower semicontinuity of the energy and passage to the constraints under trace-norm convergence. Photon localization gives compactness under a condition on photon number.

Lemma 5.1. *Let $\mathfrak{K}$ be a Hilbert space. A positive trace-class operator Γ on $\mathfrak{K}$ with $\operatorname{Tr}\Gamma \le 1$ and an orthogonal projection S on $\mathfrak{K}$ satisfy*

$$\|\Gamma - S\Gamma S\|_{\mathfrak{S}_1} \le 2\big(\operatorname{Tr}((1-S)\Gamma)\big)^{1/2}. \tag{110}$$

Moreover, a sequence (Γ_j) of positive trace-class operators on $\mathfrak{K}$, with $\operatorname{Tr}\Gamma_j \le 1$ for every j, is precompact in trace norm if, for every $\varepsilon > 0$, there is a finite-rank orthogonal projection S with $\sup_j \operatorname{Tr}((1-S)\Gamma_j) < \varepsilon$.

Proof. Writing $\Gamma - S\Gamma S = (1-S)\Gamma + S\Gamma(1-S)$ and factoring through $\sqrt{\Gamma}$, the Hilbert–Schmidt ideal inequality gives

$$\|\Gamma - S\Gamma S\|_{\mathfrak{S}_1} \le 2\|\sqrt{\Gamma}\|_{\mathfrak{S}_2}\|(1-S)\sqrt{\Gamma}\|_{\mathfrak{S}_2} \le 2\big(\operatorname{Tr}((1-S)\Gamma)\big)^{1/2}.$$

To prove precompactness, let $\delta > 0$ and choose a finite-rank orthogonal projection S with $\sup_j \operatorname{Tr}((1-S)\Gamma_j) < \delta^2/16$. The bound (110) then gives the uniform approximation

$$\sup_j \|\Gamma_j - S\Gamma_j S\|_{\mathfrak{S}_1} < \frac{\delta}{2}.$$

Each compression is positive and satisfies

$$\operatorname{Tr}(S\Gamma_j S) = \operatorname{Tr}(S\Gamma_j) \le \operatorname{Tr}\Gamma_j \le 1.$$

Thus all the compressions belong to

$$\mathcal{K}_S := \{A \in \mathfrak{S}_1(\mathfrak{K}) : A = SAS,\ A \ge 0,\ \operatorname{Tr}A \le 1\}.$$

This set is closed in trace norm: the map $A \mapsto SAS$ and the trace are continuous, and positivity is preserved under trace-norm limits. It is bounded because $\|A\|_{\mathfrak{S}_1} = \operatorname{Tr}A \le 1$ for $A \in \mathcal{K}_S$. Moreover, the condition $A = SAS$ identifies these operators with operators on the finite-dimensional space $\operatorname{ran}S$. Hence $\mathcal{K}_S$ is compact in trace norm.

Choose a finite $\delta/2$-net $A_1, \dots, A_m$ for $\mathcal{K}_S$. For each j, some $k \in \{1, \dots, m\}$ therefore satisfies $\|S\Gamma_j S - A_k\|_{\mathfrak{S}_1} < \delta/2$, and the triangle inequality gives

$$\|\Gamma_j - A_k\|_{\mathfrak{S}_1} \le \|\Gamma_j - S\Gamma_j S\|_{\mathfrak{S}_1} + \|S\Gamma_j S - A_k\|_{\mathfrak{S}_1} < \delta.$$

The sequence is thus covered by finitely many trace-norm balls of radius δ. Since $\delta > 0$ was arbitrary, the set $\{\Gamma_j : j \ge 1\}$ is totally bounded. The trace class $\mathfrak{S}_1(\mathfrak{K})$ is complete, so the closure of this set is compact, which proves precompactness in trace norm. □

For a positive trace-class operator $\mathbf{\Gamma}$ on $\mathcal{H}_N$ with $\operatorname{Tr}\mathbf{\Gamma} \le 1$, not necessarily equal to one, define the internal energy $\operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) \in [0,\infty]$ by the spectral sum following (32), and similarly the trace of $\mathbf{\Gamma}$ against any nonnegative quadratic form in place of $H^{0,0}$. When the internal energy is finite, define the density $\rho_{\mathbf{\Gamma}}$ and the combined current density $\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}$ by (47). These definitions are linear in $\mathbf{\Gamma}$ and agree with the earlier ones on $\mathcal{D}$.

Lemma 5.2 (Lower semicontinuity and passage to the constraints)**.** *Let $\mathbf{\Gamma}_j$ be positive trace-class operators on $\mathcal{H}_N$ with $\operatorname{Tr}\mathbf{\Gamma}_j \le 1$ and uniformly bounded internal energies,*

$$\sup_j \operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}_j\big) < \infty,$$

and suppose that $\mathbf{\Gamma}_j \to \mathbf{\Gamma}$ *in trace norm. Then* $\mathbf{\Gamma}$ *is positive,* $\operatorname{Tr}\mathbf{\Gamma} = \lim_j \operatorname{Tr}\mathbf{\Gamma}_j$*, and*

$$\operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) \le \liminf_j \operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}_j\big). \tag{111}$$

In particular, $\mathbf{\Gamma}$ *has finite internal energy, so* $\rho_{\mathbf{\Gamma}}$ *and* $\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}$ *are defined. The same liminf inequality holds for every nonnegative quadratic form on* $Q(H^{0,0})$ *bounded relative to* $H^{0,0}+1$*. For bounded scalar* f *and real* $\boldsymbol{\zeta} \in C_c^\infty(\mathbb{R}^3,\mathbb{R}^3)$*,*

$$\int_{\mathbb{R}^3} f\rho_{\mathbf{\Gamma}_j} \longrightarrow \int_{\mathbb{R}^3} f\rho_{\mathbf{\Gamma}}, \tag{112}$$

$$\int_{\mathbb{R}^3} \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_j} \longrightarrow \int_{\mathbb{R}^3} \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}. \tag{113}$$

Proof. Positivity and convergence of the traces follow from trace-norm convergence. The Powers–Størmer inequality gives

$$\|\sqrt{\mathbf{\Gamma}_j} - \sqrt{\mathbf{\Gamma}}\|_{\mathfrak{S}_2}^2 \le \|\mathbf{\Gamma}_j - \mathbf{\Gamma}\|_{\mathfrak{S}_1} \longrightarrow 0.$$

Equip the form domain $Q(H^{0,0})$ with the energy norm $u \mapsto \langle u, (H^{0,0}+1)u\rangle^{1/2}$, making it a Hilbert space continuously embedded in $\mathcal{H}_N$. Let $\mathfrak{S}_2(\mathcal{H}_N, Q(H^{0,0}))$ be the Hilbert–Schmidt operators from $\mathcal{H}_N$ into this space. Thus an operator T on $\mathcal{H}_N$ belongs to it when its range lies in the form domain and $(H^{0,0}+1)^{1/2}T$ is Hilbert–Schmidt, and then $\|T\|_{\mathfrak{S}_2(\mathcal{H}_N,Q(H^{0,0}))} = \|(H^{0,0}+1)^{1/2}T\|_{\mathfrak{S}_2}$. Evaluating this norm on an eigenbasis of $\mathbf{\Gamma}_j$ gives

$$\|\sqrt{\mathbf{\Gamma}_j}\|^2_{\mathfrak{S}_2(\mathcal{H}_N,Q(H^{0,0}))} = \operatorname{Tr}\mathbf{\Gamma}_j + \operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}_j\big),$$

which is uniformly bounded. The continuous embedding into $\mathfrak{S}_2$ and the strong convergence there identify every weak subsequential limit in this stronger Hilbert space with $\sqrt{\mathbf{\Gamma}}$. Thus $\sqrt{\mathbf{\Gamma}}$ belongs to that space and $\sqrt{\mathbf{\Gamma}_j} \rightharpoonup \sqrt{\mathbf{\Gamma}}$ there. Weak lower semicontinuity proves (111). A nonnegative form bounded relative to $H^{0,0}+1$ is $u \mapsto \|Bu\|^2$ for some operator B bounded from $Q(H^{0,0})$ into a Hilbert space. Composition with B preserves weak Hilbert–Schmidt convergence, so weak lower semicontinuity applies to it as well.

For the density, test the trace-norm convergence $\mathbf{\Gamma}_j \to \mathbf{\Gamma}$ against the multiplication operator $M_f := \sum_{i=1}^N f(\mathbf{x}_i)$, acting as the identity on the photon factor. It preserves electronic antisymmetry and satisfies $\|M_f\|_{\mathrm{op}} \le N\|f\|_\infty$. Hence

$$\begin{aligned}\left|\int_{\mathbb{R}^3} f(\rho_{\mathbf{\Gamma}_j} - \rho_{\mathbf{\Gamma}})\right| &= \left|\operatorname{Tr}\left(M_f(\mathbf{\Gamma}_j - \mathbf{\Gamma})\right)\right| \\ &\le N\|f\|_\infty \|\mathbf{\Gamma}_j - \mathbf{\Gamma}\|_{\mathfrak{S}_1} \longrightarrow 0,\end{aligned}$$

which proves (112).

For the current density, recall from Section 3.4 that $\mathbf{D}_1 = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1} - e\mathfrak{A}(\mathbf{x}_1)$ is the covariant momentum of the first electron. Every term in (26) is nonnegative, so $\|\mathbf{D}_1 u\|^2 \le 2\langle u, H^{0,0}u\rangle$ for $u \in Q(H^{0,0})$. Hence $\mathbf{D}_1$ is bounded from $Q(H^{0,0})$, with its energy norm, to the ambient vector-valued electron–photon L^2 space. We therefore also have $\mathbf{D}_1\sqrt{\mathbf{\Gamma}_j} \rightharpoonup \mathbf{D}_1\sqrt{\mathbf{\Gamma}}$ in the corresponding Hilbert–Schmidt class. As operators into this vector-valued space, the factors $\boldsymbol{\zeta}(\mathbf{x}_1)\sqrt{\mathbf{\Gamma}_j}$ and $\mathbf{D}_1\sqrt{\mathbf{\Gamma}_j}$ converge strongly and weakly in $\mathfrak{S}_2$, respectively. The product of the adjoint of the

first factor with the second is trace class, and

$$\int_{\mathbb{R}^3} \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}_j} = N\,\mathrm{Re}\,\mathrm{Tr}\left[\left(\boldsymbol{\zeta}(\mathbf{x}_1)\sqrt{\boldsymbol{\Gamma}_j}\right)^{\dagger}\mathbf{D}_1\sqrt{\boldsymbol{\Gamma}_j}\right]$$
$$\longrightarrow N\,\mathrm{Re}\,\mathrm{Tr}\left[\left(\boldsymbol{\zeta}(\mathbf{x}_1)\sqrt{\boldsymbol{\Gamma}}\right)^{\dagger}\mathbf{D}_1\sqrt{\boldsymbol{\Gamma}}\right] = \int_{\mathbb{R}^3}\boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}}.$$

This proves (113). □

Remark 1 (Continuum compactness obstruction). Uniform energy bounds and a fixed electronic density do not ensure trace-norm compactness in the continuum. Choose an orthonormal sequence $\xi_n \in \mathfrak{H}_{\mathrm{ph}}$ in a bounded momentum shell and a normalized smooth compactly supported electronic state Φ. Then $\Psi_n = \Phi\otimes a^{\dagger}(\xi_n)\Omega$ has fixed density, one photon, and bounded energy, while $|\Psi_n\rangle\langle\Psi_n|$ has no trace-norm convergent subsequence. Photon loss must therefore be allowed in constructing limits. Lemma 5.7 implements this using localization and partial trace, and Section 4.4 supplies its photon-number condition by modifying minimizing sequences at fixed density and combined current density.

Photon loss can be measured by localization, which preserves normalization but can turn a pure state into a mixed state. We use geometric localization in Fock space, as developed in [30, Section 3].

We first recall the notation of Sections 2.1 and 2.3, specialized to the photon Fock space $\mathcal{F}_{\mathrm{ph}} = \mathcal{F}_s(\mathfrak{H}_{\mathrm{ph}})$. For $f\in\mathfrak{H}_{\mathrm{ph}}$, the Segal field $\Phi(f)$ is the self-adjoint closure of $a^{\dagger}(f)+a(f)$, initially defined on the finite-particle space $\mathcal{F}^{\mathrm{fin}}_{\mathrm{ph}}$. It depends real-linearly on f, the conjugate field is $\Pi(f)=\Phi(\mathrm{i}f)$, and the vector potential (15) is $\mathfrak{A}^{\mu}(\mathbf{x})=\Phi(G^{\mu}_{\mathbf{x}})$. In the vacuum, $\langle\Omega,\Phi(f)\Omega\rangle=0$ and $\|\Phi(f)\Omega\|=\|f\|$. For a self-adjoint operator b on $\mathfrak{H}_{\mathrm{ph}}$, its second quantization $\mathrm{d}\Gamma(b)=\bigoplus_{M\geq 0}b^{(M)}$ acts on the M-photon sector as the closure of $\sum_{j=1}^{M}b_j$, where b_j acts on the jth photon variable. For nonnegative b, the same symbol denotes the corresponding nonnegative quadratic form. For a unitary T on $\mathfrak{H}_{\mathrm{ph}}$, or on $\mathfrak{H}_{\mathrm{ph}}\oplus\mathfrak{H}_{\mathrm{ph}}$ as below, the multiplicative second quantization $\Gamma(T)=\bigoplus_{M\geq 0}T^{\otimes M}$, restricted to symmetric tensors, is unitary on the corresponding bosonic Fock space and satisfies $\Gamma(T)\Phi(f)\Gamma(T)^{\dagger}=\Phi(Tf)$. Finally, the Weyl operator (200) is $W(f)=\exp\bigl(a^{\dagger}(f)-a(f)\bigr)$, so that $W(\mathrm{i}f)=e^{\mathrm{i}\Phi(f)}$.

Fix the polarization representation $L^2(\mathbb{R}^3\times\{1,2\})$ and Fourier transform each photon momentum to a position variable $\mathbf{y}$. Then $H_{\mathrm{rad}}=\mathrm{d}\Gamma(\sqrt{-\Delta})$, and $\mathcal{N}=\mathrm{d}\Gamma(1)$ denotes photon number. Here $\sqrt{-\Delta}$ is the Fourier multiplier $|\mathbf{k}|$. The variable $\mathbf{y}$ is a technical device rather than a physical photon position.[5] Fix smooth real functions θ_1,φ_1 on $\mathbb{R}^3$ with $0\leq\theta_1,\varphi_1\leq 1$, $\theta_1^2+\varphi_1^2=1$, $\theta_1=1$ on B_1, and $\theta_1=0$ outside B_2. For $R>0$, set $\theta_R(\mathbf{y}):=\theta_1(\mathbf{y}/R)$ and $\varphi_R(\mathbf{y}):=\varphi_1(\mathbf{y}/R)$. Thus $\theta_R^2+\varphi_R^2=1$, $\theta_R=1$ on B_R, and $\theta_R=0$ outside B_{2R}. The one-photon isometry

[5] It is the Fourier dual of $\mathbf{k}$ in the fixed polarization frame $\boldsymbol{\varepsilon}_{\lambda}$, which cannot be continuous on spheres $\{|\mathbf{k}|=r\}$ by the hairy ball theorem, so the localization below depends on this frame. We use the polarization representation because its one-photon space is all of $L^2(\mathbb{R}^3;\mathbb{C}^2)$, so multiplication by functions of $\mathbf{y}$ is available; in the solenoidal representation it would not preserve the divergence-free constraint. Only the photon-number hypothesis (122) of Lemma 5.7 refers to the frame; its conclusion involves only the density, the combined current density, and the internal energy.

$f \mapsto \theta_R f \oplus \varphi_R f$ induces a Fock-space isometry $\mathcal{U}_R$. With the electronic identity suppressed, set

$$\mathcal{L}_R(\mathbf{\Gamma}) := \mathrm{Tr}_{\mathrm{out}}(\mathcal{U}_R \mathbf{\Gamma} \mathcal{U}_R^\dagger).$$

Thus $\mathcal{L}_R$ retains nearby photons and traces out the second photon factor.

Lemma 5.3 (Photon localization and field identities)**.** *For every $R > 0$, the map $\mathcal{L}_R$ is positive and trace preserving, and leaves the electronic reduced state unchanged. For $f \in \mathfrak{H}_{\mathrm{ph}}$, its adjoint with respect to the trace pairing satisfies*

$$\mathcal{L}_R^\dagger(\Phi(f)) = \Phi(\theta_R f), \tag{114}$$

$$\mathcal{L}_R^\dagger(\Phi(f)^2) = \Phi(\theta_R f)^2 + \|\varphi_R f\|^2 \mathbb{1}. \tag{115}$$

These identities are understood as quadratic-form identities on $D(\Phi(\theta_R f))$, with the electronic identity suppressed.

Proof. Since $\mathcal{U}_R^\dagger \mathcal{U}_R = \mathbb{1}$, conjugation by $\mathcal{U}_R$ followed by partial trace is positive and trace preserving. For every bounded electronic operator A,

$$\mathcal{U}_R^\dagger (A \otimes \mathbb{1} \otimes \mathbb{1}) \mathcal{U}_R = A \otimes \mathbb{1}.$$

Thus the electronic reduced state is unchanged. By monotone spectral truncation, this also preserves the expectations of nonnegative unbounded electronic observables, including the ordinary kinetic energy and the Coulomb interaction.

To prove the field identities, complete the one-photon isometry $j_R u = (\theta_R u, \varphi_R u)$ to the unitary

$$T_R = \begin{pmatrix} \theta_R & -\varphi_R \\ \varphi_R & \theta_R \end{pmatrix} \quad \text{on } \mathfrak{H}_{\mathrm{ph}} \oplus \mathfrak{H}_{\mathrm{ph}}.$$

Unitarity follows from $\theta_R^2 + \varphi_R^2 = 1$ and commutation of these multiplication operators. Under the canonical identification $\mathcal{F}_s(\mathfrak{H}_{\mathrm{ph}} \oplus \mathfrak{H}_{\mathrm{ph}}) \simeq \mathcal{F}_{\mathrm{ph}} \otimes \mathcal{F}_{\mathrm{ph}}$, write $V_R = \Gamma(T_R)$ for its second quantization. Then

$$\mathcal{U}_R \Psi = V_R(\Psi \otimes \Omega), \qquad V_R^\dagger (\Phi(f) \otimes \mathbb{1}) V_R = \Phi(\theta_R f) \otimes \mathbb{1} - \mathbb{1} \otimes \Phi(\varphi_R f).$$

For the second identity, (207) and (208) give, for $s \in \mathbb{R}$,

$$V_R^\dagger \big(e^{\mathrm{i}s\Phi(f)} \otimes \mathbb{1}\big) V_R = W\big(\mathrm{i}s T_R^\dagger (f \oplus 0)\big) = e^{\mathrm{i}s\Phi(\theta_R f)} \otimes e^{-\mathrm{i}s\Phi(\varphi_R f)},$$

and the generators of the two sides agree. Since

$$\langle \Omega, \Phi(\varphi_R f)\Omega \rangle = 0, \qquad \|\Phi(\varphi_R f)\Omega\|^2 = \|\varphi_R f\|^2,$$

vacuum compression gives (114) and

$$\|(\Phi(f) \otimes \mathbb{1}) \mathcal{U}_R \Psi\|^2 = \|\Phi(\theta_R f)\Psi\|^2 + \|\varphi_R f\|^2 \|\Psi\|^2.$$

This proves (115) by polarization. The two fields on the separate factors strongly commute. Their joint spectral calculus, and the finite second moment of the vacuum in the second factor, show that the norm on the left is finite exactly when $\Psi \in D(\Phi(\theta_R f))$. Thus these are identities on the stated form domain, without a mean-photon-number assumption. The extra scalar term is the vacuum fluctuation in the discarded modes. □

Lemma 5.4 (Localization of one-photon forms)**.** *For every $R > 0$ and nonnegative self-adjoint one-photon operator b, the corresponding nonnegative forms obey*

$$\mathcal{L}_R^\dagger(\mathrm{d}\Gamma(b)) = \mathrm{d}\Gamma(\theta_R b \theta_R), \tag{116}$$

where $\theta_R b \theta_R$ denotes the form $u \mapsto \|\sqrt{b}\theta_R u\|^2$. Moreover, with C depending only on θ_1,

$$\theta_R^2 \le CR\sqrt{-\Delta}, \qquad \theta_R\sqrt{-\Delta}\theta_R \le C\sqrt{-\Delta} \tag{117}$$

as forms on $H^{1/2}(\mathbb{R}^3;\mathbb{C}^2)$, uniformly for $R>0$.

Proof. Write $j_R u = (\theta_R u, \varphi_R u)$ for the one-photon localization isometry. For (116), observe that $\mathrm{d}\Gamma(b)\otimes\mathbb{1}$ corresponds to $\mathrm{d}\Gamma(b\oplus 0)$ and

$$j_R^\dagger (b\oplus 0) j_R = \theta_R b \theta_R.$$

Since $\mathcal{U}_R$ is induced by j_R, it preserves the total photon number and acts on the m-photon sector as $j_R^{\otimes m}$, followed by the canonical identification. On this sector, write B_k for the operator $b\oplus 0$ acting on the kth photon variable, so that $\mathrm{d}\Gamma(b\oplus 0) = \sum_{k=1}^m B_k$ there. Each term factors over the m photon variables, and since $j_R^\dagger j_R = \mathbb{1}$,

$$(j_R^{\otimes m})^\dagger B_k\, j_R^{\otimes m} = j_R^\dagger j_R \otimes\cdots\otimes j_R^\dagger (b\oplus 0) j_R \otimes\cdots\otimes j_R^\dagger j_R = \mathbb{1}\otimes\cdots\otimes \theta_R b\theta_R \otimes\cdots\otimes\mathbb{1},$$

with the nontrivial factor in the kth position. Summing over k gives $\mathrm{d}\Gamma(\theta_R b\theta_R)$ on the m-photon sector, and summing over m gives the asserted identity. The argument first applies to bounded b on finitely many sectors. Spectral truncation of b and monotone convergence over the sectors give the identity for arbitrary nonnegative b, with possibly infinite form values.

We next prove (117). Work first with $u\in C_c^\infty(\mathbb{R}^3;\mathbb{C}^2)$, with the two components corresponding to the photon polarizations. The fractional Hardy inequality, applied to each component, gives

$$\int_{\mathbb{R}^3} \frac{|u(\mathbf{y})|^2}{|\mathbf{y}|}\mathrm{d}\mathbf{y} \le C_{\mathrm{H}} \|(-\Delta)^{1/4}u\|^2;$$

see [14, Section 2]. Since $0\le\theta_R\le 1$ and $\theta_R = 0$ outside B_{2R}, we have $\theta_R(\mathbf{y})^2 \le 2R/|\mathbf{y}|$ almost everywhere. Thus

$$\|\theta_R u\|^2 \le 2R\int_{\mathbb{R}^3}\frac{|u(\mathbf{y})|^2}{|\mathbf{y}|}\mathrm{d}\mathbf{y} \le 2C_{\mathrm{H}}R\|(-\Delta)^{1/4}u\|^2,$$

which proves the first inequality.

For the second inequality, use the integral representation

$$\|(-\Delta)^{1/4}u\|^2 = c_3 \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(\mathbf{y})-u(\mathbf{z})|^2}{|\mathbf{y}-\mathbf{z}|^4}\mathrm{d}\mathbf{y}\mathrm{d}\mathbf{z}, \qquad c_3>0.$$

Expanding the difference as

$$\theta_R(\mathbf{y})u(\mathbf{y}) - \theta_R(\mathbf{z})u(\mathbf{z}) = \theta_R(\mathbf{y})\big(u(\mathbf{y})-u(\mathbf{z})\big) + \big(\theta_R(\mathbf{y})-\theta_R(\mathbf{z})\big)u(\mathbf{z})$$

and using $|a+b|^2\le 2|a|^2+2|b|^2$ yields

$$\|(-\Delta)^{1/4}(\theta_R u)\|^2 \le 2\|(-\Delta)^{1/4}u\|^2 + 2c_3\int_{\mathbb{R}^3} K_R(\mathbf{z})|u(\mathbf{z})|^2\mathrm{d}\mathbf{z},$$

$$K_R(\mathbf{z}) := \int_{\mathbb{R}^3}\frac{|\theta_R(\mathbf{y})-\theta_R(\mathbf{z})|^2}{|\mathbf{y}-\mathbf{z}|^4}\mathrm{d}\mathbf{y}.$$

We claim that $K_R(\mathbf{z})\le C/|\mathbf{z}|$ for $\mathbf{z}\neq 0$. Indeed, since $\theta_R(\mathbf{y}) = \theta_1(\mathbf{y}/R)$, smoothness and boundedness of θ_1 give

$$|\theta_R(\mathbf{y})-\theta_R(\mathbf{z})| \le C\min\{|\mathbf{y}-\mathbf{z}|/R, 1\}.$$

Splitting the integral at $|\mathbf{y}-\mathbf{z}| = R$ and using spherical coordinates therefore gives, for every $\mathbf{z}$,

$$K_R(\mathbf{z}) \leq C\left(R^{-2}\int_0^R \mathrm{d}r + \int_R^\infty r^{-2}\mathrm{d}r\right) \leq \frac{C}{R}.$$

For $0 < |\mathbf{z}| \leq 4R$ this is at most $4C/|\mathbf{z}|$. If $|\mathbf{z}| > 4R$, then $\theta_R(\mathbf{z}) = 0$, and on the support of θ_R we have $|\mathbf{y}-\mathbf{z}| \geq |\mathbf{z}|/2$. Hence

$$K_R(\mathbf{z}) = \int_{B_{2R}} \frac{\theta_R(\mathbf{y})^2}{|\mathbf{y}-\mathbf{z}|^4}\mathrm{d}\mathbf{y} \leq \frac{CR^3}{|\mathbf{z}|^4} \leq \frac{C}{|\mathbf{z}|},$$

which proves the claim. Applying the Hardy inequality once more, we obtain

$$\begin{aligned}\|(-\Delta)^{1/4}(\theta_R u)\|^2 &\leq 2\|(-\Delta)^{1/4}u\|^2 + C\int_{\mathbb{R}^3}\frac{|u(\mathbf{z})|^2}{|\mathbf{z}|}\mathrm{d}\mathbf{z}\\ &\leq C\|(-\Delta)^{1/4}u\|^2.\end{aligned}$$

By density of $C_c^\infty(\mathbb{R}^3;\mathbb{C}^2)$ in $H^{1/2}(\mathbb{R}^3;\mathbb{C}^2)$ and boundedness of multiplication by θ_R on L^2, these estimates extend to all of $H^{1/2}(\mathbb{R}^3;\mathbb{C}^2)$. In particular, θ_R preserves this form domain. This proves both form inequalities with constants depending only on θ_1. □

Lemma 5.5 (Photon-number and energy bounds)**.** *There is a constant C, depending only on θ_1, such that for every $R > 0$ and every positive trace-class operator $\mathbf{\Gamma}$,*

$$\mathrm{Tr}(\mathcal{N}\mathcal{L}_R\mathbf{\Gamma}) = \mathrm{Tr}\left(\mathrm{d}\Gamma(\theta_R^2)\mathbf{\Gamma}\right) \leq \mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}), \tag{118}$$

$$\mathrm{Tr}(\mathcal{N}\mathcal{L}_R\mathbf{\Gamma}) \leq CR\,\mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}), \tag{119}$$

$$\mathrm{Tr}(H_{\mathrm{rad}}\mathcal{L}_R\mathbf{\Gamma}) \leq C\,\mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}). \tag{120}$$

The nonnegative traces may take the value $+\infty$. In particular, $\mathcal{L}_R$ maps $\mathcal{D}$ into $\mathcal{D}$, and

$$\mathrm{Tr}\big(H^{0,0}\mathcal{L}_R\mathbf{\Gamma}\big) \leq C\big(\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \mathrm{Tr}\,\mathbf{\Gamma}\big) \tag{121}$$

for positive $\mathbf{\Gamma}$ of finite internal energy, with C independent of R (but also depending on N, e, and the form factor).

Proof. Second quantization preserves nonnegative form inequalities by summing them over the photons in each sector. Taking $b = 1$ in (116) and using $0 \leq \theta_R^2 \leq 1$ therefore proves (118). Taking $b = 1, \sqrt{-\Delta}$ and applying (117) gives (119) and (120). The trace assertions follow by summing the vector identities and inequalities over a spectral decomposition of $\mathbf{\Gamma}$, using monotone convergence. In particular, the localized mean photon number is finite whenever the original radiation energy is finite, even if $\mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}) = \infty$.

By Lemma 5.3, the ordinary electronic kinetic energy is unchanged, while (120) bounds the radiation energy uniformly in R. Applying the form-norm equivalence (27) before and after localization proves (121). Positivity and preservation of the trace then show that $\mathcal{L}_R(\mathcal{D}) \subset \mathcal{D}$. □

Lemma 5.6 (Trace-norm bound for photon localization)**.** *Let $0 \leq \eta \leq 1$ be an operator on $\mathfrak{H}_{\mathrm{ph}}$, and let $\mathcal{U}_\eta$ be the Fock-space localization isometry induced by $u \mapsto \eta u \oplus \sqrt{1-\eta^2}\,u$. With the electronic identity suppressed, define*

$$\mathcal{L}_\eta(\tau) := \mathrm{Tr}_{\mathrm{out}}(\mathcal{U}_\eta\tau\mathcal{U}_\eta^\dagger).$$

Then

$$\|\tau - \mathcal{L}_\eta \tau\|_{\mathfrak{S}_1} \le 2\sqrt{t} + t,$$
$$t := \mathrm{Tr}\left((1 - \Gamma(\eta^2))\tau\right) \le \mathrm{Tr}\left(\mathrm{d}\Gamma(1-\eta^2)\tau\right)$$

for every positive trace-one operator τ on $\mathcal{H}_N$.

Here

$$\Gamma(\eta) := \bigoplus_{m\ge 0} \eta^{\otimes m}\big|_{\mathfrak{H}_{\mathrm{ph}}^{\otimes_s m}}, \qquad \eta^{\otimes 0} = 1,$$

is the multiplicative second quantization, extending the earlier $\Gamma(U)$ construction from unitaries to contractions. The additive lift $\mathrm{d}\Gamma(b)$ acts on the m-photon sector as $\sum_{j=1}^m b_j$ and vanishes on the vacuum.

Proof. Projecting the discarded factor onto its vacuum gives

$$K_0 := (\mathbb{1} \otimes \langle\Omega|)\mathcal{U}_\eta = \Gamma(\eta).$$

Indeed, on the m-photon sector this projection retains precisely the term $\eta^{\otimes m}$. Splitting the partial trace into the discarded vacuum and its orthogonal complement yields

$$\mathcal{L}_\eta \tau = K_0 \tau K_0 + \sigma, \qquad \sigma \ge 0, \qquad \mathrm{Tr}\,\sigma = \mathrm{Tr}\left((1 - K_0^2)\tau\right) = t,$$

where $K_0^2 = \Gamma(\eta^2)$. Thus $t \in [0,1]$ is the probability that the discarded factor contains at least one photon. Since K_0 is a positive contraction and $(1-K_0)^2 \le 1 - K_0^2$, Hilbert–Schmidt factorization gives $\|\tau - K_0\tau K_0\|_{\mathfrak{S}_1} \le 2\sqrt{t}$. The triangle inequality and $\|\sigma\|_{\mathfrak{S}_1} = t$ prove the trace-norm bound. Finally, on each photon sector the commuting contractions $(\eta^2)_j$ satisfy $1 - \prod_j (\eta^2)_j \le \sum_j (1 - (\eta^2)_j)$. Summing over sectors gives $1 - \Gamma(\eta^2) \le \mathrm{d}\Gamma(1-\eta^2)$ and hence the bound on t. □

We now combine Lemma 5.2 with the localization bounds of Lemmas 5.3 to 5.6 to construct a limit state that has the limiting density and current, and whose internal energy is at most the liminf of the internal energies along the sequence. Photons are localized at the scales $R = 3^m$, and those that escape to infinity are discarded.

Lemma 5.7 (Lower semicontinuity with photon loss)**.** *Let $(\mathbf{\Gamma}_j) \subset \mathcal{D}$ have uniformly bounded internal energies and uniformly tight electronic densities:*

$$\sup_j \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_j\big) < \infty,$$
$$\lim_{R\to\infty} \sup_j \int_{|\mathbf{x}|>R} \rho_{\mathbf{\Gamma}_j}(\mathbf{x})\mathrm{d}\mathbf{x} = 0.$$

Suppose also that the photon-number distributions of the localized states $\mathcal{L}_{3^m}\mathbf{\Gamma}_j$ are asymptotically tight, uniformly in m:

$$\lim_{M\to\infty} \sup_{m\ge 1} \limsup_{j\to\infty} \mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\mathcal{L}_{3^m}\mathbf{\Gamma}_j\right) = 0. \tag{122}$$

If $(\rho_{\mathbf{\Gamma}_j}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_j}) \to (\rho, \mathbf{j}^{\mathrm{c}})$ in the sense of distributions, then there is a $\mathbf{\Gamma} \in \mathcal{D}$ such that

$$\rho_{\mathbf{\Gamma}} = \rho, \qquad \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} = \mathbf{j}^{\mathrm{c}}, \qquad \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) \le \liminf_{j\to\infty} \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_j\big). \tag{123}$$

A sufficient condition for (122) is

$$\lim_{M\to\infty} \sup_j \mathrm{Tr}\big(\mathbb{1}_{\{\mathcal{N}>M\}}\mathbf{\Gamma}_j\big) = 0;$$

in particular, a uniform bound on $\mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}_j)$ *suffices.*

Note that neither a bound on mean photon number nor photon-position tightness is assumed, and the original sequence need not converge in trace norm.

The order of limits in (122) matters. For each fixed localization scale 3^m, the limit superior as $j \to \infty$ is taken first, so only the eventual behavior of the localized states at that scale enters. The resulting photon-number tails, one for each m, are then required to vanish uniformly in m as $M \to \infty$. Explicitly, for every $\varepsilon > 0$ there is an M such that, for every $m \geq 1$, some j_0 satisfies

$$\mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\mathcal{L}_{3^m}\mathbf{\Gamma}_j\right) < \varepsilon \qquad \text{for all } j \geq j_0.$$

The threshold j_0 may depend on m, as well as on ε. A uniform bound on the original mean photon number is much stronger. By (118) and $\mathbb{1}_{\{\mathcal{N}>M\}} \leq \mathcal{N}/M$, it gives

$$\mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\mathcal{L}_{3^m}\mathbf{\Gamma}_j\right) \leq \frac{1}{M}\sup_i \mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}_i)$$

for all j and m at once, with no threshold. In contrast, (122) constrains only the photons retained at each fixed scale, and only for large j. This permits the removal of arbitrarily many soft photons.

For example, let ξ be a normalized smooth one-photon function supported in $\{0 < |\mathbf{k}| < 1\}$, put $\xi_j(\mathbf{k},\lambda) = j^3\xi(j^2\mathbf{k},\lambda)$, and set $\Xi_j = (j!)^{-1/2}a^\dagger(\xi_j)^j\Omega$. Then

$$\langle \Xi_j, \mathcal{N}\Xi_j\rangle = j, \qquad \langle \Xi_j, H_{\mathrm{rad}}\Xi_j\rangle = j^{-1}\langle \xi, \omega\xi\rangle.$$

Write $\check{\xi}$ for the inverse Fourier transform of ξ in $\mathbf{k}$, taken separately for each polarization λ, so that $\check{\xi}$ is ξ in the photon position variable $\mathbf{y}$. Then $\check{\xi}_j(\mathbf{y}) = j^{-3}\check{\xi}(\mathbf{y}/j^2)$, so for each fixed R,

$$\mathrm{Tr}\left(\mathcal{N}\mathcal{L}_R(|\Xi_j\rangle\langle\Xi_j|)\right) = j\|\theta_R\check{\xi}_j\|^2 \leq CR^3j^{-5} \longrightarrow 0.$$

Thus the localized states converge to the vacuum and satisfy (122), although their original photon-number distributions are not uniformly tight.

Now fix a normalized $\Phi \in Q(H^0_{\mathrm{el}})$ and set $\Psi_j = \Phi \otimes \Xi_j$. We compare Ψ_j with the vacuum product $\Phi \otimes \Omega$. Since Ξ_j is normalized, $\rho_{\Psi_j} = \rho_\Phi$ and $\mathbf{j}^{\mathrm{p}}_{\Psi_j} = \mathbf{j}^{\mathrm{p}}_\Phi$. Since Ξ_j has exactly j photons and $\mathfrak{A}^\mu(\mathbf{x})$ changes the photon number by one, $\langle \Xi_j, \mathfrak{A}^\mu(\mathbf{x})\Xi_j\rangle = 0$. Hence $\mathbf{j}^{\mathrm{ph}}_{\Psi_j} = 0$, and Ψ_j has the same density and combined current density $\mathbf{j}^{\mathrm{c}}_{\Psi_j} = \mathbf{j}^{\mathrm{p}}_\Phi$ as $\Phi \otimes \Omega$.

The internal energies differ only through the radiation energy and the field fluctuations. The cross terms in $\|\mathbf{D}_n\Psi_j\|^2$ vanish because the field expectation in Ξ_j is zero, and the canonical commutation relations give

$$\|\mathfrak{A}^\mu(\mathbf{x})\Xi_j\|^2 = \|G^\mu_{\mathbf{x}}\|^2 + 2j|\langle G^\mu_{\mathbf{x}}, \xi_j\rangle|^2,$$

whose first term is the vacuum value. The Cauchy–Schwarz inequality, (14), and the identity $\|\sqrt{\omega}\xi_j\|^2 = j^{-2}\langle \xi, \omega\xi\rangle$ bound the sum over μ of the second term by $2j^{-1}\|\widehat{\chi}/\sqrt{\omega}\|^2\langle \xi, \omega\xi\rangle$. Integrating against $|\Phi|^2$, summing over the electrons, and using $\int_{\mathbb{R}^3}\rho_\Phi = N$, we find that the additional internal energy obeys

$$0 \leq \langle \Psi_j, H^{0,0}\Psi_j\rangle - \langle \Phi\otimes\Omega, H^{0,0}(\Phi\otimes\Omega)\rangle \leq \frac{1}{j}\left(1 + e^2N\left\|\frac{\widehat{\chi}}{\sqrt{\omega}}\right\|^2\right)\langle \xi, \omega\xi\rangle.$$

Thus the states $|\Psi_j\rangle\langle\Psi_j|$ satisfy all hypotheses of Lemma 5.7, with constant density and current, although $\langle \Psi_j, \mathcal{N}\Psi_j\rangle = j \to \infty$. By the photon-number computation

above, their localized states converge in trace norm to $|\Phi\otimes\Omega\rangle\langle\Phi\otimes\Omega|$, so all j photons are lost in the limit. The limit state $\mathbf{\Gamma}=|\Phi\otimes\Omega\rangle\langle\Phi\otimes\Omega|$ satisfies (123) with equality.

Proof of Lemma 5.7. Write $H=H^{0,0}$ and first pass to a subsequence realizing the energy liminf. The form-norm equivalence controls the ordinary electronic kinetic energy and $H_{\rm rad}$ uniformly.

By Lemmas 5.3 and 5.5, the localized states have the same electronic reduced state, their radiation energies are uniformly bounded, and

$$\operatorname{Tr}(\mathcal{N}\mathcal{L}_R\mathbf{\Gamma}_j)\le CR\operatorname{Tr}(H_{\rm rad}\mathbf{\Gamma}_j).$$

Their full internal energies are uniformly bounded in both j and $R>0$ by (121).

Step 1. Local trace-norm compactness. Fix $R>0$. Set

$$-\mathbf{\Delta}:=\sum_{n=1}^{N}(-\Delta_{\mathbf{x}_n}),\qquad E:=1+\sup_j\operatorname{Tr}(H\mathbf{\Gamma}_j)<\infty.$$

The form-norm equivalence and the preceding estimates give

$$\sup_j\operatorname{Tr}\left((1-\mathbf{\Delta}+H_{\rm rad})\mathcal{L}_R\mathbf{\Gamma}_j\right)\le CE,\qquad \sup_j\operatorname{Tr}(\mathcal{N}\mathcal{L}_R\mathbf{\Gamma}_j)\le CRE.$$

All constants in the estimates below are independent of j,R,M,L,s. We construct finite-rank orthogonal projections whose complements have uniformly small expectation in $\mathcal{L}_R\mathbf{\Gamma}_j$.

First, denote the photon number cutoff by

$$P_M=\mathbb{1}_{\{\mathcal{N}\le M\}},$$

for integers $M\ge 0$. The electron–photon interaction terms in the internal Hamiltonian $H=H^{0,0}$ can change photon number, so P_M need not commute with H. We deal with these terms later.

Since $1-P_M\le\mathcal{N}/(M+1)$,

$$\sup_j\operatorname{Tr}\left((1-P_M)\mathcal{L}_R\mathbf{\Gamma}_j\right)\le\frac{1}{M+1}\sup_j\operatorname{Tr}(\mathcal{N}\mathcal{L}_R\mathbf{\Gamma}_j)\le\frac{CRE}{M+1}.$$

Next choose a fixed $\zeta\in C_c^\infty(\mathbb{R}^3)$ with $0\le\zeta\le 1$, equal to one on B_1 and zero outside B_2, and define the symmetric electronic cutoff

$$\zeta_L(\mathbf{x}_1,\dots,\mathbf{x}_N):=\prod_{n=1}^{N}\zeta(\mathbf{x}_n/L),\qquad L\ge 1.$$

Thus $0\le\zeta_L\le 1$, $\zeta_L=1$ on $(B_L)^N$, and $\operatorname{supp}\zeta_L\subset(\overline{B_{2L}})^N$: the cutoff localizes all N electrons in the ball B_{2L}. Electronic tightness is used through the quantity

$$\varepsilon_{\rm el}(L):=\sup_j\int_{|\mathbf{x}|>L}\rho_{\mathbf{\Gamma}_j}(\mathbf{x})\mathrm{d}\mathbf{x},$$

which tends to zero as $L\to\infty$ by the assumed uniform tightness of the electronic densities. Using the elementary fact that

$$(1-\zeta_L)^2\le\mathbb{1}_{\{\max_n|\mathbf{x}_n|>L\}}\le\sum_{n=1}^{N}\mathbb{1}_{\{|\mathbf{x}_n|>L\}}$$

and taking expectations and suprema of both sides yields

$$\sup_j \mathrm{Tr}\big((1-\zeta_L)^2\mathcal{L}_R\mathbf{\Gamma}_j\big) \le \sup_j \int_{|\mathbf{x}|>L} \rho_{\mathcal{L}_R\mathbf{\Gamma}_j}(\mathbf{x})\mathrm{d}\mathbf{x} = \varepsilon_{\mathrm{el}}(L).$$

Indeed, photon localization leaves the electronic reduced state, and hence the density, unchanged: $\rho_{\mathcal{L}_R\mathbf{\Gamma}_j} = \rho_{\mathbf{\Gamma}_j}$ by Lemma 5.3.

Further, the positive contractions P_M and ζ_L commute. Thus

$$(1-\zeta_L P_M)^2 = (1-P_M) + P_M(1-\zeta_L)^2,$$

and hence

$$\begin{aligned}\sup_j \|(1-\zeta_L P_M)\sqrt{\mathcal{L}_R\mathbf{\Gamma}_j}\|_{\mathfrak{S}_2}^2 &\le \sup_j \mathrm{Tr}\left((1-P_M)\mathcal{L}_R\mathbf{\Gamma}_j\right) + \sup_j \mathrm{Tr}\left((1-\zeta_L)^2\mathcal{L}_R\mathbf{\Gamma}_j\right)\\ &\le \frac{CRE}{M+1} + \varepsilon_{\mathrm{el}}(L). \end{aligned} \tag{124}$$

The cutoff also preserves the required regularity with an explicit bound. We have

$$\sum_{n=1}^N |\boldsymbol{\nabla}_{\mathbf{x}_n}\zeta_L|^2 \le \frac{1}{L^2}\sum_{n=1}^N \big|(\boldsymbol{\nabla}\zeta)(\mathbf{x}_n/L)\big|^2 \le \frac{N\|\boldsymbol{\nabla}\zeta\|_\infty^2}{L^2}.$$

Let $\psi \in Q(-\mathbf{\Delta})$ and put $\varphi = P_M\psi$. Since P_M acts only on the photon factor, it commutes with the electronic derivatives, so $\|\boldsymbol{\nabla}_{\mathbf{x}_n}\varphi\| \le \|\boldsymbol{\nabla}_{\mathbf{x}_n}\psi\|$ and $\|\varphi\| \le \|\psi\|$. The product rule and $0 \le \zeta_L \le 1$ give

$$\begin{aligned}\sum_{n=1}^N \|\boldsymbol{\nabla}_{\mathbf{x}_n}(\zeta_L P_M\psi)\|^2 &\le 2\sum_{n=1}^N \|\boldsymbol{\nabla}_{\mathbf{x}_n}\varphi\|^2 + 2\Big\langle\varphi, \sum_{n=1}^N |\boldsymbol{\nabla}_{\mathbf{x}_n}\zeta_L|^2\varphi\Big\rangle\\ &\le 2\sum_{n=1}^N \|\boldsymbol{\nabla}_{\mathbf{x}_n}\psi\|^2 + \frac{CN}{L^2}\|\psi\|^2.\end{aligned}$$

Applying this to the vectors in a spectral decomposition of $\mathcal{L}_R\mathbf{\Gamma}_j$ and summing, with $\mathrm{Tr}\,\mathcal{L}_R\mathbf{\Gamma}_j = 1$, gives

$$\mathrm{Tr}\left((-\mathbf{\Delta})\zeta_L P_M(\mathcal{L}_R\mathbf{\Gamma}_j)P_M\zeta_L\right) \le 2\,\mathrm{Tr}\left((-\mathbf{\Delta})\mathcal{L}_R\mathbf{\Gamma}_j\right) + \frac{CN}{L^2}.$$

Moreover, $\zeta_L P_M$ commutes with H_{rad} and is a contraction, so

$$\begin{aligned}\mathrm{Tr}\left(H_{\mathrm{rad}}\zeta_L P_M(\mathcal{L}_R\mathbf{\Gamma}_j)P_M\zeta_L\right) &\le \mathrm{Tr}(H_{\mathrm{rad}}\mathcal{L}_R\mathbf{\Gamma}_j),\\ \mathrm{Tr}\left((1-\mathbf{\Delta}+H_{\mathrm{rad}})\zeta_L P_M(\mathcal{L}_R\mathbf{\Gamma}_j)P_M\zeta_L\right) &\le C(E+N/L^2).\end{aligned}$$

We now apply Rellich compactness after both cutoffs. In the m-photon sector of $\mathcal{L}_R\mathbf{\Gamma}_j$, every retained photon is supported in B_{2R}, because its localization factor is θ_R. Consequently, $\zeta_L P_M\sqrt{\mathcal{L}_R\mathbf{\Gamma}_j}$ takes values in the closed subspace

$$\mathscr{H}_{L,R,M} := \bigoplus_{m=0}^M \big\{\psi^{(m)} \in \mathfrak{H}_{\mathrm{el}}^N \otimes L^2_s((\mathbb{R}^3\times\{1,2\})^m) : \psi^{(m)} \equiv 0 \text{ a.e. outside } \Omega_{L,R,m}\big\},$$

where

$$\Omega_{L,R,m} := (B_{2L})^N \times (B_{2R})^m.$$

Here the photon variables $(\mathbf{y}_l, \lambda_l)$ are in the position representation, and the support condition is imposed for every value of the polarization indices λ_l. On this subspace

we restrict the closed form of $1-\boldsymbol{\Delta}+H_{\mathrm{rad}}$, computing all derivatives after extension by zero to the full configuration space. This gives the form

$$k_{L,R,M}[\psi] := \sum_{m=0}^{M} k_m[\psi^{(m)}], \qquad \psi = \bigoplus_{m=0}^{M} \psi^{(m)} \in \mathscr{H}_{L,R,M},$$

whose value in the m-photon sector is

$$k_m[\psi^{(m)}] = \|\psi^{(m)}\|^2 + \sum_{n=1}^{N} \|\boldsymbol{\nabla}_{\mathbf{x}_n}\psi^{(m)}\|^2 + \sum_{l=1}^{m} \big\|(-\Delta_{\mathbf{y}_l})^{1/4}\psi^{(m)}\big\|^2.$$

Its domain $Q(k_{L,R,M})$ consists of those $\psi \in \mathscr{H}_{L,R,M}$ for which every $k_m[\psi^{(m)}]$ is finite. The form $k_{L,R,M}$ is closed because $\mathscr{H}_{L,R,M}$ is closed in $\mathcal{H}_N$. It is densely defined because smooth functions compactly supported in $\Omega_{L,R,m}$, with the prescribed symmetries, are dense in the corresponding L^2 space. The form $k_m[\cdot]$ controls the $H^{1/2}$ norm in all $3(N+m)$ variables jointly. Indeed, by Plancherel's theorem, with $\boldsymbol{\xi}_n$ dual to $\mathbf{x}_n$ and $\mathbf{k}_l$ dual to $\mathbf{y}_l$, the Fourier symbol of $k_m[\cdot]$ is $1+\sum_n |\boldsymbol{\xi}_n|^2+\sum_l |\mathbf{k}_l|$. Using $\sum_l |\mathbf{k}_l|^2 \le \big(\sum_l |\mathbf{k}_l|\big)^2$, $\sqrt{s+t} \le \sqrt{s}+\sqrt{t}$ for $s,t \ge 0$, and $\sqrt{1+s} \le 1+s$, we obtain

$$\begin{aligned}\left(1+\sum_{n=1}^{N}|\boldsymbol{\xi}_n|^2+\sum_{l=1}^{m}|\mathbf{k}_l|^2\right)^{1/2} &\le \left(1+\sum_{n=1}^{N}|\boldsymbol{\xi}_n|^2\right)^{1/2} + \sum_{l=1}^{m}|\mathbf{k}_l| \\ &\le 1+\sum_{n=1}^{N}|\boldsymbol{\xi}_n|^2+\sum_{l=1}^{m}|\mathbf{k}_l|,\end{aligned}$$

and hence $\|u\|^2_{H^{1/2}(\mathbb{R}^{3(N+m)})} \le k_m[u]$. Since $\Omega_{L,R,m}$ is a bounded convex domain and hence a Lipschitz domain, the Rellich–Kondrashov theorem for $H^{1/2}$ gives a compact embedding of the m-photon component of $Q(k_{L,R,M})$ into $L^2(\Omega_{L,R,m})$ [11, Theorem 7.1]: the Gagliardo seminorm on $\Omega_{L,R,m}$ is bounded by the $H^{1/2}(\mathbb{R}^{3(N+m)})$ norm [11, Proposition 3.4], and Lipschitz domains are extension domains [11, Theorem 5.4]. There are only finitely many sectors and finitely many polarization components in each. Therefore $Q(k_{L,R,M})$, normed by $k_{L,R,M}[\cdot]^{1/2}$, embeds compactly into $\mathscr{H}_{L,R,M}$.

Let $K_{L,R,M} \ge 1$ be the self-adjoint operator on $\mathscr{H}_{L,R,M}$ associated with the closed form $k_{L,R,M}[\cdot]$. It has compact resolvent, so for each $s \ge 1$ its spectral projection

$$S := \mathbb{1}_{[0,s]}(K_{L,R,M}),$$

extended by zero on $\mathscr{H}_{L,R,M}^{\perp}$, is a finite-rank orthogonal projection on $\mathcal{H}_N$. The spectral theorem gives

$$\begin{aligned}\|(1-S)\zeta_L P_M \sqrt{\mathcal{L}_R\boldsymbol{\Gamma}_j}\|^2_{\mathfrak{S}_2} &= \operatorname{Tr}\big((1-S)\zeta_L P_M(\mathcal{L}_R\boldsymbol{\Gamma}_j)P_M\zeta_L\big) \\ &\le s^{-1}\operatorname{Tr}\big(K_{L,R,M}\zeta_L P_M(\mathcal{L}_R\boldsymbol{\Gamma}_j)P_M\zeta_L\big) \le \frac{C(E+N/L^2)}{s}.\end{aligned}$$

Combining this with the preceding cutoff error (124), we obtain

$$\begin{aligned}\operatorname{Tr}\big((1-S)\mathcal{L}_R\mathbf{\Gamma}_j\big) &= \|(1-S)\sqrt{\mathcal{L}_R\mathbf{\Gamma}_j}\|_{\mathfrak{S}_2}^2 \\ &\le 2\|(1-\zeta_L P_M)\sqrt{\mathcal{L}_R\mathbf{\Gamma}_j}\|_{\mathfrak{S}_2}^2 + 2\|(1-S)\zeta_L P_M\sqrt{\mathcal{L}_R\mathbf{\Gamma}_j}\|_{\mathfrak{S}_2}^2 \\ &\le \frac{2CRE}{M+1} + 2\varepsilon_{\mathrm{el}}(L) + \frac{C(E+N/L^2)}{s}.\end{aligned}$$

For fixed R, first choose M, then L, and finally s sufficiently large to make this bound arbitrarily small, uniformly in j. The states $\mathcal{L}_R\mathbf{\Gamma}_j$ are positive with unit trace, so the compactness part of Lemma 5.1 shows that the sequence $(\mathcal{L}_R\mathbf{\Gamma}_j)_j$ is precompact in trace norm.

Step 2. A trace-norm limit of the retained states. A diagonal extraction gives a subsequence, still denoted $(\mathbf{\Gamma}_j)$, such that

$$\mathcal{L}_{3^m}\mathbf{\Gamma}_j \longrightarrow \mathbf{\Gamma}^{(m)} \quad \text{in trace norm as } j\to\infty, \text{ for every } m\ge 1.$$

Localization maps compose according to multiplication of their one-photon contractions. For $l > m$, the function θ_{3^m} vanishes outside $B_{2\cdot 3^m}$, while $\theta_{3^l} = 1$ on $B_{3^l} \supset B_{3^{m+1}} \supset B_{2\cdot 3^m}$. Hence $\theta_{3^m}\theta_{3^l} = \theta_{3^m}$, and therefore

$$\mathcal{L}_{3^m}\mathbf{\Gamma}^{(l)} = \mathbf{\Gamma}^{(m)}.$$

Since photon-sector projections are bounded, the hypothesis implies

$$\delta(M) := \sup_m \operatorname{Tr}\Big(\mathbb{1}_{\{\mathcal{N}>M\}}\mathbf{\Gamma}^{(m)}\Big) \longrightarrow 0.$$

We next show that $(\mathbf{\Gamma}^{(m)})$ is Cauchy in trace norm, using Lemma 5.6 with $\tau = \mathbf{\Gamma}^{(l)}$ and $\eta = \theta_{3^m}$ for $l > m$. For this, the probability that passing from $\mathbf{\Gamma}^{(l)}$ to $\mathbf{\Gamma}^{(m)}$ discards at least one photon must be small. The bound on this probability in Lemma 5.6 involves the mean photon number, which need not be finite here. We therefore track instead the expectation of the bounded function $n \mapsto 2^{-n}$ of the photon number,

$$b_m := \operatorname{Tr}\Big(2^{-\mathcal{N}}\mathbf{\Gamma}^{(m)}\Big) \in [0,1],$$

which is finite for every state. We show below that discarding photons can only increase this expectation, so (b_m) is nonincreasing and converges. Its decrease $b_m - b_l$, together with the photon-number tightness $\delta(M)$, then controls the probability of discarding a photon.

For $l > m$, the localization isometry $\mathcal{U}_{3^m}$ underlying $\mathcal{L}_{3^m}$ takes values in $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\mathrm{ph}}^{\mathrm{in}} \otimes \mathcal{F}_{\mathrm{ph}}^{\mathrm{out}}$, where the two Fock factors contain the retained and discarded photons, respectively. In photon position, the retained photons carry the factor θ_{3^m} and are supported in the ball $B_{2\cdot 3^m}$, while the discarded photons carry the factor φ_{3^m}, which vanishes on B_{3^m}. Define their number operators by

$$\mathcal{N}_{\mathrm{in}} := \mathbb{1}_{\mathfrak{H}_{\mathrm{el}}^N} \otimes \mathcal{N} \otimes \mathbb{1}_{\mathcal{F}_{\mathrm{ph}}^{\mathrm{out}}}, \qquad \mathcal{N}_{\mathrm{out}} := \mathbb{1}_{\mathfrak{H}_{\mathrm{el}}^N} \otimes \mathbb{1}_{\mathcal{F}_{\mathrm{ph}}^{\mathrm{in}}} \otimes \mathcal{N}.$$

Thus on the sector with p retained and q discarded photons they act as multiplication by p and q, respectively, and strongly commute. Recall that $\mathcal{U}_{3^m} = \Gamma(j_{3^m})$ is the second quantization of the one-photon isometry $j_{3^m} f = (\theta_{3^m} f, \varphi_{3^m} f)$, followed by the identification $\mathcal{F}_s(\mathfrak{H}_{\mathrm{ph}} \oplus \mathfrak{H}_{\mathrm{ph}}) \simeq \mathcal{F}_{\mathrm{ph}}^{\mathrm{in}} \otimes \mathcal{F}_{\mathrm{ph}}^{\mathrm{out}}$, with the electronic identity suppressed, and that $\mathcal{L}_{3^m}(\mathbf{\Gamma}) = \operatorname{Tr}_{\mathrm{out}}(\mathcal{U}_{3^m}\mathbf{\Gamma}\mathcal{U}_{3^m}^\dagger)$. In the joint state $\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger$, their sum has the number distribution of $\mathbf{\Gamma}^{(l)}$, and the first has that of $\mathbf{\Gamma}^{(m)}$. Indeed, $\mathcal{U}_{3^m}$ maps the n-photon sector into the sum of the sectors with $p+q=n$,

so $\mathcal{U}_{3^m}^\dagger f(\mathcal{N}_{\rm in}+\mathcal{N}_{\rm out})\mathcal{U}_{3^m} = f(\mathcal{N})$ for every bounded function f on $\{0,1,2,\dots\}$. Moreover, $f(\mathcal{N}_{\rm in})$ acts trivially on the discarded factor, and the partial trace over that factor is $\mathcal{L}_{3^m}\mathbf{\Gamma}^{(l)} = \mathbf{\Gamma}^{(m)}$. Hence

$$\mathrm{Tr}\Big(f(\mathcal{N}_{\rm in}+\mathcal{N}_{\rm out})\,\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big) = \mathrm{Tr}\left(f(\mathcal{N})\mathbf{\Gamma}^{(l)}\right),$$
$$\mathrm{Tr}\Big(f(\mathcal{N}_{\rm in})\,\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big) = \mathrm{Tr}\left(f(\mathcal{N})\mathbf{\Gamma}^{(m)}\right).$$

Take $f(n) = 2^{-n}$. The operators $\mathcal{N}_{\rm in}$ and $\mathcal{N}_{\rm out}$ strongly commute, so $2^{-(\mathcal{N}_{\rm in}+\mathcal{N}_{\rm out})} = 2^{-\mathcal{N}_{\rm in}}2^{-\mathcal{N}_{\rm out}}$, and the two identities give

$$b_l = \mathrm{Tr}\Big(2^{-\mathcal{N}_{\rm in}}2^{-\mathcal{N}_{\rm out}}\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big),$$
$$b_m = \mathrm{Tr}\Big(2^{-\mathcal{N}_{\rm in}}\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big).$$

Subtracting, we obtain

$$b_m - b_l = \mathrm{Tr}\Big(2^{-\mathcal{N}_{\rm in}}(1-2^{-\mathcal{N}_{\rm out}})\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big) \geq 0,$$

where the inequality holds because $2^{-p}(1-2^{-q}) \geq 0$ for all integers $p, q \geq 0$. In particular, the sequence (b_m) is nonincreasing. Let

$$t_{m,l} := \mathrm{Tr}\Big(\mathbb{1}_{\{\mathcal{N}_{\rm out}\geq 1\}}\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big)$$

denote the probability that at least one photon is discarded. Splitting according to $\mathcal{N}_{\rm in} > M$ and $\mathcal{N}_{\rm in} \leq M$ gives

$$\begin{aligned} t_{m,l} &\leq \mathrm{Tr}\Big(\mathbb{1}_{\{\mathcal{N}_{\rm in}>M\}}\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big) \\ &\quad + \mathrm{Tr}\Big(\mathbb{1}_{\{\mathcal{N}_{\rm in}\leq M\}}\mathbb{1}_{\{\mathcal{N}_{\rm out}\geq 1\}}\mathcal{U}_{3^m}\mathbf{\Gamma}^{(l)}\mathcal{U}_{3^m}^\dagger\Big) \\ &\leq \delta(M) + 2^{M+1}(b_m - b_l). \end{aligned}$$

For the first term, we take $f = \mathbb{1}_{(M,\infty)}$ in the second trace identity above. This shows that the first term equals $\mathrm{Tr}\big(\mathbb{1}_{\{\mathcal{N}>M\}}\mathbf{\Gamma}^{(m)}\big)$, which is at most $\delta(M)$. For the second term, the operator $2^{-\mathcal{N}_{\rm in}}(1-2^{-\mathcal{N}_{\rm out}})$ is at least 2^{-M-1} on the joint spectral subspace $\mathcal{N}_{\rm in} \leq M$, $\mathcal{N}_{\rm out} \geq 1$, so the formula for $b_m - b_l$ bounds this term by $2^{M+1}(b_m - b_l)$. Finally, $t_{m,l}$ is the quantity t of Lemma 5.6 for $\tau = \mathbf{\Gamma}^{(l)}$ and $\eta = \theta_{3^m}$, and $\mathcal{L}_{3^m}\mathbf{\Gamma}^{(l)} = \mathbf{\Gamma}^{(m)}$, so

$$\|\mathbf{\Gamma}^{(l)} - \mathbf{\Gamma}^{(m)}\|_{\mathfrak{S}_1} \leq 2\sqrt{t_{m,l}} + t_{m,l}.$$

The nonincreasing sequence b_m has a limit. First choose M so that $\delta(M)$ is small, then m so that $b_m - b_l$ is small uniformly for $l > m$. Hence $\mathbf{\Gamma}^{(m)}$ is Cauchy in trace norm and converges to a density matrix $\mathbf{\Gamma}$ on the original space $\mathcal{H}_N$, possibly with infinite mean photon number. The rough energy bound (121) gives

$$\sup_{j,m} \mathrm{Tr}(H\mathcal{L}_{3^m}\mathbf{\Gamma}_j) \leq CE.$$

Applying Lemma 5.2 first to $\mathcal{L}_{3^m}\mathbf{\Gamma}_j \to \mathbf{\Gamma}^{(m)}$ and then to $\mathbf{\Gamma}^{(m)} \to \mathbf{\Gamma}$ yields

$$\sup_m \mathrm{Tr}\Big(H\mathbf{\Gamma}^{(m)}\Big) \leq CE, \qquad \mathrm{Tr}(H\mathbf{\Gamma}) \leq CE < \infty,$$

and hence $\mathbf{\Gamma} \in \mathcal{D}$. We next prove the sharp energy inequality.

Step 3. The energy inequality. The argument involves an electronic cutoff at scale L, the photon localization scale $R = 3^m$, and a truncation of $H_{\rm rad}$ by second

quantizations of one-photon operators of rank K, all introduced below. We pass to the limits in a fixed order: first $j \to \infty$, then $R = 3^m \to \infty$ with L and K fixed, then $K \to \infty$, and finally $L \to \infty$. The order matters because the bound on the localized truncated radiation energy below carries an error $\delta_K(R)$ that is established only for fixed K, and tends to zero as $R \to \infty$ but not uniformly in K.

To control the interaction error, we first choose a symmetric electronic cutoff η_L, equal to one when $\max_i |\mathbf{x}_i| \leq L$ and zero when $\max_i |\mathbf{x}_i| \geq 2L$, together with a smooth complementary cutoff $\widetilde{\eta}_L$. For example, using the electronic cutoff ζ_L constructed above, take

$$\eta_L = \sin\Big(\frac{\pi}{2}\zeta_L\Big), \qquad \widetilde{\eta}_L = \cos\Big(\frac{\pi}{2}\zeta_L\Big).$$

Then $\eta_L^2 + \widetilde{\eta}_L^2 = 1$ and

$$\sum_{i=1}^{N} \big(|\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L|^2 + |\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L|^2\big) = \frac{\pi^2}{4}\sum_{i=1}^{N} |\boldsymbol{\nabla}_{\mathbf{x}_i}\zeta_L|^2 \leq \frac{C}{L^2}.$$

Both cutoffs preserve $Q(H)$: their bounded gradients preserve the electronic H^1 regularity, and they commute with $\sqrt{H_{\mathrm{rad}}}$.

For either cutoff $f \in \{\eta_L, \widetilde{\eta}_L\}$, the covariant derivative obeys

$$\mathbf{D}_i(f\Psi) = f\mathbf{D}_i\Psi - \mathrm{i}(\boldsymbol{\nabla}_{\mathbf{x}_i} f)\Psi, \qquad \mathbf{D}_i = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_i} - e\mathfrak{A}(\mathbf{x}_i),$$

because f commutes with the field operator $\mathfrak{A}(\mathbf{x}_i)$. Since η_L and $\widetilde{\eta}_L$ are real, expanding gives

$$\begin{aligned}
&\|\mathbf{D}_i(\eta_L\Psi)\|^2 + \|\mathbf{D}_i(\widetilde{\eta}_L\Psi)\|^2 \\
&\quad = \langle \mathbf{D}_i\Psi, (\eta_L^2 + \widetilde{\eta}_L^2)\mathbf{D}_i\Psi\rangle + \|(\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L)\Psi\|^2 + \|(\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L)\Psi\|^2 \\
&\qquad + 2\,\mathrm{Re}\langle \mathbf{D}_i\Psi, -\mathrm{i}\big(\eta_L\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L + \widetilde{\eta}_L\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L\big)\Psi\rangle \\
&\quad = \|\mathbf{D}_i\Psi\|^2 + \|(\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L)\Psi\|^2 + \|(\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L)\Psi\|^2.
\end{aligned}$$

In the last step we used $\eta_L^2 + \widetilde{\eta}_L^2 = 1$, and the cross terms cancel because

$$\eta_L\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L + \widetilde{\eta}_L\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L = \tfrac{1}{2}\boldsymbol{\nabla}_{\mathbf{x}_i}(\eta_L^2 + \widetilde{\eta}_L^2) = 0.$$

The Coulomb interaction is an electronic multiplication operator, and H_{rad} acts only on the photon factor. Their localized forms therefore sum exactly to their original forms, using $\eta_L^2 + \widetilde{\eta}_L^2 = 1$. With the factor $1/2$ in the kinetic energy, the resulting covariant IMS identity is

$$\begin{aligned}
&\langle \eta_L\Psi, H\eta_L\Psi\rangle + \langle \widetilde{\eta}_L\Psi, H\widetilde{\eta}_L\Psi\rangle \\
&\quad = \langle \Psi, H\Psi\rangle + \frac{1}{2}\sum_{i=1}^{N}\big(\|(\boldsymbol{\nabla}_{\mathbf{x}_i}\eta_L)\Psi\|^2 + \|(\boldsymbol{\nabla}_{\mathbf{x}_i}\widetilde{\eta}_L)\Psi\|^2\big) \\
&\quad \leq \langle \Psi, H\Psi\rangle + \frac{C}{L^2}\|\Psi\|^2.
\end{aligned}$$

The computation first holds on the form core and extends to $Q(H)$ by continuity. Applying it to the vectors in a spectral decomposition of $\boldsymbol{\Gamma}_j$ and summing, with $\mathrm{Tr}\,\boldsymbol{\Gamma}_j = 1$, gives

$$\mathrm{Tr}(H\eta_L\boldsymbol{\Gamma}_j\eta_L) + \mathrm{Tr}(H\widetilde{\eta}_L\boldsymbol{\Gamma}_j\widetilde{\eta}_L) \leq \mathrm{Tr}(H\boldsymbol{\Gamma}_j) + \frac{C}{L^2}.$$

Since $H \geq 0$, the second term on the left is nonnegative and can be dropped. Thus

$$\operatorname{Tr}(H\eta_L \mathbf{\Gamma}_j \eta_L) \leq \operatorname{Tr}(H\mathbf{\Gamma}_j) + C/L^2.$$

Let $\mathbf{\Gamma}$ be a positive trace-class operator with $\operatorname{Tr}(H\mathbf{\Gamma}) < \infty$. Every term in (26) is nonnegative, so $\operatorname{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}) \leq \operatorname{Tr}(H\mathbf{\Gamma}) < \infty$, and we may define

$$\mathcal{E}(\mathbf{\Gamma}) := \operatorname{Tr}(H\mathbf{\Gamma}) - \operatorname{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}),$$

the internal energy with the free-photon contribution removed. It still contains the electron–photon coupling through the covariant kinetic energy, as well as the Coulomb repulsion. The field identities (114) and (115), the annihilation–creation bounds (18) and (19) relative to $\sqrt{H_{\mathrm{rad}}}$, and Cauchy–Schwarz give

$$\mathcal{E}\big(\mathcal{L}_R(\eta_L \mathbf{\Gamma}_j \eta_L)\big) \leq \mathcal{E}(\eta_L \mathbf{\Gamma}_j \eta_L) + C\varepsilon_L(R) + C\varepsilon_L(R)^2,$$

where

$$\varepsilon_L(R) := \max_{\mu} \sup_{|\mathbf{x}| \leq 2L} \big(\|(1-\theta_R) G^\mu_{\mathbf{x}}\| + \|(-\Delta)^{-1/4}(1-\theta_R) G^\mu_{\mathbf{x}}\| + \|\varphi_R G^\mu_{\mathbf{x}}\| \big).$$

Here the negative Sobolev norm is $\|f\|_{\dot{H}^{-1/2}} = \|(-\Delta)^{-1/4} f\|$ in photon position representation. The Coulomb term is unchanged and the quadratic-field identity includes the vacuum fluctuations. The constants are uniform in j for fixed L.

We now show that $\varepsilon_L(R) \to 0$ as $R \to \infty$ for fixed L. Since $0 \leq 1-\theta_R, \varphi_R \leq 1$ and both vanish on B_R, dominated convergence gives $(1-\theta_R)f \to 0$ and $\varphi_R f \to 0$ in $\mathfrak{H}_{\mathrm{ph}}$ for every $f \in \mathfrak{H}_{\mathrm{ph}}$. Smooth multiplication by θ_R is uniformly bounded on $\dot{H}^{1/2}$, and therefore by duality on $\dot{H}^{-1/2}$. Density of compactly supported smooth functions shows that $\theta_R \to 1$ strongly in both spaces. The map $\mathbf{x} \mapsto G^\mu_{\mathbf{x}}$ is continuous into $\mathfrak{H}_{\mathrm{ph}}$ and into $\dot{H}^{-1/2}$, as noted after (14). Hence the form factors $G^\mu_{\mathbf{x}}$ with $|\mathbf{x}| \leq 2L$ and $\mu = 1,2,3$ form a compact family in both norms. The operators $1-\theta_R$ on both spaces and φ_R on $\mathfrak{H}_{\mathrm{ph}}$ are uniformly bounded in R and converge strongly to zero, and strong convergence of uniformly bounded operators is uniform on compact sets. The supremum over $|\mathbf{x}| \leq 2L$ in the definition of $\varepsilon_L(R)$ is therefore harmless, and

$$\lim_{R \to \infty} \varepsilon_L(R) = 0.$$

The rough bound (120) only controls the localized radiation energy up to a constant factor. To obtain it with coefficient one, we truncate H_{rad} from below by second quantizations of finite-rank one-photon operators: choose an orthonormal basis (e_k) whose finite span is a core for $(-\Delta)^{1/4}$, and set

$$f_k = (-\Delta)^{1/4} e_k, \qquad t_K = \sum_{k=1}^{K} |f_k\rangle\langle f_k| \leq \sqrt{-\Delta},$$

$$T_K = \mathrm{d}\Gamma(t_K) = \sum_{k=1}^{K} a^\dagger(f_k) a(f_k).$$

Then $T_K \uparrow H_{\mathrm{rad}}$ in the form sense.

Claim. For fixed K there are numbers $\delta_K(R) \to 0$ as $R \to \infty$ such that

$$\theta_R t_K \theta_R \leq \big(1 + \delta_K(R)\big)\sqrt{-\Delta}$$

in the sense of quadratic forms.

Proof of the claim. Since $\|(-\Delta)^{-1/4} f_k\| = \|e_k\| = 1$, each f_k lies in $\dot{H}^{-1/2}$, and the strong convergence $\theta_R \to 1$ on $\dot{H}^{-1/2}$ established above gives

$$e_{k,R} := (-\Delta)^{-1/4} \theta_R f_k \longrightarrow e_k \quad \text{in } \mathfrak{H}_{\mathrm{ph}}, \qquad k = 1, \dots, K.$$

Let Π_K be the orthogonal projection onto the span of $e_1, \dots, e_K$, and put

$$\delta_K(R) := \Big\| \sum_{k=1}^{K} |e_{k,R}\rangle\langle e_{k,R}| - \Pi_K \Big\| \le \sum_{k=1}^{K} \big(\|e_{k,R}\| + 1\big) \|e_{k,R} - e_k\| \longrightarrow 0.$$

Let ψ be in the form domain of $\sqrt{-\Delta}$. Since θ_R is real, moving $(-\Delta)^{\pm 1/4}$ across the inner product gives

$$\begin{aligned} \langle \psi, \theta_R t_K \theta_R \psi \rangle &= \sum_{k=1}^{K} |\langle \theta_R f_k, \psi \rangle|^2 = \sum_{k=1}^{K} \big|\langle e_{k,R}, (-\Delta)^{1/4} \psi \rangle\big|^2 \\ &= \Big\langle (-\Delta)^{1/4} \psi, \sum_{k=1}^{K} |e_{k,R}\rangle\langle e_{k,R}| \, (-\Delta)^{1/4} \psi \Big\rangle \\ &\le \big(\|\Pi_K\| + \delta_K(R)\big) \|(-\Delta)^{1/4} \psi\|^2 = \big(1 + \delta_K(R)\big) \langle \psi, \sqrt{-\Delta}\, \psi \rangle. \end{aligned}$$

This proves the claim.

The convergence $\delta_K(R) \to 0$ is not uniform in K. Since second quantization preserves form inequalities, (116) and the claim give

$$\mathrm{Tr}\,\big(T_K \mathcal{L}_R(\eta_L \mathbf{\Gamma}_j \eta_L)\big) = \mathrm{Tr}\,\big(\mathrm{d}\Gamma(\theta_R t_K \theta_R) \eta_L \mathbf{\Gamma}_j \eta_L\big) \le \big(1 + \delta_K(R)\big)\, \mathrm{Tr}(H_{\mathrm{rad}} \eta_L \mathbf{\Gamma}_j \eta_L).$$

Combining the last two estimates before taking any limits yields

$$\mathcal{E}\big(\mathcal{L}_R(\eta_L \mathbf{\Gamma}_j \eta_L)\big) + \mathrm{Tr}\,\big(T_K \mathcal{L}_R(\eta_L \mathbf{\Gamma}_j \eta_L)\big) \le \mathrm{Tr}(H \mathbf{\Gamma}_j) + C/L^2 + o_R(1). \tag{125}$$

Here $o_R(1)$ denotes an error that tends to zero as $R \to \infty$, uniformly in j, for fixed L and K. It collects the term $C\varepsilon_L(R) + C\varepsilon_L(R)^2$ from the first estimate and the term $\delta_K(R)\,\mathrm{Tr}(H_{\mathrm{rad}} \eta_L \mathbf{\Gamma}_j \eta_L) \le \delta_K(R)(E + C/L^2)$ from the second, and both are bounded independently of j. We justify the two limit passages for fixed L, K in detail. Since photon localization commutes with the electronic multiplier η_L, the positive, possibly subnormalized operators

$$\sigma_{j,m} := \mathcal{L}_{3^m}(\eta_L \mathbf{\Gamma}_j \eta_L) = \eta_L (\mathcal{L}_{3^m} \mathbf{\Gamma}_j) \eta_L, \qquad \sigma_m := \eta_L \mathbf{\Gamma}^{(m)} \eta_L, \qquad \sigma := \eta_L \mathbf{\Gamma} \eta_L$$

satisfy $\sigma_{j,m} \to \sigma_m$ in trace norm as $j \to \infty$ for each m, and $\sigma_m \to \sigma$ in trace norm as $m \to \infty$. Indeed, multiplication on both sides by η_L is a contraction in trace norm. The rough energy bound (121) for $\mathcal{L}_{3^m} \mathbf{\Gamma}_j$, followed by the covariant IMS estimate, gives

$$\sup_{j,m} \big(\mathrm{Tr}\, \sigma_{j,m} + \mathrm{Tr}(H \sigma_{j,m}) \big) \le C_L < \infty.$$

By Lemma 5.2, the same bound holds for σ_m, uniformly in m, and for σ.

Write $W = \sum_{n<m} |\mathbf{x}_n - \mathbf{x}_m|^{-1}$. Since $T_K \le H_{\mathrm{rad}}$, for $\Psi \in Q(H)$

$$\frac{1}{2} \sum_{i=1}^{N} \|\mathbf{D}_i \Psi\|^2 + \|\sqrt{W}\Psi\|^2 + \|\sqrt{T_K}\Psi\|^2 \le \|\sqrt{H}\Psi\|^2.$$

Thus $\mathcal{E}(\cdot) + \mathrm{Tr}(T_K \cdot)$ is the trace of a nonnegative form bounded relative to $H + 1$, and the final assertion of Lemma 5.2 applies to it along trace-norm convergent

sequences with uniformly bounded energy. Apply it first to $\sigma_{j,m} \to \sigma_m$ with m fixed. The combined energy estimate (125) yields

$$\begin{aligned}\mathcal{E}(\sigma_m) + \operatorname{Tr}(T_K\sigma_m) &\le \liminf_j \left[\mathcal{E}(\sigma_{j,m}) + \operatorname{Tr}(T_K\sigma_{j,m})\right] \\ &\le \liminf_j \operatorname{Tr}(H\mathbf{\Gamma}_j) + C/L^2 + o_m(1),\end{aligned}$$

where $o_m(1)$ is the error $o_R(1)$ at $R = 3^m$. Applying the same assertion to $\sigma_m \to \sigma$ and then letting $m \to \infty$ gives

$$\mathcal{E}(\eta_L\mathbf{\Gamma}\eta_L) + \operatorname{Tr}(T_K\eta_L\mathbf{\Gamma}\eta_L) \le \liminf_j \operatorname{Tr}(H\mathbf{\Gamma}_j) + C/L^2.$$

For fixed L, the nonnegative forms T_K increase to H_{rad}. Monotone convergence of their traces and the definition of $\mathcal{E}$ therefore give

$$\operatorname{Tr}(H\eta_L\mathbf{\Gamma}\eta_L) \le \liminf_j \operatorname{Tr}(H\mathbf{\Gamma}_j) + C/L^2.$$

Next, $\zeta_L \to 1$ pointwise as $L \to \infty$, so $\eta_L \to 1$ pointwise with $0 \le \eta_L \le 1$. By dominated convergence, $\eta_L \to 1$ strongly as multiplication operators on $\mathcal{H}_N$. Since $\sqrt{\mathbf{\Gamma}}$ is Hilbert–Schmidt, dominated convergence over an orthonormal basis gives $\|(1-\eta_L)\sqrt{\mathbf{\Gamma}}\|_{\mathfrak{S}_2} \to 0$. Factoring through $\sqrt{\mathbf{\Gamma}}$ and using $\operatorname{Tr}\mathbf{\Gamma} = 1$, we obtain

$$\|\eta_L\mathbf{\Gamma}\eta_L - \mathbf{\Gamma}\|_{\mathfrak{S}_1} \le 2\|(1-\eta_L)\sqrt{\mathbf{\Gamma}}\|_{\mathfrak{S}_2} \longrightarrow 0.$$

The preceding energy bound allows us to apply Lemma 5.2 to this trace-norm convergence. Hence

$$\operatorname{Tr}(H\mathbf{\Gamma}) \le \liminf_{L\to\infty} \operatorname{Tr}(H\eta_L\mathbf{\Gamma}\eta_L) \le \liminf_j \operatorname{Tr}(H\mathbf{\Gamma}_j).$$

Step 4. The constraints. We first pass the density through the two successive limits. For $f \in C_c^\infty(\mathbb{R}^3)$ and fixed m, invariance of the electronic reduced state under photon localization and (112) give

$$\int_{\mathbb{R}^3} f\rho_{\mathbf{\Gamma}^{(m)}} = \lim_{j\to\infty} \int_{\mathbb{R}^3} f\rho_{\mathcal{L}_{3^m}\mathbf{\Gamma}_j} = \lim_{j\to\infty} \int_{\mathbb{R}^3} f\rho_{\mathbf{\Gamma}_j} = \int_{\mathbb{R}^3} f\rho.$$

Since $\mathbf{\Gamma}^{(m)} \to \mathbf{\Gamma}$ in trace norm, a second application of (112) gives $\int f\rho_{\mathbf{\Gamma}} = \int f\rho$. Thus $\rho_{\mathbf{\Gamma}} = \rho$ in distributions.

For the current density, fix real $\boldsymbol{\zeta} \in C_c^\infty(\mathbb{R}^3, \mathbb{R}^3)$ and choose L with $\operatorname{supp}\boldsymbol{\zeta} \subset B_{2L}$. Put

$$h^\mu_{R,\mathbf{x}} := (1-\theta_R)G^\mu_{\mathbf{x}}, \qquad A_{R,\boldsymbol{\zeta}} := e\sum_{i=1}^N \sum_{\mu=1}^3 \zeta^\mu(\mathbf{x}_i)\Phi(h^\mu_{R,\mathbf{x}_i}).$$

Photon localization preserves the paramagnetic current density, since it depends only on the electronic reduced state. Using $\mathbf{j}^{\mathrm{c}} = \mathbf{j}^{\mathrm{p}} + \mathbf{j}^{\mathrm{ph}}$ and (114), we consequently have the form identity

$$\int_{\mathbb{R}^3} \boldsymbol{\zeta}\cdot(\mathbf{j}^{\mathrm{c}}_{\mathcal{L}_R\mathbf{\Gamma}_j} - \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_j}) = \operatorname{Tr}(A_{R,\boldsymbol{\zeta}}\mathbf{\Gamma}_j).$$

The definition of $\varepsilon_L(R)$ and the field bounds (18) and (19) imply

$$\|A_{R,\boldsymbol{\zeta}}\Psi\| \le C_{\boldsymbol{\zeta}}\varepsilon_L(R)\big(\|\sqrt{H_{\mathrm{rad}}}\Psi\| + \|\Psi\|\big), \qquad \Psi \in Q(H).$$

Thus the trace pairing is well defined without a mean-photon-number bound. Hilbert–Schmidt Cauchy–Schwarz yields

$$\begin{aligned}|\mathrm{Tr}(A_{R,\boldsymbol{\zeta}}\boldsymbol{\Gamma}_j)| &\le \|\sqrt{\boldsymbol{\Gamma}_j}\|_{\mathfrak{S}_2}\|A_{R,\boldsymbol{\zeta}}\sqrt{\boldsymbol{\Gamma}_j}\|_{\mathfrak{S}_2}\\ &\le C_{\boldsymbol{\zeta}}\varepsilon_L(R)\big(1+\mathrm{Tr}(H_{\mathrm{rad}}\boldsymbol{\Gamma}_j)\big)^{1/2} \le C_{\boldsymbol{\zeta}}\varepsilon_L(R)E^{1/2},\end{aligned}$$

where $E = 1 + \sup_j \mathrm{Tr}(H\boldsymbol{\Gamma}_j)$ was fixed above.

Now fix m and take $R = 3^m$. The states $\mathcal{L}_{3^m}\boldsymbol{\Gamma}_j$ converge in trace norm to $\boldsymbol{\Gamma}^{(m)}$ and have uniformly bounded internal energies. Hence (113) passes their tested current densities to the limit as $j \to \infty$. Combining this with the assumed distributional convergence of $\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}_j}$ gives

$$\left|\int_{\mathbb{R}^3} \boldsymbol{\zeta}\cdot(\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}^{(m)}} - \mathbf{j}^{\mathrm{c}})\right| \le C_{\boldsymbol{\zeta}}\varepsilon_L(3^m)E^{1/2}.$$

The energies of $\boldsymbol{\Gamma}^{(m)}$ are bounded uniformly in m, so (113) also applies to $\boldsymbol{\Gamma}^{(m)} \to \boldsymbol{\Gamma}$. Letting $m \to \infty$ in the last inequality, and using $\varepsilon_L(3^m) \to 0$ for this fixed L, proves $\int \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} = \int \boldsymbol{\zeta}\cdot\mathbf{j}^{\mathrm{c}}$. This identifies the combined current density in distributions. Since $\boldsymbol{\Gamma} \in \mathcal{D}$, Proposition 4.1 and the mixed-state series (47), which converge in L^1 by normalization and finite energy, show that both $\rho_{\boldsymbol{\Gamma}}$ and $\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}}$ lie in L^1. Hence these distributional identities hold almost everywhere, and in particular ρ and $\mathbf{j}^{\mathrm{c}}$ are integrable functions. This completes (123).

Step 5. Sufficient photon-number conditions. On the input k-photon sector, $\mathcal{U}_R$ takes values in the sum of retained/discarded sectors with $p + q = k$. Since $p \le k$,

$$\mathcal{U}_R^\dagger(\mathbb{1}_{\{\mathcal{N}>M\}}\otimes\mathbb{1})\mathcal{U}_R \le \mathbb{1}_{\{\mathcal{N}>M\}}.$$

Taking the trace against $\boldsymbol{\Gamma}_j$ and then the indicated limits gives

$$\sup_{m\ge1}\limsup_{j\to\infty}\mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\mathcal{L}_{3^m}\boldsymbol{\Gamma}_j\right) \le \sup_j \mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\boldsymbol{\Gamma}_j\right).$$

Uniform tails on the right therefore imply (122). If the mean photon numbers are uniformly bounded, the spectral inequality $\mathbb{1}_{\{\mathcal{N}>M\}} \le \mathcal{N}/(M+1)$ for integers $M \ge 0$ gives

$$\sup_j \mathrm{Tr}\left(\mathbb{1}_{\{\mathcal{N}>M\}}\boldsymbol{\Gamma}_j\right) \le \frac{\sup_j \mathrm{Tr}(\mathcal{N}\boldsymbol{\Gamma}_j)}{M+1} \longrightarrow 0,$$

which proves the final assertion. □

5.7. **Soft photon removal lemma.** In this section, we prove Lemma 5.8, which is a central technical ingredient in the proofs of mixed-state attainment, soft-photon purification, and infrared bounds on optimizers.

First, we split the photon space into soft- and hard-photon parts. For $\kappa > 0$, let

$$\mathfrak{H}_{\ge\kappa} = \mathbb{1}_{\{\omega\ge\kappa\}}\mathfrak{H}_{\mathrm{ph}}, \qquad \mathfrak{H}_{<\kappa} = \mathbb{1}_{\{\omega<\kappa\}}\mathfrak{H}_{\mathrm{ph}}$$

be the hard and soft one-photon spaces, so that $\mathfrak{H}_{\mathrm{ph}} = \mathfrak{H}_{\ge\kappa} \oplus \mathfrak{H}_{<\kappa}$, and let $\mathcal{F}_{\ge\kappa} = \mathcal{F}_s(\mathfrak{H}_{\ge\kappa})$ and $\mathcal{F}_{<\kappa} = \mathcal{F}_s(\mathfrak{H}_{<\kappa})$. The exponential law for Fock spaces gives the factorization

$$\mathcal{H}_N \simeq \mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa} \otimes \mathcal{F}_{<\kappa}.$$

Accordingly, $\mathfrak{A}^\mu(\mathbf{x}) = \mathfrak{A}^\mu_{\ge\kappa}(\mathbf{x}) + \mathfrak{A}^\mu_{<\kappa}(\mathbf{x})$, where $\mathfrak{A}^\mu_{\ge\kappa}(\mathbf{x}) = \Phi(\mathbb{1}_{\{\omega\ge\kappa\}}G^\mu_{\mathbf{x}})$ acts on $\mathcal{F}_{\ge\kappa}$ and $\mathfrak{A}^\mu_{<\kappa}(\mathbf{x}) = \Phi(\mathbb{1}_{\{\omega<\kappa\}}G^\mu_{\mathbf{x}})$ acts on $\mathcal{F}_{<\kappa}$. Similarly, $H_{\mathrm{rad}} = H_{\mathrm{rad},\ge\kappa} + H_{\mathrm{rad},<\kappa}$ with

$$H_{\mathrm{rad},\ge\kappa} = \mathrm{d}\Gamma(\omega\mathbb{1}_{\{\omega\ge\kappa\}}), \qquad H_{\mathrm{rad},<\kappa} = \mathrm{d}\Gamma(\omega\mathbb{1}_{\{\omega<\kappa\}}).$$

The *hard model* is the internal Pauli–Fierz Hamiltonian $H^{0,0}_{\geq\kappa}$ on $\mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_{\geq\kappa}$ with field $\mathfrak{A}_{\geq\kappa}$ and radiation energy $H_{\mathrm{rad},\geq\kappa}$. The restricted form factor still satisfies (9), so the form construction above applies to it. The notation $\mathrm{Tr}_{\mathrm{el},<\kappa}\,\boldsymbol{\Gamma}$ denotes the partial trace over the electronic and soft-photon factors, leaving the reduced state on $\mathcal{F}_{\geq\kappa}$. Similarly, $\mathrm{Tr}_{<\kappa}$ denotes the partial trace over $\mathcal{F}_{<\kappa}$ alone, leaving an operator on $\mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_{\geq\kappa}$. We write $\Omega_{<\kappa}$ for the normalized vacuum in $\mathcal{F}_{<\kappa}$, so that $|\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|$ is the state with no photons in the modes $\omega < \kappa$.

We are now in a position to state and prove the main result of this section.

Lemma 5.8 (Exact soft-photon removal)**.** *Fix $N \in \mathbb{N}$. For every $\boldsymbol{\Gamma} \in \mathcal{D}$ and $0 < \kappa \leq 1$, there is a $\boldsymbol{\Gamma}_\kappa \in \mathcal{D}$ with $\rho_{\boldsymbol{\Gamma}_\kappa} = \rho_{\boldsymbol{\Gamma}}$ and $\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}_\kappa} = \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}}$, and with photon marginal*

$$\mathrm{Tr}_{\mathrm{el}}\,\boldsymbol{\Gamma}_\kappa = \big(\mathrm{Tr}_{\mathrm{el},<\kappa}\,\boldsymbol{\Gamma}\big) \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|. \tag{126}$$

Put $E_< = \mathrm{Tr}(H_{\mathrm{rad},<\kappa}\boldsymbol{\Gamma})$. There exists a constant C, independent of $\boldsymbol{\Gamma}$ and κ (but allowed to depend on N), such that

$$\begin{aligned}\mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}_\kappa\big) \leq \mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}\big) - E_< \\ + C\Big(\kappa^2 + e^2 b_\kappa^2 + e\kappa\sqrt{a_\kappa^2 E_< + b_\kappa^2} + e^2\kappa^2\big(a_\kappa^2 E_< + b_\kappa^2\big)\Big).\end{aligned} \tag{127}$$

In particular, $\mathrm{Tr}(\mathcal{N}\boldsymbol{\Gamma}_\kappa) \leq \kappa^{-1}\,\mathrm{Tr}(H_{\mathrm{rad}}\boldsymbol{\Gamma})$.

The quantities a_κ, b_κ defined in (71) both tend to zero as $\kappa \downarrow 0$.

Proof. Replacing the soft photons by the vacuum removes their radiation energy $E_<$, but it also removes the contribution of the soft field to the combined current density, so by itself it would violate the current constraint. We compensate for this loss by converting the field-induced current density carried by the soft photons into an equal paramagnetic current density. The components of the soft field commute, so we can condition on their values u. For each u, the soft field becomes a classical vector potential $\mathbf{a}_u$ that varies on the scale κ^{-1}. After the electrons are localized into clusters of diameter $O(R)$, the field $\mathbf{a}_u$ is nearly constant on each cluster. Its constant part is removed exactly by a suitable gauge transformation in the electronic variables. The small remainder is removed by the current shift of Lemma C.2, at a kinetic cost controlled by κR and the infrared quantities a_κ, b_κ.

Step 1. Electronic localization. Fix a cluster scale $1 \leq R \leq \kappa^{-1}$, to be chosen in Step 6. Choose a locally finite smooth partition $(\eta_a)_{a\in\mathbb{N}}$ on $\mathbb{R}^3$ with $\sum_a \eta_a^2 = 1$, $\operatorname{supp}\eta_a \subset B(c_a, c_0 R)$, and $\sum_a |\boldsymbol{\nabla}\eta_a|^2 \leq C/R^2$. For each multi-index $\alpha = (\alpha_1, \dots, \alpha_N) \in \mathbb{N}^N$ with $\alpha_1 \leq \cdots \leq \alpha_N$, let $\mathscr{S}_N\alpha$ be the set of its distinct rearrangements $(\alpha_{\pi(1)}, \dots, \alpha_{\pi(N)})$, $\pi \in \mathscr{S}_N$, and put

$$\zeta_\alpha(\mathbf{X}) = \left(\sum_{(a_1,\dots,a_N)\in\mathscr{S}_N\alpha} \prod_{i=1}^N \eta_{a_i}(\mathbf{x}_i)^2\right)^{1/2}.$$

These are real symmetric $W^{1,\infty}$ multipliers. Since $\mathbb{N}^N$ is the disjoint union of the sets $\mathscr{S}_N\alpha$, expanding $\prod_{i=1}^N \sum_a \eta_a(\mathbf{x}_i)^2 = 1$ gives $\sum_\alpha \zeta_\alpha^2 = 1$. Moreover, ζ_α is the Euclidean norm of the vector $\big(\prod_i \eta_{a_i}(\mathbf{x}_i)\big)_{(a_1,\dots,a_N)\in\mathscr{S}_N\alpha}$, and the gradient of a norm is bounded by the norm of the gradient. Hence

$$\sum_\alpha \sum_{i=1}^N |\boldsymbol{\nabla}_{\mathbf{x}_i}\zeta_\alpha|^2 \leq \sum_{i=1}^N \sum_{(a_1,\dots,a_N)\in\mathbb{N}^N} \Big|\boldsymbol{\nabla}_{\mathbf{x}_i} \prod_{j=1}^N \eta_{a_j}(\mathbf{x}_j)\Big|^2 = \sum_{i=1}^N \sum_a |\boldsymbol{\nabla}\eta_a(\mathbf{x}_i)|^2 \leq \frac{C_N}{R^2}.$$

Set

$$\mathbf{\Gamma}_\alpha = \zeta_\alpha \mathbf{\Gamma} \zeta_\alpha, \qquad E_\alpha = \mathrm{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}_\alpha).$$

All these operators act within the antisymmetric space. Real multiplication and the covariant IMS identity give

$$\sum_\alpha (\rho_{\mathbf{\Gamma}_\alpha}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_\alpha}) = (\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}), \qquad \sum_\alpha \mathrm{Tr}\,\mathbf{\Gamma}_\alpha = 1, \qquad \sum_\alpha E_\alpha = E_<,$$
$$\sum_\alpha \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\alpha\big) \le \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + C/R^2. \tag{128}$$

Here densities, current densities, and form traces are extended linearly to positive trace-class operators of arbitrary finite trace. Whenever current densities are used, the operator is assumed to have finite energy in the relevant model.

Step 2. Conditioning on the soft field. We use the Gaussian representation and the unnormalized conditional operators constructed in Appendix D, with the soft space $\mathfrak{h} = \mathfrak{H}_{<\kappa}$ and $\mathcal{K} = \mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa}$. Under $\mathbb{1}\otimes\mathcal{G}$, the soft field $\mathfrak{A}_{<\kappa}(\mathbf{x})$ becomes multiplication by the real random field $\mathbf{a}_u(\mathbf{x})$ with components

$$a^\mu_u(\mathbf{x}) = \sum_{n\ge1} \langle \xi_n, \mathbb{1}_{\{\omega<\kappa\}} G^\mu_{\mathbf{x}}\rangle\, u_n,$$

where $(\xi_n)_{n\ge1}$ is a J-real orthonormal basis of $\mathfrak{H}_{<\kappa}$ and $u = (u_n)_{n\ge1} \in \mathcal{Q} = \mathbb{R}^{\mathbb{N}}$ carries independent standard Gaussian coordinates. Let $\Theta_\alpha(u)$ be the family $\Theta(u)$ of Lemma D.1 for $\mathbf{\Gamma}_\alpha$. These are unnormalized conditional operators for the electrons and hard photons at the soft-field value u. They satisfy

$$\int_{\mathcal{Q}} \mathrm{Tr}\,\Theta_\alpha(u)\mathrm{d}\mu(u) = \mathrm{Tr}\,\mathbf{\Gamma}_\alpha \le 1,$$

but their individual traces can exceed one. More precisely, for every bounded operator B on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa}$ and every bounded measurable function f on $\mathcal{Q}$,

$$\mathrm{Tr}\left(\mathbf{\Gamma}_\alpha\,(B\otimes\mathcal{G}^{-1}M_f\mathcal{G})\right) = \int_{\mathcal{Q}} f(u)\,\mathrm{Tr}\left(B\Theta_\alpha(u)\right)\mathrm{d}\mu(u), \tag{129}$$

where M_f is multiplication by f on $L^2(\mathcal{Q},\mu)$. Explicitly, if $(\Psi_j)_{j\ge1}$ is an orthonormal basis of $\mathcal{H}_N$, then

$$\Theta_\alpha(u) = \sum_{j\ge1} \big|\big((\mathbb{1}\otimes\mathcal{G})\sqrt{\mathbf{\Gamma}_\alpha}\Psi_j\big)(u)\big\rangle\big\langle\big((\mathbb{1}\otimes\mathcal{G})\sqrt{\mathbf{\Gamma}_\alpha}\Psi_j\big)(u)\big|,$$

where $(\mathbb{1}\otimes\mathcal{G})\sqrt{\mathbf{\Gamma}_\alpha}\Psi_j$ is regarded as an element of $L^2(\mathcal{Q},\mu;\mathfrak{H}_{\mathrm{el}}^N\otimes\mathcal{F}_{\ge\kappa})$. The series converges in trace norm for μ-almost every u, and by Lemma D.1(iii) the result does not depend on the choice of the basis, up to a μ-null set.

The electronic coordinates remain in the union of support balls selected by ζ_α, without assigning fixed particle labels. The unitary $\mathbb{1}\otimes\mathcal{G}$ acts only on the soft factor. It therefore commutes with electronic differentiation and with hard-photon operators, and it maps $\mathfrak{A}_{<\kappa}(\mathbf{x}_i)$ to multiplication by $\mathbf{a}_u(\mathbf{x}_i)$. Writing

$$\mathbf{D}_{i,\ge\kappa} = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_i} - e\mathfrak{A}_{\ge\kappa}(\mathbf{x}_i), \qquad \mathbf{D}_i = \mathbf{D}_{i,\ge\kappa} - e\mathfrak{A}_{<\kappa}(\mathbf{x}_i),$$

we obtain, for μ-almost every u,

$$\big((\mathbb{1}\otimes\mathcal{G})\mathbf{D}_i\Psi\big)(u) = \big(\mathbf{D}_{i,\ge\kappa} - e\mathbf{a}_u(\mathbf{x}_i)\big)\big((\mathbb{1}\otimes\mathcal{G})\Psi\big)(u),$$

first for Ψ in the finite-particle core and then, by the field bounds, for every Ψ in the form domain. Apply this to $\Psi = \sqrt{\mathbf{\Gamma}_\alpha}\Psi_j$, where $(\Psi_j)_{j\ge1}$ is the orthonormal

basis used in the series representation of Θ_α above. For $\Theta = \sum_j |v_j\rangle\langle v_j|$ one has $\sum_j \|Xv_j\|^2 = \|X\sqrt{\Theta}\|_{\mathfrak{S}_2}^2$, so Tonelli's theorem shows that the kinetic energy of $\mathbf{\Gamma}_\alpha$ is exactly

$$\begin{aligned}\frac{1}{2}\sum_{i=1}^N \|\mathbf{D}_i\sqrt{\mathbf{\Gamma}_\alpha}\|_{\mathfrak{S}_2}^2 &= \frac{1}{2}\sum_{i=1}^N\sum_{j\geq 1}\|\mathbf{D}_i\sqrt{\mathbf{\Gamma}_\alpha}\Psi_j\|^2 \\ &= \frac{1}{2}\int_{\mathcal{Q}}\sum_{i=1}^N \|(\mathbf{D}_{i,\geq\kappa} - e\mathbf{a}_u(\mathbf{x}_i))\sqrt{\Theta_\alpha(u)}\|_{\mathfrak{S}_2}^2 \mathrm{d}\mu(u).\end{aligned} \tag{130}$$

We next derive the corresponding formula for the current density. For a positive trace-class operator Θ on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\geq\kappa}$ with $\mathrm{Tr}\big(H_{\geq\kappa}^{0,0}\Theta\big) < \infty$, let $\mathbf{j}^{\mathrm{c}}_{\Theta,\geq\kappa}$ denote the combined current density of Θ in the hard model, defined by (36) with $\mathfrak{A}$ replaced by $\mathfrak{A}_{\geq\kappa}$. Fix $\boldsymbol{\zeta} \in C_c^\infty(\mathbb{R}^3,\mathbb{R}^3)$, let Ψ be in the form domain, and write $\psi_u = ((\mathbb{1}\otimes\mathcal{G})\Psi)(u)$ for its fibers. Integrating (36) against $\boldsymbol{\zeta}$ turns the partial inner product into a full one, and $-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1} - e\mathfrak{A}(\mathbf{x}_1) = \mathbf{D}_{1,\geq\kappa} - e\mathfrak{A}_{<\kappa}(\mathbf{x}_1)$. Hence

$$\begin{aligned}\int_{\mathbb{R}^3}\boldsymbol{\zeta}(\mathbf{x})\cdot\mathbf{j}^{\mathrm{c}}_\Psi(\mathbf{x})\mathrm{d}\mathbf{x} &= N\,\mathrm{Re}\langle\Psi, \boldsymbol{\zeta}(\mathbf{x}_1)\cdot\big(\mathbf{D}_{1,\geq\kappa} - e\mathfrak{A}_{<\kappa}(\mathbf{x}_1)\big)\Psi\rangle \\ &= N\,\mathrm{Re}\int_{\mathcal{Q}}\langle\psi_u, \boldsymbol{\zeta}(\mathbf{x}_1)\cdot\big(\mathbf{D}_{1,\geq\kappa} - e\mathbf{a}_u(\mathbf{x}_1)\big)\psi_u\rangle\mathrm{d}\mu(u) \\ &= \int_{\mathcal{Q}}\int_{\mathbb{R}^3}\boldsymbol{\zeta}(\mathbf{x})\cdot\big(\mathbf{j}^{\mathrm{c}}_{\psi_u,\geq\kappa}(\mathbf{x}) - e\mathbf{a}_u(\mathbf{x})\rho_{\psi_u}(\mathbf{x})\big)\mathrm{d}\mathbf{x}\,\mathrm{d}\mu(u).\end{aligned}$$

The second line uses the unitarity of $\mathbb{1}\otimes\mathcal{G}$, which commutes with $\boldsymbol{\zeta}(\mathbf{x}_1)$, and the fiberwise identity for $\mathbf{D}_1$ above. In the third line, the hard part is the hard-model current density of ψ_u tested against $\boldsymbol{\zeta}$. For the soft part, $\mathbf{a}_u(\mathbf{x}_1)$ is real, so $N\,\mathrm{Re}\langle\psi_u, \boldsymbol{\zeta}(\mathbf{x}_1)\cdot\mathbf{a}_u(\mathbf{x}_1)\psi_u\rangle = \int_{\mathbb{R}^3}\boldsymbol{\zeta}\cdot\mathbf{a}_u\,\rho_{\psi_u}$ by (33). Densities and current densities are linear in the state. Apply the last identity to $\Psi = \sqrt{\mathbf{\Gamma}_\alpha}\Psi_j$ and sum over j. By (20), applied to $\mathfrak{A}_{\geq\kappa}$ and $\mathfrak{A}_{<\kappa}$, the resulting integrand $\mathbf{j}^{\mathrm{c}}_{\Theta_\alpha(u),\geq\kappa}(\mathbf{x}) - e\rho_{\Theta_\alpha(u)}(\mathbf{x})\mathbf{a}_u(\mathbf{x})$ is integrable over $\mathbb{R}^3\times\mathcal{Q}$, which justifies exchanging the sum with the integrals. Since $\boldsymbol{\zeta}$ is arbitrary, Fubini's theorem and the fundamental lemma of the calculus of variations give

$$\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_\alpha}(\mathbf{x}) = \int_{\mathcal{Q}}\big(\mathbf{j}^{\mathrm{c}}_{\Theta_\alpha(u),\geq\kappa}(\mathbf{x}) - e\rho_{\Theta_\alpha(u)}(\mathbf{x})\mathbf{a}_u(\mathbf{x})\big)\mathrm{d}\mu(u) \qquad \text{for a.e. } \mathbf{x}\in\mathbb{R}^3. \tag{131}$$

Since $\mathbb{1}_{\{\omega<\kappa\}}G^\mu_{\mathbf{x}}$ has norms at most those of $G^\mu_{\mathbf{x}}$, the estimates (18) and (19) and hence (20) also hold for the removed field $\mathfrak{A}_{<\kappa}(\mathbf{x})$. As $\mathbf{D}_{i,\geq\kappa} = \mathbf{D}_i + e\mathfrak{A}_{<\kappa}(\mathbf{x}_i)$ and $\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\alpha\big) < \infty$, this gives

$$\sum_{i=1}^N\|\mathbf{D}_{i,\geq\kappa}\sqrt{\mathbf{\Gamma}_\alpha}\|_{\mathfrak{S}_2}^2 \leq 2\sum_{i=1}^N\|\mathbf{D}_i\sqrt{\mathbf{\Gamma}_\alpha}\|_{\mathfrak{S}_2}^2 + 2e^2NC_\chi\big(\mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}_\alpha) + \mathrm{Tr}\,\mathbf{\Gamma}_\alpha\big) < \infty.$$

The computation leading to (130), with $\mathbf{D}_i$ replaced by $\mathbf{D}_{i,\geq\kappa}$, and the fact that $H_{\mathrm{rad},\geq\kappa}$ acts only on $\mathcal{F}_{\geq\kappa}$ therefore give

$$\int_{\mathcal{Q}}\Big(\sum_{i=1}^N\|\mathbf{D}_{i,\geq\kappa}\sqrt{\Theta_\alpha(u)}\|_{\mathfrak{S}_2}^2 + \mathrm{Tr}(H_{\mathrm{rad},\geq\kappa}\Theta_\alpha(u))\Big)\mathrm{d}\mu(u) < \infty.$$

The Coulomb interaction $W = \sum_{n<m} |\mathbf{x}_n - \mathbf{x}_m|^{-1}$ acts only on the electronic variables and hence commutes with $\mathbb{1} \otimes \mathcal{G}$. The argument leading to (130) therefore gives

$$\operatorname{Tr}(W\mathbf{\Gamma}_\alpha) = \int_{\mathcal{Q}} \operatorname{Tr}\big(W\Theta_\alpha(u)\big)\mathrm{d}\mu(u).$$

Together, these estimates show that $\operatorname{Tr}\Big(H^{0,0}_{\geq\kappa}\Theta_\alpha(u)\Big) < \infty$ for almost every u. For $\operatorname{Tr}\Theta_\alpha(u) > 0$, the density matrix $\Theta_\alpha(u)/\operatorname{Tr}\Theta_\alpha(u)$ has finite hard-model energy. The operations applied to $\Theta_\alpha(u)$ in Step 4, namely multiplication by a phase of modulus one and the current shift of Lemma C.2, leave $\operatorname{Tr}(W\Theta_\alpha(u))$ unchanged. Hence only the kinetic and radiation energies change in the remaining steps.

Step 3. Local bounds on the measured field. Fix a multi-index β and $\mathbf{x} \in \mathbb{R}^3$. The differentiated soft field $\partial^\beta_{\mathbf{x}}\mathfrak{A}^\mu_{<\kappa}(\mathbf{x})$ is the Segal field with kernel $\partial^\beta_{\mathbf{x}}(\mathbb{1}_{\{\omega<\kappa\}}G^\mu_{\mathbf{x}}) = (-\mathrm{i}\mathbf{k})^\beta \mathbb{1}_{\{\omega<\kappa\}}G^\mu_{\mathbf{x}}$. Since $|\mathbf{k}| < \kappa$ on the soft region, the projector identity behind (14) gives

$$\sum_{\mu=1}^{3} \Big\| \frac{(-\mathrm{i}\mathbf{k})^\beta \mathbb{1}_{\{\omega<\kappa\}} G^\mu_{\mathbf{x}}}{\sqrt{\omega}} \Big\|^2 \leq \kappa^{2|\beta|} a_\kappa^2, \qquad \sum_{\mu=1}^{3} \big\| (-\mathrm{i}\mathbf{k})^\beta \mathbb{1}_{\{\omega<\kappa\}} G^\mu_{\mathbf{x}} \big\|^2 \leq \kappa^{2|\beta|} b_\kappa^2,$$

with a_κ, b_κ as in (71). These kernels are soft, that is, they vanish for $\omega \geq \kappa$, so (18) and (19) hold with $H_{\mathrm{rad},<\kappa}$ in place of H_{rad} and give

$$\sum_{\mu=1}^{3} \|\partial^\beta_{\mathbf{x}}\mathfrak{A}^\mu_{<\kappa}(\mathbf{x})\Psi\|^2 \leq C\kappa^{2|\beta|}\big(a_\kappa^2 \|\sqrt{H_{\mathrm{rad},<\kappa}}\Psi\|^2 + b_\kappa^2\|\Psi\|^2\big).$$

Apply this to $\Psi = \sqrt{\mathbf{\Gamma}_\alpha}\Psi_j$ and sum over j. Then use (129) with $B = \mathbb{1}$ and the unbounded function $f(u) = |\partial^\beta \mathbf{a}_u(\mathbf{x})|^2$, to which the identity extends by monotone convergence. As $E_\alpha = \operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}_\alpha)$, we obtain

$$\int_{\mathcal{Q}} \operatorname{Tr}\Theta_\alpha(u)|\partial^\beta \mathbf{a}_u(\mathbf{x})|^2 \mathrm{d}\mu(u) \leq C_\beta \kappa^{2|\beta|}\big(a_\kappa^2 E_\alpha + b_\kappa^2 \operatorname{Tr}\mathbf{\Gamma}_\alpha\big), \tag{132}$$

uniformly in $\mathbf{x}$ and α. The fields have smooth versions locally: this follows from these Gaussian derivative moments and local Sobolev embedding, and remains true under the measures $\operatorname{Tr}\Theta_\alpha(u)\mathrm{d}\mu(u)$.

For a fixed α, every electron in $\mathbf{\Gamma}_\alpha$ lies in one of the balls $B(c_{\alpha_i}, c_0 R)$. Consider the graph whose vertices are the distinct centers among $c_{\alpha_1}, \ldots, c_{\alpha_N}$, two centers being joined by an edge if their distance is at most $4c_0R$. We call the vertex sets of its connected components the *clusters* of α and index them by s. A cluster has at most N centers, so its diameter is at most $4(N-1)c_0R \leq C_N R$, while centers in different clusters are more than $4c_0R$ apart. The measured soft field varies on the scale $\kappa^{-1} \geq R$, so in Step 4 it will be replaced on each cluster by a constant. Choose one center of each cluster as its anchor $c_{\alpha,s}$. The construction is illustrated in Fig. 2. Let $\theta_a = 1$ on a neighborhood of $B(c_a, c_0R)$, with $\operatorname{supp}\theta_a \subset B(c_a, 3c_0R/2)$ and $|\nabla\theta_a| \leq C/R$, and define the cluster cutoff

$$\theta_{\alpha,s} = 1 - \prod_{a \text{ in cluster } s} (1 - \theta_a).$$

Then

$$\theta_{\alpha,s} = 1 \ \text{ on } \bigcup_{a \text{ in cluster } s} B(c_a, c_0 R), \qquad \operatorname{supp}\theta_{\alpha,s} \subset \bigcup_{a \text{ in cluster } s} B(c_a, 3c_0 R/2),$$
$$|\boldsymbol{\nabla}\theta_{\alpha,s}| \le \frac{C_N}{R}.$$

Since centers in different clusters are more than $4c_0R$ apart, the supports of $\theta_{\alpha,s}$ for different s are disjoint. Let $\mathcal{B}_{\alpha,s}$ be a ball centered at $c_{\alpha,s}$ of radius $C_N R$ containing $\operatorname{supp}\theta_{\alpha,s}$. All constants are independent of the separation between clusters. Put $Z_\alpha(u) = \max_s \sup_{\mathcal{B}_{\alpha,s}} |\boldsymbol{\nabla}\mathbf{a}_u|$. For a ball $B \subset \mathbb{R}^3$ of radius r and $f \in H^2(B)$, the Sobolev inequality

$$\sup_B |f|^2 \le C \sum_{|\beta|\le 2} r^{2|\beta|-3} \int_B |\partial^\beta f|^2 \mathrm{d}\mathbf{x}$$

holds with C independent of r. Apply it with $r = C_N R$ to the components of $\boldsymbol{\nabla}\mathbf{a}_u$ on each $\mathcal{B}_{\alpha,s}$, multiply by $\operatorname{Tr}\Theta_\alpha(u)$, and integrate over u. By (132) for multi-indices of order $|\beta|+1$, and since $|\mathcal{B}_{\alpha,s}| \le CR^3$, this yields

$$\begin{aligned}\int_{\mathcal{Q}} \operatorname{Tr}\Theta_\alpha(u) Z_\alpha(u)^2 \mathrm{d}\mu(u) &\le C \sum_s \sum_{|\beta|\le 2} R^{2|\beta|-3} \int_{\mathcal{B}_{\alpha,s}} \int_{\mathcal{Q}} \operatorname{Tr}\Theta_\alpha(u) |\partial^\beta \boldsymbol{\nabla}\mathbf{a}_u|^2 \mathrm{d}\mu(u)\mathrm{d}\mathbf{x} \\ &\le C\kappa^2 \big(a_\kappa^2 E_\alpha + b_\kappa^2 \operatorname{Tr}\boldsymbol{\Gamma}_\alpha\big),\end{aligned}$$

because $\kappa R \le 1$ and there are at most N clusters (the constant may depend on N). No global supremum of the random field is used.

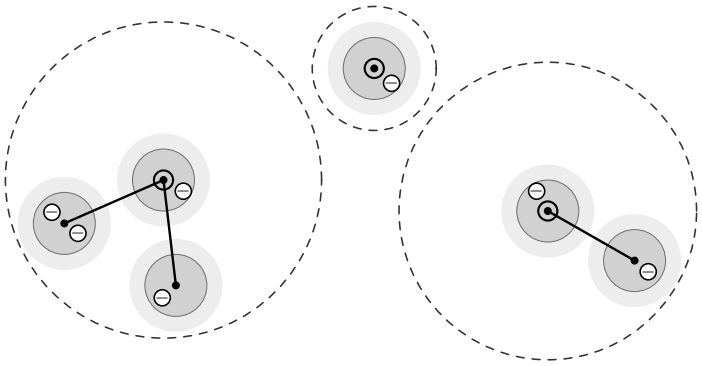


FIGURE 2. The clusters of a multi-index α ($N = 7$, $\alpha_1 = \alpha_2$). Centers at distance at most $4c_0R$ are joined. Anchors are ringed and the balls $\mathcal{B}_{\alpha,s}$ are dashed.

Step 4. Current shift on each conditional state. For almost every u, define the one-body phase and residual velocity

$$\varphi_{\alpha,u}(\mathbf{x}) = -e \sum_s \theta_{\alpha,s}(\mathbf{x}) \mathbf{a}_u(c_{\alpha,s}) \cdot (\mathbf{x} - c_{\alpha,s}),$$
$$\mathbf{v}_{\alpha,u}(\mathbf{x}) = -e \sum_s \theta_{\alpha,s}(\mathbf{x}) \big(\mathbf{a}_u(\mathbf{x}) - \mathbf{a}_u(c_{\alpha,s})\big).$$

In the electronic variables, let $U_{\alpha,u}$ be multiplication by the permutation-symmetric phase

$$\exp\Big(\mathrm{i}\sum_{i=1}^{N}\varphi_{\alpha,u}(\mathbf{x}_i)\Big).$$

First replace $\Theta_\alpha(u)$ by $U_{\alpha,u}\Theta_\alpha(u)U_{\alpha,u}^\dagger$. This leaves the density and the photon marginal unchanged and adds $\rho_{\Theta_\alpha(u)}\boldsymbol{\nabla}\varphi_{\alpha,u}$ to the current density. Where $\theta_{\alpha,s}=1$, the velocity $\boldsymbol{\nabla}\varphi_{\alpha,u}=-e\mathbf{a}_u(c_{\alpha,s})$ is constant, and $\boldsymbol{\nabla}\varphi_{\alpha,u}+\mathbf{v}_{\alpha,u}=-e\mathbf{a}_u$. Next apply Lemma C.2 with velocity $\mathbf{v}_{\alpha,u}$ to the hard model $H^{0,0}_{\geq\kappa}$ instead of $H^{0,0}$. Its proof applies verbatim, since the multipliers act only on the electronic variables. If $\operatorname{Tr}\Theta_\alpha(u)=0$, set $\widetilde{\Theta}_\alpha(u)=0$. Positivity gives $\Theta_\alpha(u)=0$ in this case. If $\operatorname{Tr}\Theta_\alpha(u)>0$, apply it to the normalized state $U_{\alpha,u}\Theta_\alpha(u)U_{\alpha,u}^\dagger/\operatorname{Tr}\Theta_\alpha(u)$, multiply the result by $\operatorname{Tr}\Theta_\alpha(u)$, and call the resulting operator $\widetilde{\Theta}_\alpha(u)$. Its current density is $\mathbf{j}^{\mathrm{c}}_{\Theta_\alpha(u),\geq\kappa}-e\rho_{\Theta_\alpha(u)}\mathbf{a}_u$, the integrand in (131), while

$$\|\mathbf{v}_{\alpha,u}\|_\infty\leq CeRZ_\alpha(u),\qquad \|\boldsymbol{\nabla}\mathbf{v}_{\alpha,u}\|_\infty\leq CeZ_\alpha(u).$$

The wavenumber chosen in the proof of Lemma C.2 depends measurably on $\mathbf{v}_{\alpha,u}$. When the velocity vanishes, use the identity channel. The tensor lift is fixed independently of the velocity, so this defines a measurable family of channels. The kinetic remainder on an unnormalized conditional operator is bounded by

$$C\operatorname{Tr}\Theta_\alpha(u)(\|\mathbf{v}_{\alpha,u}\|_\infty^2+\|\boldsymbol{\nabla}\mathbf{v}_{\alpha,u}\|_\infty).$$

We now compare the hard-model kinetic energy of the output with the integrand of (130), that is, we estimate

$$\delta_\alpha(u)=\frac{1}{2}\sum_{i=1}^{N}\Big\|\mathbf{D}_{i,\geq\kappa}\sqrt{\widetilde{\Theta}_\alpha(u)}\Big\|_{\mathfrak{S}_2}^2-\frac{1}{2}\sum_{i=1}^{N}\Big\|(\mathbf{D}_{i,\geq\kappa}-e\mathbf{a}_u(\mathbf{x}_i))\sqrt{\Theta_\alpha(u)}\Big\|_{\mathfrak{S}_2}^2.$$

The phase is exact: since $\mathbf{D}_{i,\geq\kappa}U_{\alpha,u}=U_{\alpha,u}(\mathbf{D}_{i,\geq\kappa}+\boldsymbol{\nabla}\varphi_{\alpha,u}(\mathbf{x}_i))$, it replaces $\mathbf{D}_{i,\geq\kappa}$ by $\mathbf{D}_{i,\geq\kappa}+\boldsymbol{\nabla}\varphi_{\alpha,u}(\mathbf{x}_i)$. By (241), the current shift then adds

$$\int_{\mathbb{R}^3}\mathbf{j}^{\mathrm{c}}_{U_{\alpha,u}\Theta_\alpha(u)U_{\alpha,u}^\dagger,\geq\kappa}\cdot\mathbf{v}_{\alpha,u},$$

the hard-model current density of $U_{\alpha,u}\Theta_\alpha(u)U_{\alpha,u}^\dagger$ paired with $\mathbf{v}_{\alpha,u}$, plus the kinetic remainder. For the square completion, abbreviate $\Theta=\Theta_\alpha(u)$, $\mathbf{g}=\boldsymbol{\nabla}\varphi_{\alpha,u}$, $\mathbf{v}=\mathbf{v}_{\alpha,u}$, and $\mathbf{D}_i^{\mathrm{h}}=\mathbf{D}_{i,\geq\kappa}$. The phase-transformed current is $\mathbf{j}^{\mathrm{c}}_{\Theta,\geq\kappa}+\rho_\Theta\mathbf{g}$, so

$$\begin{aligned}
&\frac{1}{2}\sum_{i=1}^{N}\big\|(\mathbf{D}_i^{\mathrm{h}}+\mathbf{g}(\mathbf{x}_i))\sqrt{\Theta}\big\|_{\mathfrak{S}_2}^2+\int_{\mathbb{R}^3}(\mathbf{j}^{\mathrm{c}}_{\Theta,\geq\kappa}+\rho_\Theta\mathbf{g})\cdot\mathbf{v}\\
&\quad=\frac{1}{2}\sum_{i=1}^{N}\big\|(\mathbf{D}_i^{\mathrm{h}}+\mathbf{g}(\mathbf{x}_i)+\mathbf{v}(\mathbf{x}_i))\sqrt{\Theta}\big\|_{\mathfrak{S}_2}^2-\frac{1}{2}\int_{\mathbb{R}^3}\rho_\Theta|\mathbf{v}|^2\\
&\quad=\frac{1}{2}\sum_{i=1}^{N}\big\|(\mathbf{D}_i^{\mathrm{h}}-e\mathbf{a}_u(\mathbf{x}_i))\sqrt{\Theta}\big\|_{\mathfrak{S}_2}^2-\frac{1}{2}\int_{\mathbb{R}^3}\rho_\Theta|\mathbf{v}|^2.
\end{aligned}$$

The last equality uses $\mathbf{g}+\mathbf{v}=-e\mathbf{a}_u$ on the electronic support. Dropping this nonpositive term and using the bounds on $\mathbf{v}_{\alpha,u}$,

$$\delta_\alpha(u)\leq C\operatorname{Tr}\Theta_\alpha(u)\big(\|\mathbf{v}_{\alpha,u}\|_\infty^2+\|\boldsymbol{\nabla}\mathbf{v}_{\alpha,u}\|_\infty\big)\leq C\operatorname{Tr}\Theta_\alpha(u)\big(e^2R^2Z_\alpha(u)^2+eZ_\alpha(u)\big).$$

Integrate over u. The first term is controlled by the Step 3 bound on the integral of $\operatorname{Tr}\Theta_\alpha(u)Z_\alpha(u)^2$. For the second, the Cauchy–Schwarz inequality, together with $\int_{\mathcal{Q}}\operatorname{Tr}\Theta_\alpha \mathrm{d}\mu = \operatorname{Tr}\mathbf{\Gamma}_\alpha$, gives the same bound under a square root. Hence

$$\int_{\mathcal{Q}} \delta_\alpha(u)\mathrm{d}\mu(u) \le Ce^2\kappa^2R^2\big(a_\kappa^2E_\alpha + b_\kappa^2\operatorname{Tr}\mathbf{\Gamma}_\alpha\big) + Ce\kappa\sqrt{\big(a_\kappa^2E_\alpha + b_\kappa^2\operatorname{Tr}\mathbf{\Gamma}_\alpha\big)\operatorname{Tr}\mathbf{\Gamma}_\alpha}.$$

Thus constant measured fields on each cluster are compensated without a kinetic remainder depending on their magnitude.

Step 5. Assembly. Using $\mathcal{H}_N \simeq \mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa} \otimes \mathcal{F}_{<\kappa}$, define

$$\mathbf{\Gamma}_{\kappa,R} = \sum_\alpha \int_{\mathcal{Q}} \widetilde{\Theta}_\alpha(u) \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}| \mathrm{d}\mu(u).$$

The map $u \mapsto \widetilde{\Theta}_\alpha(u)$ is measurable by Step 4, and the integral converges in trace norm because the conditional operations preserve traces, so that $\operatorname{Tr}\widetilde{\Theta}_\alpha(u) = \operatorname{Tr}\Theta_\alpha(u)$. They also preserve photon marginals. By (129) with $f=1$, $\int_{\mathcal{Q}}\Theta_\alpha\mathrm{d}\mu = \operatorname{Tr}_{<\kappa}\mathbf{\Gamma}_\alpha$, and $\mathbf{\Gamma}_{\kappa,R}$ is therefore a positive trace-class operator with

$$\operatorname{Tr}\mathbf{\Gamma}_{\kappa,R} = \sum_\alpha \operatorname{Tr}\big(\operatorname{Tr}_{<\kappa}\mathbf{\Gamma}_\alpha\big) = \sum_\alpha \operatorname{Tr}\mathbf{\Gamma}_\alpha = 1,$$

and its photon marginal is

$$\sum_\alpha \operatorname{Tr}_{\mathrm{el}}\big(\operatorname{Tr}_{<\kappa}\mathbf{\Gamma}_\alpha\big) \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}| = \big(\operatorname{Tr}_{\mathrm{el},<\kappa}\mathbf{\Gamma}\big) \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|,$$

since $\sum_\alpha \zeta_\alpha^2 = 1$. This is (126). Preparing the soft vacuum adds only its covariant-kinetic contribution $e^2Nb_\kappa^2/2$, and the soft radiation energy $E_<$ is removed. For the constraints, let Θ be a positive trace-class operator on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa}$ with finite hard-model energy, $\operatorname{Tr}\big(H_{\ge\kappa}^{0,0}\Theta\big) < \infty$. Since $\langle\Omega_{<\kappa}, \mathfrak{A}_{<\kappa}^\mu(\mathbf{x})\Omega_{<\kappa}\rangle = 0$, the definitions (33) and (36) give

$$\rho_{\Theta\otimes|\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|} = \rho_\Theta, \qquad \mathbf{j}^{\mathrm{c}}_{\Theta\otimes|\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|} = \mathbf{j}^{\mathrm{c}}_{\Theta,\ge\kappa}.$$

By linearity in the state, Step 4, (131), and (128), for almost every $\mathbf{x}$,

$$\begin{aligned}
\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_{\kappa,R}}(\mathbf{x}) &= \sum_\alpha \int_{\mathcal{Q}} \mathbf{j}^{\mathrm{c}}_{\widetilde{\Theta}_\alpha(u),\ge\kappa}(\mathbf{x})\mathrm{d}\mu(u) \\
&= \sum_\alpha \int_{\mathcal{Q}} \big(\mathbf{j}^{\mathrm{c}}_{\Theta_\alpha(u),\ge\kappa}(\mathbf{x}) - e\rho_{\Theta_\alpha(u)}(\mathbf{x})\mathbf{a}_u(\mathbf{x})\big)\mathrm{d}\mu(u) \\
&= \sum_\alpha \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_\alpha}(\mathbf{x}) = \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}(\mathbf{x}).
\end{aligned}$$

The phase and the current shift leave the density unchanged, and the density depends only on the electronic reduced state. Hence (129) with $f=1$ and (128) give

$$\rho_{\mathbf{\Gamma}_{\kappa,R}} = \sum_\alpha \int_{\mathcal{Q}} \rho_{\Theta_\alpha(u)}\mathrm{d}\mu(u) = \sum_\alpha \rho_{\mathbf{\Gamma}_\alpha} = \rho_{\mathbf{\Gamma}}.$$

Since $\sum_\alpha(a_\kappa^2E_\alpha + b_\kappa^2\operatorname{Tr}\mathbf{\Gamma}_\alpha) = a_\kappa^2E_< + b_\kappa^2$ and, by the Cauchy–Schwarz inequality,

$$\sum_\alpha \sqrt{\big(a_\kappa^2E_\alpha + b_\kappa^2\operatorname{Tr}\mathbf{\Gamma}_\alpha\big)\operatorname{Tr}\mathbf{\Gamma}_\alpha} \le \sqrt{a_\kappa^2E_< + b_\kappa^2},$$

we obtain

$$\begin{aligned}\operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}_{\kappa,R}\bigr) \le \operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}\bigr) - E_< + C\Bigl(R^{-2} + e^2 b_\kappa^2 + e^2\kappa^2 R^2\bigl(a_\kappa^2 E_< + b_\kappa^2\bigr) \\ + e\kappa\sqrt{a_\kappa^2 E_< + b_\kappa^2}\Bigr),\end{aligned} \tag{133}$$

with C independent of $\mathbf{\Gamma}$, κ and R. It also proves finite form energy of the output. Only the output is asserted to have finite full form energy, so no soft-radiation regularity of an intermediate measured state is needed. The marginal identity proves the photon-number bound.

Step 6. Choice of the cluster scale. Only the terms R^{-2} and $e^2\kappa^2R^2(a_\kappa^2E_<+b_\kappa^2)$ in (133) depend on R. Put $q = e\kappa\sqrt{a_\kappa^2E_< + b_\kappa^2} \ge 0$. If $\kappa^2 \le q \le 1$, then $q > 0$, and we choose $R = q^{-1/2} \in [1, \kappa^{-1}]$. The two terms then balance and both equal q. If $q < \kappa^2$, including $q = 0$, take $R = \kappa^{-1}$. Then $e^2(a_\kappa^2E_< + b_\kappa^2) < \kappa^2$, so the two terms add up to less than $2\kappa^2$. If $q > 1$, take $R = 1$. Then the two terms add up to less than $2q^2 = 2e^2\kappa^2(a_\kappa^2E_< + b_\kappa^2)$. In each case, $\mathbf{\Gamma}_\kappa = \mathbf{\Gamma}_{\kappa,R}$ satisfies (127) after changing C. The constant C in (133) does not depend on $\mathbf{\Gamma}$, so R may depend on $E_<$. □

5.8. **The proof of Theorem 4.8.** We remove the soft photons of near-minimizers using Lemma 5.8, which keeps ρ and $\mathbf{j}^c$ fixed at a small energy cost and bounds the mean photon number. Lemma 5.7 then gives a minimizer and lower semicontinuity, and convex conjugation identifies the functional with $F_{\mathrm{PFL}}^{e,\chi}$.

Step 1. Soft energy of near-minimizers. Apply Lemma 5.8, with $H_{\mathrm{rad},<\kappa}$ as defined above. The resulting state $\mathbf{\Gamma}_\kappa$ replaces photons with $\omega < \kappa$ by the vacuum and adjusts the electronic current density so that its density and combined current density agree exactly with those of $\mathbf{\Gamma}$. The estimate (127), together with $\sqrt{s+t} \le \sqrt{s} + \sqrt{t}$ and $\kappa \le 1$, gives

$$\begin{aligned}&\operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}_\kappa\bigr) - \operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}\bigr) + \operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}) \\ &\quad\le C\Bigl[\kappa^2 + e^2b_\kappa^2 + e^2\kappa^2a_\kappa^2\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}) + e\kappa a_\kappa\sqrt{\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma})} + e\kappa b_\kappa\Bigr].\end{aligned}$$

Since $\kappa a_\kappa \to 0$, choose $\kappa_0 \le 1$, depending only on N, e and χ, so the term proportional to $\kappa^2a_\kappa^2\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma})$ can be absorbed by the term $\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma})$ on the left-hand side for $0 < \kappa \le \kappa_0$. Young's inequality absorbs the square-root term as well, giving

$$\operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}_\kappa\bigr) \le \operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}\bigr) - \tfrac{1}{2}\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}) + C_{N,e,\chi}(\kappa^2 + b_\kappa^2). \tag{134}$$

For an exact feasible $\mathbf{\Gamma}$, set $d_{\mathbf{\Gamma}} = \operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}\bigr) - \widetilde{F}_{\mathrm{PFL}}^{e,\chi}(\rho, \mathbf{j}^c)$. The competitor $\mathbf{\Gamma}_\kappa$ has exactly the same constraints. Consequently

$$\operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma}) \le 2d_{\mathbf{\Gamma}} + C_{N,e,\chi}(\kappa^2 + b_\kappa^2), \qquad 0 < \kappa \le \kappa_0. \tag{135}$$

Step 2. A uniformly number-bounded minimizing sequence. For $0 < \kappa < \kappa_0$, the pointwise inequality

$$\mathbb{1}_{\{\omega\ge\kappa\}} \le \frac{\omega}{\kappa_0} + \omega\int_\kappa^{\kappa_0}\frac{\mathbb{1}_{\{\omega<t\}}}{t^2}\mathrm{d}t$$

and (126) imply

$$\operatorname{Tr}(\mathcal{N}\mathbf{\Gamma}_\kappa) \le \frac{\operatorname{Tr}\bigl(H^{0,0}\mathbf{\Gamma}\bigr)}{\kappa_0} + \int_\kappa^{\kappa_0}\frac{\operatorname{Tr}(H_{\mathrm{rad},<t}\mathbf{\Gamma})}{t^2}\mathrm{d}t.$$

The weighted condition $\widehat{\chi}/\sqrt{\omega} \in L^2$ in (9) gives, by Tonelli's theorem,

$$\int_0^{\kappa_0} \frac{b_t^2}{t^2}\mathrm{d}t = \int_{\omega<\kappa_0} |\widehat{\chi}(\mathbf{k})|^2 \left(\frac{1}{\omega(\mathbf{k})} - \frac{1}{\kappa_0}\right) \mathrm{d}\mathbf{k} \leq a_{\kappa_0}^2 < \infty.$$

Thus (135) yields

$$\mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}_\kappa) \leq \frac{\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big)}{\kappa_0} + \frac{2d_{\mathbf{\Gamma}}}{\kappa} + C_{N,e,\chi}. \tag{136}$$

Now take any minimizing sequence $\mathbf{\Gamma}_n \in \mathcal{D}$ with $(\rho_{\mathbf{\Gamma}_n}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_n}) = (\rho, \mathbf{j}^{\mathrm{c}})$, with excess energies $d_n \to 0$, and choose $\kappa_n \to 0$ with $d_n/\kappa_n \to 0$, for example $\kappa_n = \max\{\sqrt{d_n}, 1/n\}$ for all sufficiently large n. Set $\widetilde{\mathbf{\Gamma}}_n = (\mathbf{\Gamma}_n)_{\kappa_n}$, using the output of Lemma 5.8 with the cluster scale chosen in Step 6 of its proof. These states satisfy $(\rho_{\widetilde{\mathbf{\Gamma}}_n}, \mathbf{j}^{\mathrm{c}}_{\widetilde{\mathbf{\Gamma}}_n}) = (\rho, \mathbf{j}^{\mathrm{c}})$ by Lemma 5.8, so $\mathrm{Tr}\Big(H^{0,0}\widetilde{\mathbf{\Gamma}}_n\Big) \geq \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$. For n large enough that $\kappa_n \leq \kappa_0$, dropping the nonpositive term in (134) gives

$$\mathrm{Tr}\Big(H^{0,0}\widetilde{\mathbf{\Gamma}}_n\Big) \leq \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) + d_n + C_{N,e,\chi}\big(\kappa_n^2 + b_{\kappa_n}^2\big).$$

Since $d_n \to 0$, $\kappa_n \to 0$, and $b_\kappa \to 0$ as $\kappa \downarrow 0$, their energies converge to $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$. Moreover, since $d_n/\kappa_n \to 0$ and the energies $\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_n\big)$ are bounded, (136) gives a uniform bound on the mean photon numbers of $\widetilde{\mathbf{\Gamma}}_n$. The fixed density supplies electronic tightness. Hence Lemma 5.7 applies and produces a minimizer $\mathbf{\Gamma} \in \mathcal{D}$ with $(\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}) = (\rho, \mathbf{j}^{\mathrm{c}})$.

Now let $\mathbf{\Gamma}$ be any minimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$, not only the one just constructed. Then $d_{\mathbf{\Gamma}} = 0$. Using the same pointwise inequality and then letting $\kappa \downarrow 0$ in (135) gives

$$\mathrm{Tr}(\mathcal{N}\mathbf{\Gamma}) \leq C_{N,e,\chi}\big(1 + \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})\big). \tag{137}$$

In particular, every optimizer has finite mean photon number.

Step 3. Lower semicontinuity and identification of the functional. Take pairs $(\rho_k, \mathbf{j}^{\mathrm{c}}_k)$ converging in $X \times Y$ along a subsequence on which $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho_k, \mathbf{j}^{\mathrm{c}}_k)$ has finite liminf, and choose the minimizers just constructed. Their energies and mean photon numbers are uniformly bounded by (137). Convergence of their densities in L^1 gives uniform electronic tightness. A further application of Lemma 5.7 preserves the limiting pair and proves the energy liminf inequality. Finally, we identify the functional. Fix $(u, \mathbf{A}) \in X^* \times Y^*$ and put $v = u - \frac{1}{2}|\mathbf{A}|^2$. By linearity in the state, (37) extends to density matrices:

$$\mathrm{Tr}\big(H^{v,\mathbf{A}}\mathbf{\Gamma}\big) = \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \langle u, \rho_{\mathbf{\Gamma}}\rangle + \langle \mathbf{A}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}\rangle, \qquad \mathbf{\Gamma} \in \mathcal{D}.$$

Minimizing first over $\mathbf{\Gamma}$ at fixed $(\rho, \mathbf{j}^{\mathrm{c}})$ and then over $(\rho, \mathbf{j}^{\mathrm{c}})$ gives

$$\inf_{(\rho,\mathbf{j}^{\mathrm{c}})\in X\times Y} \Big[\widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) + \langle u, \rho\rangle + \langle \mathbf{A}, \mathbf{j}^{\mathrm{c}}\rangle\Big] = \inf_{\mathbf{\Gamma}\in\mathcal{D}} \mathrm{Tr}\big(H^{v,\mathbf{A}}\mathbf{\Gamma}\big) = \bar{E}(u, \mathbf{A}).$$

The last equality holds because density matrices and pure states have the same spectral infimum. Indeed, pure states are density matrices, and for a spectral decomposition $\mathbf{\Gamma} = \sum_r p_r |\Psi_r\rangle\langle\Psi_r|$,

$$\mathrm{Tr}\big(H^{v,\mathbf{A}}\mathbf{\Gamma}\big) = \sum_r p_r \langle \Psi_r, H^{v,\mathbf{A}}\Psi_r\rangle \geq E(v, \mathbf{A}).$$

Let $(\widetilde{F}^{e,\chi}_{\mathrm{PFL}})^*$ denote the convex conjugate with respect to the pairing of $X \times Y$ with $X^* \times Y^*$. The identity for the infimum over $X \times Y$ states that $(\widetilde{F}^{e,\chi}_{\mathrm{PFL}})^*(-u, -\mathbf{A}) =$

$-\bar{E}(u,\mathbf{A})$, so the definition (54) reads $F^{e,\chi}_{\mathrm{PFL}} = (\widetilde{F}^{e,\chi}_{\mathrm{PFL}})^{**}$. The functional $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$ is proper, since it is nonnegative and finite at every N-representable pair. It is convex, since $\mathcal{D}$ is convex and $\rho_{\mathbf{\Gamma}}$, $\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}$, and $\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big)$ are linear in $\mathbf{\Gamma}$. The Fenchel–Moreau theorem therefore gives, for any N,

$$F^{e,\chi}_{\mathrm{PFL}} = \overline{\widetilde{F}^{e,\chi}_{\mathrm{PFL}}}^{\,\|\cdot\|_{X\times Y}},$$

the norm-lower-semicontinuous hull of $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$; for convex functions it coincides with the weakly lower semicontinuous hull. Since $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$ is norm lower semicontinuous by the first part of this step, the hull equals $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$, which establishes (58).

5.9. **Soft-photon purification.**

Proof of Theorem 4.10. Fix $\mathbf{\Gamma} \in \mathcal{D}$ and $0 < \kappa \leq 1$. Apply Lemma 5.8 and let $\mathbf{\Gamma}_\kappa$ be its output. This state has exactly the same density and combined current density as $\mathbf{\Gamma}$. Since $a_\kappa, b_\kappa \to 0$ and $E_< \leq \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big)$, (127) gives

$$\limsup_{\kappa\downarrow 0} \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\kappa\big) \leq \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big). \tag{138}$$

Use the Fock factorization into modes with $\omega \geq \kappa$ and $\omega < \kappa$, and let $Q = 1 \otimes \big(1 - |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|\big)$ be the projection onto states with at least one soft photon. By (126), the soft marginal of $\mathbf{\Gamma}_\kappa$ is $|\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|$, so $\mathrm{Tr}(Q\mathbf{\Gamma}_\kappa Q) = \mathrm{Tr}(\mathbf{\Gamma}_\kappa Q) = 0$. Since $\mathbf{\Gamma}_\kappa \geq 0$, the operator $Q\mathbf{\Gamma}_\kappa Q$ is positive with zero trace, hence zero. Thus $\mathbf{\Gamma}_\kappa^{1/2} Q = 0$, so $\mathbf{\Gamma}_\kappa Q = Q\mathbf{\Gamma}_\kappa = 0$ and $\mathbf{\Gamma}_\kappa = (1-Q)\mathbf{\Gamma}_\kappa(1-Q)$. This is the product decomposition

$$\mathbf{\Gamma}_\kappa = \gamma_\kappa \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|, \qquad \gamma_\kappa = \sum_r p_r |\Phi_r\rangle\langle\Phi_r|, \qquad p_r > 0, \quad \sum_r p_r = 1.$$

Here (Φ_r) is orthonormal in $\mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_{\geq\kappa}$, and each Φ_r is antisymmetric in the electronic coordinates. Let $H^{0,0}_{\geq\kappa}$ be the hard model introduced before Lemma 5.8, and put $\mathbf{D}_{n,\geq\kappa} = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\mathfrak{A}_{\geq\kappa}(\mathbf{x}_n)$. The soft-vacuum expectation and (14) give the exact identity

$$\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\kappa\big) = \sum_r p_r \langle \Phi_r, H^{0,0}_{\geq\kappa}\Phi_r\rangle + \frac{Ne^2}{2} b_\kappa^2. \tag{139}$$

In particular, every Φ_r is in the hard-model form domain and the displayed sum of nonnegative form energies is finite.

The soft one-photon space $\mathfrak{H}_{<\kappa}$ is infinite dimensional. Choose an orthonormal family (f_r) in it, write $\eta_r = a^\dagger(f_r)\Omega_{<\kappa}$, and consider

$$\Psi_\kappa = \sum_r \sqrt{p_r}\, \Phi_r \otimes \eta_r. \tag{140}$$

The vectors $\Phi_r \otimes \eta_r$ are orthonormal, so the series (140) converges in norm to a unit vector. We show that it also converges in the form norm of $H^{0,0}$, so that Ψ_κ lies in its form domain $\mathcal{Q}_{\mathrm{PF}}$.

Each term of the series has exactly one soft photon. Identify $\mathfrak{H}_{<\kappa}$ with the one-photon sector of $\mathcal{F}_{<\kappa}$, and let $\Psi \in \mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_{\geq\kappa} \otimes \mathfrak{H}_{<\kappa}$. For almost every $\mathbf{X} = (\mathbf{x}_1, \ldots, \mathbf{x}_N)$, the value $\Psi(\mathbf{X})$ lies in $\mathcal{F}_{\geq\kappa} \otimes \mathfrak{H}_{<\kappa}$, and $\mathfrak{A}^\mu_{<\kappa}(\mathbf{x}_n)$ acts on it as $a^\dagger(g) + a(g)$ on the soft factor, with $g = \mathbb{1}_{\{\omega<\kappa\}} G^\mu_{\mathbf{x}_n}$. The vector $a^\dagger(g)\Psi(\mathbf{X})$ has two soft photons and $a(g)\Psi(\mathbf{X})$ has none, so these two vectors are orthogonal. Together

with the CCR $\|a^\dagger(g)\Psi(\mathbf{X})\|^2 = \|g\|^2\|\Psi(\mathbf{X})\|^2 + \|a(g)\Psi(\mathbf{X})\|^2$ and $\|a(g)\Psi(\mathbf{X})\| \le \|g\|\|\Psi(\mathbf{X})\|$, this gives

$$\|[a^\dagger(g) + a(g)]\Psi(\mathbf{X})\|^2 = \|g\|^2\|\Psi(\mathbf{X})\|^2 + 2\|a(g)\Psi(\mathbf{X})\|^2 \le 3\|g\|^2\|\Psi(\mathbf{X})\|^2.$$

By (14) restricted to $\{\omega < \kappa\}$, the sum of $\|g\|^2$ over μ is b_κ^2. Summing over μ and n and integrating over $\mathbf{X}$ therefore gives

$$\sum_{n=1}^N \|\mathfrak{A}_{<\kappa}(\mathbf{x}_n)\Psi\|^2 \le 3Nb_\kappa^2\|\Psi\|^2. \tag{141}$$

Consider a finite partial sum $\Psi_I = \sum_{r\in I}\sqrt{p_r}\,\Phi_r \otimes \eta_r$. Both Ψ_I and $\mathbf{D}_{n,\ge\kappa}\Psi_I$ have exactly one soft photon, while $\mathfrak{A}_{<\kappa}(\mathbf{x}_n)\Psi_I$ has zero or two. Since $\mathbf{D}_n = \mathbf{D}_{n,\ge\kappa} - e\mathfrak{A}_{<\kappa}(\mathbf{x}_n)$, it follows that

$$\langle \mathbf{D}_{n,\ge\kappa}\Psi_I, \mathfrak{A}_{<\kappa}(\mathbf{x}_n)\Psi_I\rangle = 0, \qquad \|\mathbf{D}_n\Psi_I\|^2 = \|\mathbf{D}_{n,\ge\kappa}\Psi_I\|^2 + e^2\|\mathfrak{A}_{<\kappa}(\mathbf{x}_n)\Psi_I\|^2.$$

Since the tags η_r are orthonormal, tracing out the soft photons gives

$$\mathrm{Tr}_{<\kappa}\,|\Psi_I\rangle\langle\Psi_I| = \sum_{r\in I} p_r|\Phi_r\rangle\langle\Phi_r|. \tag{142}$$

The hard model $H^{0,0}_{\ge\kappa}$ acts only on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa}$, so

$$\langle\Psi_I, H^{0,0}_{\ge\kappa}\Psi_I\rangle = \sum_{r\in I} p_r\langle\Phi_r, H^{0,0}_{\ge\kappa}\Phi_r\rangle.$$

By the identity for $\|\mathbf{D}_n\Psi_I\|^2$, the rest of $\langle\Psi_I, H^{0,0}\Psi_I\rangle$ is $\frac{e^2}{2}\sum_n \|\mathfrak{A}_{<\kappa}(\mathbf{x}_n)\Psi_I\|^2$, which (141) bounds, plus the soft radiation energy. Since $\omega < \kappa$ on $\mathfrak{H}_{<\kappa}$, the latter satisfies $\langle\Psi_I, H_{\mathrm{rad},<\kappa}\Psi_I\rangle \le \kappa\|\Psi_I\|^2 = \kappa\sum_{r\in I} p_r$. Hence

$$\langle\Psi_I, H^{0,0}\Psi_I\rangle \le \sum_{r\in I} p_r\langle\Phi_r, H^{0,0}_{\ge\kappa}\Phi_r\rangle + \left(\kappa + \frac{3Ne^2}{2}b_\kappa^2\right)\sum_{r\in I} p_r. \tag{143}$$

Applying this bound to tails, together with (139), proves convergence of (140) in the full form norm. Hence $\Psi_\kappa \in \mathcal{Q}_{\mathrm{PF}}$ is normalized and retains electronic antisymmetry.

Letting I increase to all indices in (142), by continuity of the partial trace in trace norm, gives

$$\mathrm{Tr}_{<\kappa}\,|\Psi_\kappa\rangle\langle\Psi_\kappa| = \gamma_\kappa = \mathrm{Tr}_{<\kappa}\,\mathbf{\Gamma}_\kappa.$$

So Ψ_κ and $\mathbf{\Gamma}_\kappa$ have the same reduced state on electrons and hard photons.

We next prove that Ψ_κ and $\mathbf{\Gamma}_\kappa$ have the same density and combined current density. Put $\Psi_r^0 = \Phi_r \otimes \Omega_{<\kappa}$, so that $\mathbf{\Gamma}_\kappa = \sum_r p_r|\Psi_r^0\rangle\langle\Psi_r^0|$, and let $\mathbf{\Gamma}_I = \sum_{r\in I} p_r|\Psi_r^0\rangle\langle\Psi_r^0|$. Let $v \in C_c^\infty(\mathbb{R}^3)$ and $\mathbf{A} \in C_c^\infty(\mathbb{R}^3;\mathbb{R}^3)$. Integrating (33) and (36) against v and $\mathbf{A}$ gives, for every $\Psi \in \mathcal{Q}_{\mathrm{PF}}$,

$$\int_{\mathbb{R}^3} v\rho_\Psi = N\langle\Psi, v(\mathbf{x}_1)\Psi\rangle, \qquad \int_{\mathbb{R}^3} \mathbf{A}\cdot\mathbf{j}^{\mathrm{c}}_\Psi = N\,\mathrm{Re}\langle\Psi, \mathbf{A}(\mathbf{x}_1)\cdot\mathbf{D}_1\Psi\rangle. \tag{144}$$

Write $\mathbf{D}_1 = \mathbf{D}_{1,\ge\kappa} - e\mathfrak{A}_{<\kappa}(\mathbf{x}_1)$. The operators $v(\mathbf{x}_1)$ and $\mathbf{A}(\mathbf{x}_1)\cdot\mathbf{D}_{1,\ge\kappa}$ act only on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_{\ge\kappa}$. Since the tags are orthonormal and $\Omega_{<\kappa}$ is normalized,

$$\langle\Psi_I, v(\mathbf{x}_1)\Psi_I\rangle = \sum_{r\in I} p_r\langle\Psi_r^0, v(\mathbf{x}_1)\Psi_r^0\rangle,$$

$$\langle\Psi_I, \mathbf{A}(\mathbf{x}_1)\cdot\mathbf{D}_{1,\ge\kappa}\Psi_I\rangle = \sum_{r\in I} p_r\langle\Psi_r^0, \mathbf{A}(\mathbf{x}_1)\cdot\mathbf{D}_{1,\ge\kappa}\Psi_r^0\rangle.$$

The soft field contributes to neither state. The vector $\mathfrak{A}_{<\kappa}(\mathbf{x}_1)\Psi_I$ has zero or two soft photons while Ψ_I has one, and $\mathfrak{A}_{<\kappa}(\mathbf{x}_1)\Psi_r^0$ has one soft photon while Ψ_r^0 has none. Hence

$$\langle \Psi_I, \mathbf{A}(\mathbf{x}_1)\cdot\mathfrak{A}_{<\kappa}(\mathbf{x}_1)\Psi_I\rangle = \langle \Psi_r^0, \mathbf{A}(\mathbf{x}_1)\cdot\mathfrak{A}_{<\kappa}(\mathbf{x}_1)\Psi_r^0\rangle = 0.$$

By (144) and linearity in the state, the last three displays give

$$\int_{\mathbb{R}^3} v\rho_{\Psi_I} = \int_{\mathbb{R}^3} v\rho_{\mathbf{\Gamma}_I}, \qquad \int_{\mathbb{R}^3} \mathbf{A}\cdot\mathbf{j}^{\mathrm{c}}_{\Psi_I} = \int_{\mathbb{R}^3} \mathbf{A}\cdot\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_I}. \tag{145}$$

Now let I increase to all indices. Then $|\Psi_I\rangle\langle\Psi_I| \to |\Psi_\kappa\rangle\langle\Psi_\kappa|$ and $\mathbf{\Gamma}_I \to \mathbf{\Gamma}_\kappa$ in trace norm. All these operators have trace at most one, and their energies are bounded uniformly in I, by (143) and by $\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_I\big) \le \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\kappa\big)$. Hence (112) and (113) of Lemma 5.2 pass both sides of (145) to the limit. Since v and $\mathbf{A}$ are arbitrary, Ψ_κ and $\mathbf{\Gamma}_\kappa$ have the same density and combined current density. Together with Lemma 5.8, this gives

$$(\rho_{\Psi_\kappa}, \mathbf{j}^{\mathrm{c}}_{\Psi_\kappa}) = (\rho_{\mathbf{\Gamma}_\kappa}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_\kappa}) = (\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}). \tag{146}$$

Passing to the limit in (143) and subtracting the vacuum contribution in (139) gives

$$\langle \Psi_\kappa, H^{0,0}\Psi_\kappa\rangle \le \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_\kappa\big) + \kappa + Ne^2 b_\kappa^2. \tag{147}$$

The last two terms tend to zero as $\kappa \downarrow 0$, since $b_\kappa \to 0$ for every form factor.

Finally, let $\mathcal{N}_{\ge\kappa} = \mathrm{d}\Gamma(\mathbb{1}_{\{\omega\ge\kappa\}})$. The soft tags have exactly one photon, so $\langle\Psi_\kappa, \mathcal{N}\Psi_\kappa\rangle = 1 + \mathrm{Tr}(\mathcal{N}_{\ge\kappa}\gamma_\kappa)$. Tracing (126) over $\mathcal{F}_{<\kappa}$ gives $\mathrm{Tr}_{\mathrm{el},<\kappa}\,\mathbf{\Gamma}_\kappa = \mathrm{Tr}_{\mathrm{el},<\kappa}\,\mathbf{\Gamma}$, so $\mathrm{Tr}(\mathcal{N}_{\ge\kappa}\gamma_\kappa) = \mathrm{Tr}(\mathcal{N}_{\ge\kappa}\mathbf{\Gamma})$. Thus

$$\langle\Psi_\kappa, \mathcal{N}\Psi_\kappa\rangle = 1 + \mathrm{Tr}(\mathcal{N}_{\ge\kappa}\mathbf{\Gamma}) \le 1 + \kappa^{-1}\,\mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}) < \infty. \tag{148}$$

Together, (138), (146) and (147) prove (59) by choosing κ sufficiently small.

Fix $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$, and let $\mathbf{\Gamma} \in \mathcal{D}$ satisfy $(\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}) = (\rho, \mathbf{j}^{\mathrm{c}})$. The pure states in (59) are admissible in (52), so $F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) \le \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \delta$ for every $\delta > 0$. Taking the infimum over $\mathbf{\Gamma}$ and using (57) proves $F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) = \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$. If no such $\mathbf{\Gamma}$ exists, then no admissible pure state exists either, since $|\Psi\rangle\langle\Psi| \in \mathcal{D}$ for every normalized $\Psi \in \mathcal{Q}_{\mathrm{PF}}$. Then $F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) = \widetilde{F}^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) = +\infty$. The equality with $F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$ follows from Theorem 4.8. If $F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty$, equality of the two searches identifies a pure minimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$ with a rank-one minimizer of the total mixed-state problem, in both directions. □

Proof of Corollary 4.11. Properness, convexity, and norm lower semicontinuity follow from (60) and the corresponding properties of $F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}})$. Every pure state defines a rank-one density matrix, and (59) provides, for every mixed state, a finite-energy pure state with the same density and combined current density. This proves the first equality in (61). Since $\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) < \infty$ for every $\mathbf{\Gamma} \in \mathcal{D}$, the middle set in (61) is the domain of $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$, and (58) identifies $\widetilde{F}^{e,\chi}_{\mathrm{PFL}}$ with $F^{e,\chi}_{\mathrm{PFL}}$. This proves the second equality. The pure-state class is therefore the domain of the convex functional $F^{e,\chi}_{\mathrm{PFL}}$, hence convex.

Fix any mixed-state minimizer $\mathbf{\Gamma}_*$ at $(\rho, \mathbf{j}^{\mathrm{c}})$. By Theorem 4.8, it has finite mean photon number. For $0 < \kappa \le 1$, let Ψ_κ be the pure state (140) built from $\mathbf{\Gamma}_*$ in the proof of Theorem 4.10. That is, first remove the soft photons from $\mathbf{\Gamma}_*$ by Lemma 5.8, then attach orthonormal one-photon soft tags to the eigenvectors of

the result. Choose a sequence $\kappa_j \downarrow 0$ and put $\Psi_j = \Psi_{\kappa_j}$. By (146), $(\rho_{\Psi_j}, \mathbf{j}^{\mathrm{c}}_{\Psi_j}) = (\rho_{\mathbf{\Gamma}_*}, \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_*}) = (\rho, \mathbf{j}^{\mathrm{c}})$ for every j. By (138) and (147) and $b_{\kappa_j} \to 0$,

$$\limsup_{j\to\infty} \langle \Psi_j, H^{0,0}\Psi_j\rangle \le \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_*\big) = F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}}),$$

where the equality holds because $\mathbf{\Gamma}_*$ is a minimizer, by (58) and (60). Each Ψ_j is admissible in (52), so $\langle \Psi_j, H^{0,0}\Psi_j\rangle \ge F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}})$, and hence $\langle \Psi_j, H^{0,0}\Psi_j\rangle \to F^{e,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{c}})$. Since $\mathcal{N}_{\ge\kappa_j} \le \mathcal{N}$, (148) and the photon-number bound in Theorem 4.8 give (62). □

Proof of Proposition 4.12. Let Θ be the time reversal (190), with the properties in Proposition A.4, and let $\mathcal{I}_N := \{\rho \ge 0 : \int_{\mathbb{R}^3} \rho = N,\ \sqrt{\rho} \in H^1(\mathbb{R}^3)\}$. We first show that, for either $F \in \{F_{\mathrm{PFLL}}, F_{\mathrm{PFL}}\}$, every $\rho \in \mathcal{I}_N$, and every $\mathbf{j}^{\mathrm{c}} \in Y$,

$$F^{e,\chi}(\rho, \mathbf{j}^{\mathrm{c}}) = F^{e,\chi}(\rho, -\mathbf{j}^{\mathrm{c}}), \qquad F^{e,\chi}(\rho, 0) \le F^{e,\chi}(\rho, \mathbf{j}^{\mathrm{c}}). \tag{149}$$

Evenness of both functionals in the current density is (194). For the PFL functional, convexity then gives

$$F^{e,\chi}_{\mathrm{PFL}}(\rho, 0) \le \frac{1}{2}\big[F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}) + F^{e,\chi}_{\mathrm{PFL}}(\rho, -\mathbf{j}^{\mathrm{c}})\big] = F^{e,\chi}_{\mathrm{PFL}}(\rho, \mathbf{j}^{\mathrm{c}}).$$

This is (149) for F_{PFL}. By (193), $\bar{E}(u, \mathbf{A}) = \bar{E}(u, -\mathbf{A})$, and concavity of $\bar{E}$ gives $\bar{E}(u, \mathbf{A}) \le \bar{E}(u, 0) = E(u, 0)$, proving (65) directly from (54). For the mixed-state search, replace any $\mathbf{\Gamma}$ by $\frac{1}{2}(\mathbf{\Gamma} + \Theta\mathbf{\Gamma}\Theta^{-1})$. This preserves its density and energy and sets its combined current density to zero. Theorem 4.8 then gives (64), including the mixed-state minimum. The minimizing density matrix can be chosen time-reversal invariant. The density bound makes $\rho \in \mathcal{I}_N$ necessary for finiteness. Conversely, every $\rho \in \mathcal{I}_N$ has a finite-kinetic-energy electronic representative [33]. Vacuum embedding and the same averaging then give a finite-energy density matrix at $(\rho, 0)$.

For the PFLL functional, to prove minimality at zero current density, take any normalized $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ with pair $(\rho, \mathbf{j}^{\mathrm{c}})$ and form

$$\mathbf{\Gamma}_\Psi = \frac{1}{2}\big(|\Psi\rangle\langle\Psi| + |\Theta\Psi\rangle\langle\Theta\Psi|\big).$$

This density matrix has pair $(\rho, 0)$ and energy $\langle \Psi, H^{0,0}\Psi\rangle$. For every $\delta > 0$, the approximation statement (59) supplies a normalized pure state Φ_δ with the exact pair $(\rho, 0)$ and

$$\langle \Phi_\delta, H^{0,0}\Phi_\delta\rangle \le \langle \Psi, H^{0,0}\Psi\rangle + \delta.$$

Letting $\delta \downarrow 0$ and taking the infimum over Ψ proves (149) for F_{PFLL}, without using its convexity or its equality with F_{PFL}. Taking the infimum over all pure states of density ρ gives (63). The density bound and the same construction applied to a vacuum-embedded electronic representative give the finite domain $\mathcal{I}_N$.

Finally, apply (59) to a PFL optimizer at $(\rho, 0)$. Letting the energy error tend to zero gives $F^{e,\chi}_{\mathrm{PFLL}}(\rho, 0) \le F^{e,\chi}_{\mathrm{PFL}}(\rho, 0)$. The reverse inequality follows from (57). Only the constructive approximation is used here, not the general equality of the two functionals. □

5.10. **Properties of optimizers.**

Proof of Proposition 4.13. For $h \in \mathfrak{H}_{\mathrm{ph}}$ with $h/\sqrt{\omega} \in \mathfrak{H}_{\mathrm{ph}}$, the annihilation estimate and Cauchy–Schwarz in a spectral decomposition of $\mathbf{\Gamma}$ give

$$|\operatorname{Tr}(a(h)\mathbf{\Gamma})| \leq \|h/\sqrt{\omega}\| \left(\operatorname{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma})\right)^{1/2}. \tag{150}$$

Thus all linear traces below are well defined, even without finite mean photon number.

For (i), put $g_j = \sum_\mu \int u_j^\mu(\mathbf{x}) G_{\mathbf{x}}^\mu \mathrm{d}\mathbf{x}$ and $\vec{\mathfrak{A}} = (\int \mathbf{u}_1 \cdot \mathfrak{A}, \dots, \int \mathbf{u}_n \cdot \mathfrak{A})$, so that $\int \mathbf{u}_j \cdot \mathfrak{A} = \Phi(g_j)$ and, as in Section 3.3, $g_j \in D(\omega)$. By the symmetry of the form factor, all scalar products among the kernels g_j, ωg_j, and $G_{\mathbf{x}}^\mu$ are real. By Proposition A.6(iii), the components of $\vec{\mathfrak{A}}$ therefore strongly commute with each other and with every $\mathfrak{A}^\mu(\mathbf{x})$, so

$$U_t = e^{\mathrm{i}t\varphi(\vec{\mathfrak{A}})}, \qquad t \in \mathbb{R},$$

is a photon unitary commuting with every $\mathfrak{A}^\mu(\mathbf{x})$. It commutes with each $\mathbf{D}_n$ and leaves the density, the paramagnetic current density, and the conditional field expectations unchanged, hence also $\mathbf{j}^{\mathrm{c}}$. For $\xi \in \mathbb{R}^n$, $e^{\mathrm{i}\xi\cdot\vec{\mathfrak{A}}} = W(\mathrm{i}\sum_j \xi_j g_j)$, and the pointwise shift (217) gives

$$a(\mathbf{k},\lambda) e^{\mathrm{i}\xi\cdot\vec{\mathfrak{A}}}\eta = e^{\mathrm{i}\xi\cdot\vec{\mathfrak{A}}}\Big(a(\mathbf{k},\lambda)\eta + \mathrm{i}\sum_{j=1}^n \xi_j g_j(\mathbf{k},\lambda)\eta\Big), \qquad \eta \in D(\sqrt{H_{\mathrm{rad}}}).$$

Since $e^{\mathrm{i}t\varphi} - 1 \in \mathcal{S}(\mathbb{R}^n)$, integrating this identity against its Fourier transform, and using closedness of the annihilation map, gives

$$a(\mathbf{k},\lambda) U_t \eta = U_t\Big(a(\mathbf{k},\lambda)\eta + \mathrm{i}t\sum_{j=1}^n g_j(\mathbf{k},\lambda)(\partial_j\varphi)(\vec{\mathfrak{A}})\eta\Big).$$

As $g_j \in D(\omega)$, U_t preserves $D(\sqrt{H_{\mathrm{rad}}})$, hence $\mathcal{Q}_{\mathrm{PF}}$, and only the radiation energy changes. Recall that $\int \mathbf{u}_j \cdot \mathfrak{E}_\perp = -\mathrm{i}\big(a^\dagger(\omega g_j) - a(\omega g_j)\big)$. Squaring and integrating against ω gives the expansion below. In its linear term we used that the commutator

$$[a(\omega g_j), (\partial_j\varphi)(\vec{\mathfrak{A}})] = \sum_{l=1}^n \langle \omega g_j, g_l\rangle (\partial_l\partial_j\varphi)(\vec{\mathfrak{A}})$$

is self-adjoint:

$$\begin{aligned}\operatorname{Tr}\Big(H^{0,0} U_t \mathbf{\Gamma} U_t^\dagger\Big) = \operatorname{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) - t\sum_{j=1}^n \operatorname{Re}\operatorname{Tr}\Big((\partial_j\varphi)(\vec{\mathfrak{A}})\int \mathbf{u}_j\cdot\mathfrak{E}_\perp\,\mathbf{\Gamma}\Big) \\ + t^2\sum_{j,l=1}^n \langle\sqrt{\omega}g_j, \sqrt{\omega}g_l\rangle \operatorname{Tr}\big((\partial_j\varphi)(\vec{\mathfrak{A}})(\partial_l\varphi)(\vec{\mathfrak{A}})\mathbf{\Gamma}\big).\end{aligned}$$

Optimality at $t = 0$ proves (66).

For (ii), apply (i) with $n = 1$, $\mathbf{u}_1 = \mathbf{u}$, and $\varphi(q) = m\psi(q/m)$, where $\psi \in \mathcal{S}(\mathbb{R})$ is real with $\psi'(0) = 1$. Then $\varphi'(\int \mathbf{u}\cdot\mathfrak{A}) = \psi'(m^{-1}\int \mathbf{u}\cdot\mathfrak{A})$ is bounded uniformly in m and converges strongly to $\mathbb{1}$ as $m \to \infty$. Since $\mathbf{\Gamma}$ has finite radiation energy, dominated convergence over a spectral decomposition of $\mathbf{\Gamma}$ gives $\operatorname{Re}\operatorname{Tr}\big(\int \mathbf{u}\cdot\mathfrak{E}_\perp\,\mathbf{\Gamma}\big) = 0$. This trace is real, because $\int \mathbf{u}\cdot\mathfrak{E}_\perp$ is self-adjoint, which proves (67).

For (iii), suppose first that $\mathbf{j}^{\mathrm{c}} = 0$. By (64), $\mathbf{\Gamma}$ also minimizes the internal energy among all density matrices with density ρ. For any $f \in D(\omega)$, Corollary A.8 shows

that $W(tf)\mathbf{\Gamma}W(tf)^\dagger$ has density ρ, and that its internal energy is the quadratic polynomial (220) in t, with linear coefficient $2\,\mathrm{Re}\,\mathrm{Tr}(a(\omega f)\mathbf{\Gamma}) - e\int \mathbf{c}_f \cdot \mathbf{j}^{\mathrm{c}}$. This coefficient vanishes. Since $\mathbf{j}^{\mathrm{c}} = 0$, using both f and $\mathrm{i}f$ gives $\mathrm{Tr}(a(\omega f)\mathbf{\Gamma}) = 0$. For any h as in (150), set

$$h_m = \mathbb{1}_{\{m^{-1}\le\omega\le m\}}h, \qquad f_m = h_m/\omega \in D(\omega).$$

Then $\|(h_m - h)/\sqrt{\omega}\| \to 0$, so (150) shows that $\mathrm{Tr}(a(h)\mathbf{\Gamma}) = 0$. Taking $h = G^\mu_{\mathbf{x}}$ proves the pointwise assertion for $\mathfrak{A}$, and taking $h = g_{\boldsymbol{\nabla}\times\mathbf{u}}$ proves it for $\mathfrak{B}$.

Finally, if $\mathbf{j}^{\mathrm{c}} = \rho\boldsymbol{\nabla}S$, the gauge covariance identities (197) to (199), applied to spectral decompositions, show that $U_{-S}\mathbf{\Gamma}U_{-S}^\dagger$ is an optimizer at $(\rho, 0)$. The electronic unitary U_{-S} leaves the photon reduced state unchanged. All coherent photon amplitudes therefore agree with those of this zero-current optimizer. □

Proof of Proposition 4.14. (i) The vacuum product $\sqrt{\rho}\otimes\Omega$ has finite energy and pair $(\rho, 0)$. By Theorem 4.8 an optimizer $\mathbf{\Gamma}_0$ at this pair exists. Gauge covariance with $S(\mathbf{x}) = \mathbf{q}\cdot\mathbf{x}$ maps it to an optimizer at $(\rho, \rho\mathbf{q})$. Proposition 4.13 gives the claimed fields for every optimizer there, and direct differentiation gives the divergence.

(ii) Write $\varphi = \sqrt{\rho}$. For any finite-energy density matrix $\mathbf{\Gamma} = \sum_r p_r|\Psi_r\rangle\langle\Psi_r|$ with density ρ, integration by parts gives

$$\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) = \frac{3}{4} + \frac{1}{2}\sum_{r,\mu} p_r\|(\partial_\mu + x^\mu)\Psi_r\|^2 + \mathrm{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}).$$

Indeed, $\int|\mathbf{x}|^2\rho = 3/2$. The identity follows first on smooth vectors and then by approximation in $H^1\cap D(|\mathbf{x}|)$. The state $\varphi\otimes\Omega$ attains $3/4$ at $(\rho, 0)$. Equality forces each occupied vector to be $\varphi\otimes\xi_r$, and $\ker H_{\mathrm{rad}} = \mathrm{Span}\{\Omega\}$ then forces the density matrix to be $|\varphi\otimes\Omega\rangle\langle\varphi\otimes\Omega|$. Gauge covariance is a bijection of the optimizer sets and proves (68) and its uniqueness.

Suppose that $\Psi_{\mathbf{q}}$ were an eigenvector of some admissible $H^{v,\mathbf{A}}$ with eigenvalue E. Removing its electronic phase makes $\varphi\otimes\Omega$ an eigenvector with vector potential $\mathbf{A}' = \mathbf{A} + \mathbf{q} \in L^3 + L^\infty$. At $e = 0$ the photon vacuum decouples. Taking the real part of the weak electronic eigenvalue equation, tested against real compactly supported functions, gives

$$-\frac{1}{2}\Delta\varphi + \left(v + \frac{1}{2}|\mathbf{A}'|^2\right)\varphi = E\varphi.$$

Since $\varphi > 0$, this implies

$$v + \frac{1}{2}|\mathbf{A}'|^2 = E + \frac{\Delta\varphi}{2\varphi} = E + \frac{|\mathbf{x}|^2 - 3}{2}.$$

The left-hand side belongs to $L^{3/2} + L^\infty$, whereas the quadratically growing right-hand side does not. This is a contradiction. Finally, time reversal maps the constraint $(\rho, \rho\mathbf{q})$ to $(\rho, -\rho\mathbf{q})$, so uniqueness at $(\rho, \rho\mathbf{q})$ does not imply time-reversal invariance. □

Proof of Proposition 4.15. (i) By Proposition A.4, Θ commutes with every $U_{\mathbf{R}}$, and $\Theta^2 = \mathbb{1}$. Thus $g\mapsto V_g$ is a strongly continuous representation of G by unitary and antiunitary operators. By (180) to (182) and (193), each V_g preserves $\mathcal{Q}_{\mathrm{PF}}$ and the energy, and maps a density matrix with pair $(\rho', \mathbf{j}')$ to one with pair $(\rho'\circ\mathbf{R}^\top, s\mathbf{R}\mathbf{j}'\circ$

$\mathbf{R}^\top$). For $g \in G$ the pair $(\rho, \mathbf{j}^{\mathrm{c}})$ is fixed, so V_g maps optimizers to optimizers, with inverse given by $V_{g^{-1}}$.

Let $\mathbf{\Gamma}$ be an optimizer, and let $\mathrm{d}g$ be the normalized Haar measure on G. Since V_g commutes with $H^{0,0}$, the map

$$g \mapsto \sqrt{H^{0,0}+1}\, V_g \mathbf{\Gamma} V_g^{-1} \sqrt{H^{0,0}+1} = V_g \sqrt{H^{0,0}+1}\, \mathbf{\Gamma} \sqrt{H^{0,0}+1}\, V_g^{-1}$$

is continuous in trace norm. Hence

$$\mathbf{\Gamma}_G = \int_G V_g \mathbf{\Gamma} V_g^{-1} \mathrm{d}g$$

is a density matrix with $\sqrt{H^{0,0}+1}\, \mathbf{\Gamma}_G \sqrt{H^{0,0}+1}$ trace class. As in the proof of Corollary A.8, the energy and the pairings of the density and of the combined current density with bounded test functions are continuous linear functionals of $\sqrt{H^{0,0}+1}\, \mathbf{\Gamma} \sqrt{H^{0,0}+1}$ in trace norm. They are constant along the orbit, so they pass to the average, and $\mathbf{\Gamma}_G$ is an optimizer at $(\rho, \mathbf{j}^{\mathrm{c}})$. Invariance of Haar measure makes it G-invariant.

(ii) Every $G^\mu_{\mathbf{x}}$ lies in $\mathfrak{H}_S^\perp$. By (208), the field acts only on the first factor, and H_{rad} is the sum of the radiation energies of the two factors. Replacing an optimizer $\mathbf{\Gamma}$ by the partial trace of $\mathbf{\Gamma}$ over the second factor, tensored with $|\Omega_S\rangle\langle\Omega_S|$, therefore preserves the density, the combined current density, and every term of the energy except the radiation energy of the second factor, which it removes. Optimality forces that term to vanish. Since $\omega > 0$ almost everywhere, the radiation energy of the second factor has kernel spanned by Ω_S, so every eigenvector of $\mathbf{\Gamma}$ with positive eigenvalue has Ω_S as its second factor. □

Proof of Proposition 4.16. The competitor in (134) has exactly the same density and combined current density as $\mathbf{\Gamma}_*$. Optimality therefore gives

$$0 \le \mathrm{Tr}\big(H^{0,0}(\mathbf{\Gamma}_{*,\kappa} - \mathbf{\Gamma}_*)\big) \le -\tfrac{1}{2} E_*(\kappa) + C(\kappa^2 + b_\kappa^2),$$

which proves (69) after changing C. No supporting external potential is needed. Tonelli's theorem and $\mathcal{U}_*(\varepsilon) = \varepsilon \mathcal{N}_*(\varepsilon)$ give the exact identity

$$N_*(\kappa) = \frac{E_*(\kappa)}{\kappa} + \int_0^\kappa \frac{E_*(t)}{t^2} \mathrm{d}t.$$

The form factor contribution obeys a second Tonelli identity,

$$\frac{b_\kappa^2}{\kappa} + \int_0^\kappa \frac{b_t^2}{t^2} \mathrm{d}t = \int_{\omega<\kappa} \frac{|\widehat{\chi}(\mathbf{k})|^2}{\omega(\mathbf{k})} \mathrm{d}\mathbf{k} = a_\kappa^2.$$

Together these prove (70). Finally, for the hard cutoff and $\kappa \le \Lambda$, $b_\kappa^2 = 2\pi\kappa^2$ and $a_\kappa^2 = 4\pi\kappa$. □

5.11. **Zero coupling.**

Proof of Theorem 4.17. Throughout the proof, $H^{0,0}$ is evaluated at $e = 0$. The equality $F^{0,\chi}_{\mathrm{PFLL}} = F^{0,\chi}_{\mathrm{PFL}}$ follows from Theorem 4.10. It remains to prove $F^{0,\chi}_{\mathrm{PFLL}} = F_{\mathrm{VR}}$ and the attainment criterion.

Step 1. The lower bound $F^{0,\chi}_{\mathrm{PFLL}} \ge F_{\mathrm{VR}}$. Let $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ be normalized and suppose that $(\rho_\Psi, \mathbf{j}^{\mathrm{p}}_\Psi) = (\rho, \mathbf{j}^{\mathrm{p}})$. Its electronic and photon reduced states are

$$\Gamma_{\mathrm{el}} := \mathrm{Tr}_{\mathrm{ph}} |\Psi\rangle\langle\Psi|, \qquad \Gamma_{\mathrm{ph}} := \mathrm{Tr}_{\mathrm{el}} |\Psi\rangle\langle\Psi|.$$

The partial-trace identity for positive observables (6), first for bounded spectral truncations and then by monotone convergence, gives

$$\langle \Psi, H^{0,0}\Psi\rangle = \mathrm{Tr}\big(H_{\mathrm{el}}^0\Gamma_{\mathrm{el}}\big) + \mathrm{Tr}(H_{\mathrm{rad}}\Gamma_{\mathrm{ph}}).$$

In particular, Γ_{el} has finite electronic energy. It has the same density as Ψ: for $v \in C_c^\infty(\mathbb{R}^3)$ and the bounded operator $V = \sum_{n=1}^N v(\mathbf{x}_n)$ on $\mathfrak{H}_{\mathrm{el}}^N$,

$$\int_{\mathbb{R}^3} v\rho_\Psi = \langle \Psi, (V \otimes \mathbb{1}_{\mathcal{F}_{\mathrm{ph}}})\Psi\rangle = \mathrm{Tr}(V\Gamma_{\mathrm{el}}) = \int_{\mathbb{R}^3} v\rho_{\Gamma_{\mathrm{el}}}.$$

It also has the same paramagnetic current density. Indeed, insert a Schmidt decomposition $\Psi = \sum_j \sqrt{p_j}\,\Phi_j \otimes \Xi_j$, for which $\Gamma_{\mathrm{el}} = \sum_j p_j|\Phi_j\rangle\langle\Phi_j|$ by (4), into (34). The gradient acts only on the electronic factor, and $\langle \Xi_j, \Xi_k\rangle = \delta_{jk}$ removes all cross terms, so

$$\mathbf{j}_\Psi^{\mathrm{p}} = \sum_j p_j \mathbf{j}_{\Phi_j}^{\mathrm{p}} = \mathbf{j}_{\Gamma_{\mathrm{el}}}^{\mathrm{p}}.$$

The convergence of these series is checked in the proof of Theorem 4.4, which holds for every $e \geq 0$. Consequently, $(\rho_{\Gamma_{\mathrm{el}}}, \mathbf{j}_{\Gamma_{\mathrm{el}}}^{\mathrm{p}}) = (\rho, \mathbf{j}^{\mathrm{p}})$, and

$$\langle \Psi, H^{0,0}\Psi\rangle \geq \mathrm{Tr}\big(H_{\mathrm{el}}^0\Gamma_{\mathrm{el}}\big) \geq F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}}).$$

Taking the infimum over admissible Ψ gives $F_{\mathrm{PFLL}}^{0,\chi}(\rho, \mathbf{j}^{\mathrm{p}}) \geq F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}})$.

Step 2. The upper bound $F_{\mathrm{PFLL}}^{0,\chi} \leq F_{\mathrm{VR}}$. We purify an arbitrary admissible electronic density matrix with soft photons. Each of its eigenvectors is paired with its own one-photon state, the photon states being orthonormal and supported at momenta below ε. The resulting pure state has this density matrix as its electronic reduced state, and hence the prescribed density and current density. Its energy exceeds the electronic energy only by the photon energy, which is at most ε and can therefore be made arbitrarily small. This is the one-photon purification (88) used in the proof of Theorem 4.4 to prove the reverse inclusions in (45) and (46). There the purification only had to realize the prescribed pair with vanishing field-induced current density. Here, at $e = 0$, the energy form factorizes, so we can also compute the energy of the purified state exactly.

More precisely, let Γ be any admissible electronic density matrix of finite energy. Writing only its nonzero eigenvalues, its spectral decomposition is

$$\Gamma = \sum_{j=1}^r p_j|\Phi_j\rangle\langle\Phi_j|, \qquad p_j > 0, \qquad \sum_{j=1}^r p_j = 1, \qquad r \in \mathbb{N} \cup \{\infty\}.$$

The vectors Φ_j are orthonormal, belong to $Q(H_{\mathrm{el}}^0)$, and satisfy

$$\sum_{j=1}^r p_j \langle \Phi_j, H_{\mathrm{el}}^0 \Phi_j\rangle = \mathrm{Tr}\big(H_{\mathrm{el}}^0\Gamma\big) < \infty.$$

Fix $\varepsilon > 0$. The one-photon space over the region $\{0 < |\mathbf{k}| < \varepsilon\}$ is infinite dimensional, so it contains an orthonormal family $\{f_j^\varepsilon\}_{j=1}^r$. Put

$$\Xi_j^\varepsilon = a^\dagger(f_j^\varepsilon)\Omega.$$

Then the Ξ_j^ε are orthonormal one-photon vectors and

$$\langle \Xi_j^\varepsilon, H_{\mathrm{rad}}\Xi_j^\varepsilon\rangle = \langle f_j^\varepsilon, |\mathbf{k}| f_j^\varepsilon\rangle \leq \varepsilon.$$

When $r = \infty$, consider first the finite sums

$$\Psi_{\varepsilon,M} = \sum_{j=1}^{M} \sqrt{p_j}\, \Phi_j \otimes \Xi_j^{\varepsilon}.$$

For $L > M$, orthogonality in both tensor factors and the form factorization at $e = 0$ give

$$\begin{aligned} &\|\Psi_{\varepsilon,L} - \Psi_{\varepsilon,M}\|^2 + \langle \Psi_{\varepsilon,L} - \Psi_{\varepsilon,M}, H^{0,0}(\Psi_{\varepsilon,L} - \Psi_{\varepsilon,M})\rangle \\ &\quad = \sum_{M<j\le L} p_j \left(1 + \langle \Phi_j, H_{\mathrm{el}}^0 \Phi_j\rangle + \langle \Xi_j^{\varepsilon}, H_{\mathrm{rad}} \Xi_j^{\varepsilon}\rangle\right). \end{aligned}$$

The series on the right is summable. Hence the partial sums converge in the form norm to a normalized vector. When $r < \infty$, this vector is simply the corresponding finite sum. In either case,

$$\Psi_{\varepsilon} = \sum_{j=1}^{r} \sqrt{p_j}\, \Phi_j \otimes \Xi_j^{\varepsilon} \in \mathcal{Q}_{\mathrm{PF}}.$$

Hilbert-space convergence implies trace-norm convergence of the corresponding rank-one density matrices, and the partial trace is trace-norm continuous. Taking the partial trace first for the finite sums and then passing to the limit therefore yields

$$\mathrm{Tr}_{\mathrm{ph}}\, |\Psi_{\varepsilon}\rangle\langle\Psi_{\varepsilon}| = \sum_{j=1}^{r} p_j |\Phi_j\rangle\langle\Phi_j| = \Gamma.$$

Thus Ψ_{ε} has precisely the prescribed density and paramagnetic current density. Its energy is

$$\begin{aligned} \langle \Psi_{\varepsilon}, H^{0,0}\Psi_{\varepsilon}\rangle &= \mathrm{Tr}\big(H_{\mathrm{el}}^0 \Gamma\big) + \sum_{j=1}^{r} p_j \langle f_j^{\varepsilon}, |\mathbf{k}| f_j^{\varepsilon}\rangle \\ &\le \mathrm{Tr}\big(H_{\mathrm{el}}^0 \Gamma\big) + \varepsilon. \end{aligned}$$

Since Ψ_{ε} is admissible for $F_{\mathrm{PFLL}}^{0,\chi}(\rho, \mathbf{j}^{\mathrm{p}})$, taking the infimum first over admissible Γ and then letting $\varepsilon \downarrow 0$ gives $F_{\mathrm{PFLL}}^{0,\chi}(\rho, \mathbf{j}^{\mathrm{p}}) \le F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}})$.

Step 3. Characterization of attainment. Suppose that a normalized Ψ_* attains the infimum on the left-hand side of (73). Its electronic marginal is admissible for the electronic minimization, and hence

$$\begin{aligned} 0 &= \langle \Psi_*, H^{0,0}\Psi_*\rangle - F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}}) \\ &= \left[\mathrm{Tr}\big(H_{\mathrm{el}}^0 \Gamma_{\mathrm{el},\Psi_*}\big) - F_{\mathrm{VR}}(\rho, \mathbf{j}^{\mathrm{p}})\right] + \mathrm{Tr}(H_{\mathrm{rad}} \Gamma_{\mathrm{ph},\Psi_*}). \end{aligned}$$

Both terms on the last line are nonnegative, so they vanish separately. Thus $\Gamma_{\mathrm{el},\Psi_*}$ is an electronic minimizer and

$$\mathrm{Tr}(H_{\mathrm{rad}} \Gamma_{\mathrm{ph},\Psi_*}) = \|\sqrt{H_{\mathrm{rad}}}\sqrt{\Gamma_{\mathrm{ph},\Psi_*}}\|_{\mathfrak{S}_2}^2 = 0.$$

It follows that the range of $\sqrt{\Gamma_{\mathrm{ph},\Psi_*}}$ lies in $\ker H_{\mathrm{rad}}$. Sector by sector, H_{rad} is multiplication on the m-photon sector by $\sum_{j=1}^{m} |\mathbf{k}_j|$, which is strictly positive almost everywhere for every $m \ge 1$. Therefore $\ker H_{\mathrm{rad}} = \mathbb{C}\Omega$ and $\Gamma_{\mathrm{ph},\Psi_*} = |\Omega\rangle\langle\Omega|$.

Since a pure state with a pure marginal is a product state, (5) gives $\Psi_* = \Phi \otimes \Omega$ for a normalized $\Phi \in Q(H_{\mathrm{el}}^0)$, and its electronic marginal $|\Phi\rangle\langle\Phi|$ is a rank-one

minimizer. Conversely, if $|\Phi\rangle\langle\Phi|$ is a rank-one electronic minimizer, then $\Phi \otimes \Omega$ is admissible and attains $F^{0,\chi}_{\mathrm{PFLL}}(\rho, \mathbf{j}^{\mathrm{p}})$. □

Proof of Theorem 4.18. Throughout the proof, the coupling and form factor are displayed in the notation $H^{0,0}_{e,\chi}$.

Step 1. Comparison of the forms at couplings e and 0. By (28), all these forms have the same domain when the form factor is fixed. Expanding the covariant kinetic energy on this domain gives

$$\begin{aligned}&\langle \Psi, H^{0,0}_{e,\chi}\Psi\rangle - \langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle \\ &\quad = -e\sum_{n=1}^{N} \mathrm{Re}\langle(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n})\Psi, \mathfrak{A}(\mathbf{x}_n)\Psi\rangle + \frac{e^2}{2}\sum_{n=1}^{N}\|\mathfrak{A}(\mathbf{x}_n)\Psi\|^2.\end{aligned}$$

For normalized Ψ, positivity of the zero-coupling form and (20) imply

$$\sum_{n=1}^{N}\|(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n})\Psi\|^2 \le 2\langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle,$$

and

$$\sum_{n=1}^{N}\|\mathfrak{A}(\mathbf{x}_n)\Psi\|^2 \le NC_\chi\left(\langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle + 1\right).$$

Cauchy–Schwarz therefore gives a constant C, depending on N and the fixed form factor but not on e or Ψ, such that

$$\left|\langle \Psi, H^{0,0}_{e,\chi}\Psi\rangle - \langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle\right| \le C(e+e^2)\left(\langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle + 1\right).$$

For all sufficiently small e, the same estimate can be rearranged as

$$\langle \Psi, H^{0,0}_{0,\chi}\Psi\rangle + 1 \le C\left(\langle \Psi, H^{0,0}_{e,\chi}\Psi\rangle + 1\right).$$

It follows in particular that a sequence with bounded $H^{0,0}_{e_k,\chi}$ energy has bounded zero-coupling energy and that the difference of the two form expectations tends to zero along that sequence.

Step 2. The lower bound (i): electronic marginals. It suffices to consider a subsequence on which the liminf in (i) is finite. Choose normalized Ψ_k satisfying

$$(\rho_{\Psi_k}, \mathbf{j}^{\mathrm{c}}_{\Psi_k}) = (\rho_k, \mathbf{j}_k), \qquad \langle \Psi_k, H^{0,0}_{e_k,\chi}\Psi_k\rangle \le F^{e_k,\chi}_{\mathrm{PFLL}}(\rho_k, \mathbf{j}_k) + \frac{1}{k}.$$

The preceding comparison gives a uniform zero-coupling energy bound. Set

$$\Gamma_k = \mathrm{Tr}_{\mathrm{ph}}\,|\Psi_k\rangle\langle\Psi_k|.$$

The zero-coupling factorization used in Theorem 4.17 yields

$$\langle \Psi_k, H^{0,0}_{0,\chi}\Psi_k\rangle = \mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma_k\big) + \langle \Psi_k, H_{\mathrm{rad}}\Psi_k\rangle.$$

In particular, the electronic form traces and the photon energies are uniformly bounded.

The electronic marginal has density ρ_k. Its paramagnetic current density is not exactly $\mathbf{j}_k$, but (36) gives

$$\mathbf{j}^{\mathrm{p}}_{\Gamma_k} = \mathbf{j}^{\mathrm{p}}_{\Psi_k} = \mathbf{j}_k - \mathbf{j}^{\mathrm{ph}}_{\Psi_k}.$$

By (39),

$$\int_{\mathbb{R}^3}\frac{|\mathbf{j}^{\mathrm{ph}}_{\Psi_k}|^2}{\rho_k} \le Ce_k^2.$$

Since $\int_{\mathbb{R}^3} \rho_k = N$ and the weakly convergent sequence (ρ_k) is bounded in X, hence in L^3, Hölder's inequality gives

$$\|\mathbf{j}^{\mathrm{ph}}_{\Psi_k}\|_1 \leq N^{1/2} \left(\int_{\mathbb{R}^3} \frac{|\mathbf{j}^{\mathrm{ph}}_{\Psi_k}|^2}{\rho_k} \right)^{1/2}, \qquad \|\mathbf{j}^{\mathrm{ph}}_{\Psi_k}\|_{3/2} \leq \|\rho_k\|_3^{1/2} \left(\int_{\mathbb{R}^3} \frac{|\mathbf{j}^{\mathrm{ph}}_{\Psi_k}|^2}{\rho_k} \right)^{1/2}.$$

Consequently,

$$\mathbf{j}^{\mathrm{ph}}_{\Psi_k} \longrightarrow 0 \quad \text{in } Y, \qquad \mathbf{j}^{\mathrm{p}}_{\Gamma_k} \rightharpoonup \mathbf{j} \quad \text{weakly in } Y.$$

Step 3. The lower bound (i): compactness of the marginals. We now use compactness only on the electronic space. The densities are uniformly tight: with $B_R = \{\mathbf{x} : |\mathbf{x}| < R\}$,

$$\lim_{R\to\infty} \sup_k \int_{B_R^c} \rho_k = 0.$$

Indeed, since $L^\infty \subset X^*$, testing $\rho_k \rightharpoonup \rho$ against the indicator of B_R^c gives

$$\int_{B_R^c} \rho_k \longrightarrow \int_{B_R^c} \rho$$

for each fixed R. Choose R first to make the latter integral small, and then enlarge it to handle the finitely many initial indices; the integrals on the left decrease as R grows. As in the proof of Lemma 5.7, the elementary inequality

$$\mathbb{1} - \prod_{n=1}^N \mathbb{1}_{B_R}(\mathbf{x}_n) = \mathbb{1}_{\{\max_n |\mathbf{x}_n| \geq R\}} \leq \sum_{n=1}^N \mathbb{1}_{B_R^c}(\mathbf{x}_n),$$

tested against Γ_k, converts this into a bound on the probability that some electron lies outside B_R:

$$\mathrm{Tr}\left[\left(\mathbb{1} - \prod_{n=1}^N \mathbb{1}_{B_R}(\mathbf{x}_n) \right) \Gamma_k \right] \leq \int_{B_R^c} \rho_k.$$

Equip $Q(H^0_{\mathrm{el}})$ with the Hilbert norm generated by $\Phi \mapsto \langle \Phi, (H^0_{\mathrm{el}} + 1)\Phi \rangle$. The uniform electronic form bound means that, for every orthonormal basis (ψ_j) of $\mathfrak{H}^N_{\mathrm{el}}$,

$$\sum_j \|\sqrt{\Gamma_k}\psi_j\|^2_{Q(H^0_{\mathrm{el}})} = 1 + \mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma_k\big) \leq C. \tag{151}$$

Choose $0 \leq \eta_R \leq 1$ smooth, equal to one on B_R and supported in B_{2R}, and put $\chi_R(\mathbf{x}_1, \ldots, \mathbf{x}_N) = \prod_{n=1}^N \eta_R(\mathbf{x}_n)$. Then

$$\|(1-\chi_R)\sqrt{\Gamma_k}\|^2_{\mathfrak{S}_2} \leq \mathrm{Tr}\big((1-\chi_R^2)\Gamma_k\big) \leq \int_{B_R^c} \rho_k.$$

For fixed R, local Rellich compactness makes multiplication by χ_R a compact map from $Q(H^0_{\mathrm{el}})$ to $\mathfrak{H}^N_{\mathrm{el}}$. Hence, for every $\delta > 0$, there is a finite-rank orthogonal projection S such that

$$\|(1-S)\chi_R\|_{Q(H^0_{\mathrm{el}}) \to \mathfrak{H}^N_{\mathrm{el}}} < \delta.$$

Now split

$$(1-S)\sqrt{\Gamma_k} = (1-S)(1-\chi_R)\sqrt{\Gamma_k} + (1-S)\chi_R\sqrt{\Gamma_k}.$$

Since $\|1-S\| \le 1$, the Hilbert–Schmidt norm of the first term is at most $\|(1-\chi_R)\sqrt{\Gamma_k}\|_{\mathfrak{S}_2}$. For the second term, each $\sqrt{\Gamma_k}\psi_j$ lies in $Q(H_{\mathrm{el}}^0)$ by (151), so the operator-norm bound on $(1-S)\chi_R$ gives

$$\|(1-S)\chi_R\sqrt{\Gamma_k}\|_{\mathfrak{S}_2}^2 = \sum_j \|(1-S)\chi_R\sqrt{\Gamma_k}\psi_j\|^2 \le \delta^2 \sum_j \|\sqrt{\Gamma_k}\psi_j\|_{Q(H_{\mathrm{el}}^0)}^2 \le C\delta^2.$$

Together,

$$\sup_k \|(1-S)\sqrt{\Gamma_k}\|_{\mathfrak{S}_2} \le \sup_k \|(1-\chi_R)\sqrt{\Gamma_k}\|_{\mathfrak{S}_2} + C^{1/2}\delta.$$

First choosing R large and then δ small makes the right-hand side arbitrarily small. Since $1-S$ is an orthogonal projection,

$$\operatorname{Tr}((1-S)\Gamma_k) = \|(1-S)\sqrt{\Gamma_k}\|_{\mathfrak{S}_2}^2,$$

so for every $\varepsilon > 0$ there is a single finite-rank orthogonal projection S with $\sup_k \operatorname{Tr}((1-S)\Gamma_k) < \varepsilon$. This is the hypothesis of Lemma 5.1. By the compression estimate (110), every Γ_k lies within $2\sqrt{\varepsilon}$ in trace norm of its compression $S\Gamma_k S$. These compressions are positive and have trace at most one, and each $A = S\Gamma_k S$ satisfies $A = SAS$, that is, it vanishes on $(\operatorname{ran} S)^\perp$ and maps into $\operatorname{ran} S$. They are therefore operators on the fixed finite-dimensional space $\operatorname{ran} S$, extended by zero, and so lie in a compact set. Since ε is arbitrary, (Γ_k) is precompact in trace norm. After passing to a subsequence,

$$\Gamma_k \longrightarrow \Gamma \quad \text{in } \mathfrak{S}_1(\mathfrak{H}_{\mathrm{el}}^N), \qquad \Gamma \ge 0, \qquad \operatorname{Tr}\Gamma = 1.$$

Step 4. The lower bound (i): passage to the limit. We pass both the full electronic form and the constraints to this limit. The Powers–Størmer inequality gives $\sqrt{\Gamma_k} \to \sqrt{\Gamma}$ in $\mathfrak{S}_2(\mathfrak{H}_{\mathrm{el}}^N)$. By (151), $\sqrt{\Gamma_k}$, regarded as a Hilbert–Schmidt operator with values in the form domain, has a weakly convergent subsequence. The continuous embedding $Q(H_{\mathrm{el}}^0) \hookrightarrow \mathfrak{H}_{\mathrm{el}}^N$ and the strong $\mathfrak{S}_2$ convergence identify its weak limit with $\sqrt{\Gamma}$. Weak lower semicontinuity therefore yields

$$\operatorname{Tr}\big(H_{\mathrm{el}}^0\Gamma\big) \le \liminf_{k\to\infty} \operatorname{Tr}\big(H_{\mathrm{el}}^0\Gamma_k\big).$$

This applies to the full electronic form, including the Coulomb many-body interaction.

Moreover, $-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1}$ is a bounded map from $Q(H_{\mathrm{el}}^0)$ to $(\mathfrak{H}_{\mathrm{el}}^N)^3$. Hence

$$(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1})\sqrt{\Gamma_k} \rightharpoonup (-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1})\sqrt{\Gamma} \quad \text{in the corresponding Hilbert–Schmidt space.}$$

Trace-norm convergence passes the density against every bounded multiplication operator. For every real $\mathbf{A} \in C_c^\infty(\mathbb{R}^3,\mathbb{R}^3)$, strong convergence of $\mathbf{A}(\mathbf{x}_1)\sqrt{\Gamma_k}$ and the preceding weak convergence give

$$\begin{aligned}\int_{\mathbb{R}^3} \mathbf{A}\cdot\mathbf{j}_{\Gamma_k}^{\mathrm{p}} &= N\operatorname{Re}\big(\mathbf{A}(\mathbf{x}_1)\sqrt{\Gamma_k}, (-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1})\sqrt{\Gamma_k}\big)_{\mathfrak{S}_2} \\ &\longrightarrow N\operatorname{Re}\big(\mathbf{A}(\mathbf{x}_1)\sqrt{\Gamma}, (-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_1})\sqrt{\Gamma}\big)_{\mathfrak{S}_2} = \int_{\mathbb{R}^3} \mathbf{A}\cdot\mathbf{j}_{\Gamma}^{\mathrm{p}}.\end{aligned}$$

Since $L^\infty \subset X^*$ and $C_c^\infty(\mathbb{R}^3,\mathbb{R}^3) \subset Y^*$, the weak convergences $\rho_k \rightharpoonup \rho$ in X and $\mathbf{j}_{\Gamma_k}^{\mathrm{p}} \rightharpoonup \mathbf{j}$ in Y also hold against these test functions. Since $\rho_k = \rho_{\Gamma_k}$, uniqueness of limits therefore gives

$$(\rho_\Gamma, \mathbf{j}_\Gamma^{\mathrm{p}}) = (\rho, \mathbf{j}).$$

Using the approximate minimality, the form comparison, and the nonnegativity of the photon energy, we conclude that

$$\begin{aligned}\liminf_{k\to\infty} F^{e_k,\chi}_{\mathrm{PFLL}}(\rho_k,\mathbf{j}_k) &\geq \liminf_{k\to\infty}\left(\langle\Psi_k, H^{0,0}_{e_k,\chi}\Psi_k\rangle - \frac{1}{k}\right)\\ &= \liminf_{k\to\infty}\langle\Psi_k, H^{0,0}_{0,\chi}\Psi_k\rangle\\ &\geq \mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma\big) \geq F_{\mathrm{VR}}(\rho,\mathbf{j}).\end{aligned}$$

This proves (i).

Step 5. The recovery bound (ii). Suppose $F_{\mathrm{VR}}(\rho,\mathbf{j}) < \infty$ and fix $\delta > 0$. Choose an admissible electronic density matrix Γ_δ with

$$\mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma_\delta\big) \leq F_{\mathrm{VR}}(\rho,\mathbf{j}) + \delta.$$

Apply the construction in (88) as detailed in Step 2 of the proof of Theorem 4.17, choosing all photon tags in $\{0 < |\mathbf{k}| < \delta\}$. The resulting normalized vector Ψ_δ has electronic marginal Γ_δ and photon energy at most δ. It lies entirely in the one-photon sector: for an infinite-rank Γ_δ, this follows because every partial sum has that property and the one-photon sector is closed. Since $\mathfrak{A}(\mathbf{x})$ maps this sector into the orthogonal sum of the vacuum and two-photon sectors, $\langle\Psi_\delta, \mathfrak{A}(\mathbf{x})\Psi_\delta\rangle_{\mathbf{x}} = 0$ almost everywhere. Thus

$$\rho_{\Psi_\delta} = \rho, \qquad \mathbf{j}^{\mathrm{p}}_{\Psi_\delta} = \mathbf{j}, \qquad \mathbf{j}^{\mathrm{ph}}_{\Psi_\delta} = 0, \qquad \langle\Psi_\delta, H_{\mathrm{rad}}\Psi_\delta\rangle \leq \delta.$$

It therefore represents the same combined-current pair $(\rho,\mathbf{j})$ at every coupling and belongs to $Q(H^{0,0}_{e,\chi})$ for every $e \geq 0$ by the common form-domain identity. The electronic derivative preserves photon number, whereas $\mathfrak{A}(\mathbf{x}_n)$ changes it by one, and hence

$$\mathrm{Re}\langle(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n})\Psi_\delta, \mathfrak{A}(\mathbf{x}_n)\Psi_\delta\rangle = 0.$$

For almost every $\mathbf{X}$, the photon factor is $\Psi_\delta(\mathbf{X}) = a^\dagger(\eta)\Omega$ for a one-photon vector η supported in $\{\omega < \delta\}$, with $\|\eta\| = \|\Psi_\delta(\mathbf{X})\|$. The canonical commutation relations give

$$\|\mathfrak{A}^\mu(\mathbf{x})a^\dagger(\eta)\Omega\|^2 = \|G^\mu_{\mathbf{x}}\|^2\|\eta\|^2 + 2|\langle G^\mu_{\mathbf{x}},\eta\rangle|^2 \leq \big(\|G^\mu_{\mathbf{x}}\|^2 + 2\|\mathbb{1}_{\{\omega<\delta\}}G^\mu_{\mathbf{x}}\|^2\big)\|\eta\|^2.$$

Summing over μ by (14), applied also to $\mathbb{1}_{\{\omega<\delta\}}\widehat{\chi}$, and integrating over the electronic variables gives

$$\|\mathfrak{A}(\mathbf{x}_n)\Psi_\delta\|^2 \leq \|\widehat{\chi}\|^2 + 2\|\mathbb{1}_{\{\omega<\delta\}}\widehat{\chi}\|^2.$$

Expanding the positive-coupling form now gives

$$\begin{aligned}F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}) &\leq \langle\Psi_\delta, H^{0,0}_{e,\chi}\Psi_\delta\rangle\\ &= \mathrm{Tr}\big(H^0_{\mathrm{el}}\Gamma_\delta\big) + \langle\Psi_\delta, H_{\mathrm{rad}}\Psi_\delta\rangle + \frac{e^2}{2}\sum_{n=1}^{N}\|\mathfrak{A}(\mathbf{x}_n)\Psi_\delta\|^2\\ &\leq F_{\mathrm{VR}}(\rho,\mathbf{j}) + 2\delta + \frac{e^2N}{2}\big(\|\widehat{\chi}\|^2 + 2\|\mathbb{1}_{\{\omega<\delta\}}\widehat{\chi}\|^2\big).\end{aligned}$$

Since $\widehat{\chi} \in L^2(\mathbb{R}^3)$, letting $\delta \downarrow 0$ at fixed e gives explicitly

$$F^{e,\chi}_{\mathrm{PFLL}}(\rho,\mathbf{j}) \leq F_{\mathrm{VR}}(\rho,\mathbf{j}) + \frac{N}{2}\|\widehat{\chi}\|^2e^2,$$

which is the quantitative estimate in (ii). The same construction proves $(\rho,\mathbf{j}) \in \mathcal{J}^{e,\chi}_N$ for every $e \geq 0$.

Step 6. The zero-coupling limit. Applying (i) to the constant constraints and combining it with (ii) gives the asserted pointwise limit on the effective domain. If $F_{\mathrm{VR}}(\rho,\mathbf{j}) = +\infty$, (i) applied to the constant sequence shows that the limit is $+\infty$. Finally, since $\mathbf{j}^{\mathrm{c}} = \mathbf{j}^{\mathrm{p}}$ at $e = 0$, (45) gives $\mathcal{J}_N^{0,\chi} = \mathcal{J}_{N,\mathrm{mix}}^{\mathrm{el}}$, and (73) identifies the limit with $F_{\mathrm{PFLL}}^{0,\chi}$. □

5.12. **The long-wavelength (dipole) limit.**

Proof of Theorem 4.19. For a finite-rank positive operator $\mathbf{\Gamma}$ whose range lies in $\mathcal{Q}_{\mathrm{PF}}$, the density $\rho_{\mathbf{\Gamma}}$ and the current densities $\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon}$ and $\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c,d}}$ are defined as for density matrices, also when $\operatorname{Tr}\mathbf{\Gamma} < 1$. All constants below may depend on N, e, and the fixed form factor, but not on $\varepsilon \in [0,1]$.

Step 1. Uniform bounds and fixed-state convergence. The field bounds (14) and (20) are uniform in the spatial argument. The proof of (27) therefore gives

$$c\|\Psi\|_{\mathcal{Q}_{\mathrm{PF}}}^2 \le \langle \Psi, H_\varepsilon^{0,0}\Psi\rangle + \|\Psi\|^2 \le C\|\Psi\|_{\mathcal{Q}_{\mathrm{PF}}}^2. \tag{152}$$

In particular, the form-domain identification is uniform in ε.

Define the modulus

$$d(r) = \sum_{\mu=1}^{3} \sup_{|\mathbf{y}|\le r} \left(\|G_{\mathbf{y}}^\mu - G_0^\mu\| + \left\| \frac{G_{\mathbf{y}}^\mu - G_0^\mu}{\sqrt{\omega}} \right\| \right). \tag{153}$$

The continuity following (14) implies $d(r) \to 0$ as $r \downarrow 0$. If Ψ is supported where $|\mathbf{x}_n| \le 2L$ for all n, then

$$\sum_{n=1}^{N} \|(\mathfrak{A}(\varepsilon\mathbf{x}_n) - \mathfrak{A}(0))\Psi\|^2 \le C d(2\varepsilon L)^2 \big(\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 + \|\Psi\|^2 \big). \tag{154}$$

Indeed, for almost every $\mathbf{X}$ in the support of Ψ, we have $\Psi(\mathbf{X}) \in D(\sqrt{H_{\mathrm{rad}}})$ and $|\varepsilon\mathbf{x}_n| \le 2\varepsilon L$ for every n. Fix such $\mathbf{X}$, an index n, and a component μ, and put $g = G_{\varepsilon\mathbf{x}_n}^\mu - G_0^\mu$. Since the Segal field is real-linear in its argument,

$$\big(\mathfrak{A}^\mu(\varepsilon\mathbf{x}_n) - \mathfrak{A}^\mu(0)\big)\Psi(\mathbf{X}) = \big(a^\dagger(g) + a(g)\big)\Psi(\mathbf{X}),$$

and the definition (153) gives $\|g\| + \|g/\sqrt{\omega}\| \le d(2\varepsilon L)$. The bounds (18) and (19), applied with g in place of $G_{\mathbf{x}}^\mu$, therefore yield

$$\begin{aligned} \big\| \big(\mathfrak{A}^\mu(\varepsilon\mathbf{x}_n) - \mathfrak{A}^\mu(0)\big)\Psi(\mathbf{X}) \big\| &\le 2\|g/\sqrt{\omega}\| \, \|\sqrt{H_{\mathrm{rad}}}\Psi(\mathbf{X})\| + \|g\| \, \|\Psi(\mathbf{X})\| \\ &\le 2d(2\varepsilon L)\big(\|\sqrt{H_{\mathrm{rad}}}\Psi(\mathbf{X})\| + \|\Psi(\mathbf{X})\| \big). \end{aligned}$$

Integrating over $\mathbf{X}$, and using $\|\sqrt{H_{\mathrm{rad}}}\Psi\|^2 = \int \|\sqrt{H_{\mathrm{rad}}}\Psi(\mathbf{X})\|^2 \mathrm{d}\mathbf{X}$ because H_{rad} acts only on the photon variables, gives (154) with $C = 24N$. Expanding the differences of the squared covariant-derivative norms, and using (152), gives

$$|\langle \Psi, H_\varepsilon^{0,0}\Psi\rangle - \langle \Psi, H_{\mathrm{d}}\Psi\rangle| \le C\big(d(2\varepsilon L) + d(2\varepsilon L)^2\big)\big(\langle \Psi, H_\varepsilon^{0,0}\Psi\rangle + \|\Psi\|^2\big). \tag{155}$$

The same estimates hold after summing over any finite-rank positive operator with this electronic support.

For a fixed $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, the field difference instead converges without a support assumption:

$$\|(\mathfrak{A}(\varepsilon\mathbf{x}_n) - \mathfrak{A}(0))\Psi\| \longrightarrow 0, \qquad \langle \Psi, H_\varepsilon^{0,0}\Psi\rangle \longrightarrow \langle \Psi, H_{\mathrm{d}}\Psi\rangle. \tag{156}$$

Indeed, for almost every electronic configuration $\mathbf{X}$, $\Psi(\mathbf{X}) \in D(\sqrt{H_{\mathrm{rad}}})$. The estimates (18) and (19) and the continuity of the kernels give pointwise convergence

on these fibers, dominated in squared norm by $C(\|\sqrt{H_{\mathrm{rad}}}\Psi(\mathbf{X})\|^2 + \|\Psi(\mathbf{X})\|^2)$. Integration and then expansion of the kinetic form prove (156).

The current convergence is in the full space Y. For a normalized pure state, put

$$b_{\varepsilon,\Psi}(\mathbf{x}) = N\|(\mathfrak{A}(\varepsilon\mathbf{x}) - \mathfrak{A}(0))\Psi\|_{\mathbf{x}}^2,$$

where the partial norm $\|\cdot\|_{\mathbf{x}}$ is summed over the three field components. Pointwise Cauchy–Schwarz and Hölder's inequality give

$$\begin{aligned} |\mathbf{j}_\Psi^{\mathrm{c},\varepsilon} - \mathbf{j}_\Psi^{\mathrm{c,d}}| &\le e\sqrt{\rho_\Psi}\sqrt{b_{\varepsilon,\Psi}}, \\ \|\mathbf{j}_\Psi^{\mathrm{c},\varepsilon} - \mathbf{j}_\Psi^{\mathrm{c,d}}\|_Y &\le e\big(\sqrt{N} + \|\sqrt{\rho_\Psi}\|_6\big)\|\sqrt{b_{\varepsilon,\Psi}}\|. \end{aligned} \tag{157}$$

For a density matrix, define $b_{\varepsilon,\mathbf{\Gamma}}$ by linear extension. Cauchy–Schwarz over the state labels proves the same estimates with Ψ replaced by $\mathbf{\Gamma}$. The Hilbert-space-valued Sobolev inequality bounds $\|\sqrt{\rho_{\mathbf{\Gamma}}}\|_6$ by the square root of the ordinary electronic kinetic energy. Consequently

$$\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon} \longrightarrow \mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c,d}} \quad \text{in } Y, \qquad \mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big) \longrightarrow \mathrm{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}) \tag{158}$$

for every fixed finite-rank density matrix of finite form energy. Moreover, by (154), the current difference in (157) tends to zero uniformly on electronically supported density matrices of bounded energy whenever $\varepsilon L \to 0$.

We will also use the uniform bound

$$\|\rho_{\mathbf{\Gamma}}\|_3 + \|\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon}\|_{3/2} + \|\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon}\|_1 \le C\big(1 + \mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big)\big) \tag{159}$$

for every density matrix $\mathbf{\Gamma}$ with $\mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big) < \infty$. To see this, regard the weighted state vectors of a density matrix as a single vector in a Hilbert-space direct sum. Its electronic derivative is controlled by (152), and its covariant derivative by $\mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big)$. Sobolev and Hölder then give (159), exactly as for pure states in Proposition 4.1.

Step 2. Finite-rank approximation of the convex relaxation. By (74), the epigraph of $F_{\mathrm{PFL},\varepsilon}$ is the norm-closed convex hull of the epigraph of $F_{\mathrm{PFLL},\varepsilon}$. Thus, whenever $F_{\mathrm{PFL},\varepsilon}(\rho,\mathbf{j}^{\mathrm{c}}) < \infty$ and $\delta > 0$, there is a finite-rank density matrix $\mathbf{\Gamma}$, made from states in $\mathcal{Q}_{\mathrm{PF}}$, such that

$$\|\rho_{\mathbf{\Gamma}} - \rho\|_X + \|\mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon} - \mathbf{j}^{\mathrm{c}}\|_Y < \delta, \qquad \mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big) < F_{\mathrm{PFL},\varepsilon}(\rho,\mathbf{j}^{\mathrm{c}}) + \delta. \tag{160}$$

To obtain this, approximate an epigraph point by a finite convex combination of epigraph points of $F_{\mathrm{PFLL},\varepsilon}$, and choose an almost minimizer in each of the finitely many pure-state searches. No attainment of either search is used. Conversely, convexity and $F_{\mathrm{PFL},\varepsilon} \le F_{\mathrm{PFLL},\varepsilon}$ give

$$F_{\mathrm{PFL},\varepsilon}(\rho_{\mathbf{\Gamma}}, \mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{c},\varepsilon}) \le \mathrm{Tr}\big(H_\varepsilon^{0,0}\mathbf{\Gamma}\big) \tag{161}$$

for every such finite-rank density matrix.

Step 3. Lower bound along weakly convergent sequences. Suppose $\varepsilon_k \to 0$ and $(\rho_k, \mathbf{j}_k^{\mathrm{c}}) \rightharpoonup (\rho,\mathbf{j}^{\mathrm{c}})$ weakly in $X \times Y$. If the energy liminf is infinite, there is nothing to prove. Otherwise pass to a subsequence on which the liminf is a finite limit and all the functional values are finite. The case of infinitely many $\varepsilon_k = 0$ follows directly from weak lower semicontinuity of F_{d}, so we may assume $\varepsilon_k > 0$. By (160), choose finite-rank density matrices $\mathbf{\Gamma}_k$ such that

$$\|\rho_{\mathbf{\Gamma}_k} - \rho_k\|_X + \|\mathbf{j}_{\mathbf{\Gamma}_k}^{\mathrm{c},\varepsilon_k} - \mathbf{j}_k^{\mathrm{c}}\|_Y \le k^{-1}, \qquad \mathrm{Tr}\big(H_{\varepsilon_k}^{0,0}\mathbf{\Gamma}_k\big) \le F_{\mathrm{PFL},\varepsilon_k}(\rho_k,\mathbf{j}_k^{\mathrm{c}}) + k^{-1}. \tag{162}$$

Their energies are uniformly bounded. Since $L^\infty \subset X^*$, $\rho_{\mathbf{\Gamma}_k}$ converges weakly in L^1 to ρ. Positivity and the test function 1 show $\rho \geq 0$ and $\int_{\mathbb{R}^3} \rho = N$. Testing against the indicator of the complement of a fixed ball gives

$$\int_{|\mathbf{x}|>R} \rho_{\mathbf{\Gamma}_k} \longrightarrow \int_{|\mathbf{x}|>R} \rho$$

for every fixed $R > 0$. Now let $\eta > 0$. Since $\rho \in L^1$, there is R_0 with $\int_{|\mathbf{x}|>R_0} \rho < \eta$, and the convergence just displayed, with $R = R_0$, gives an index K such that $\int_{|\mathbf{x}|>R_0} \rho_{\mathbf{\Gamma}_k} < \eta$ for all $k \geq K$. Each of the finitely many densities $\rho_{\mathbf{\Gamma}_1}, \dots, \rho_{\mathbf{\Gamma}_{K-1}}$ is integrable, so there is $R_1 \geq R_0$ such that $\int_{|\mathbf{x}|>R_1} \rho_{\mathbf{\Gamma}_k} < \eta$ also for $k < K$. Since these tail integrals do not increase with the radius, $\sup_k \int_{|\mathbf{x}|>R} \rho_{\mathbf{\Gamma}_k} \leq \eta$ for every $R \geq R_1$. As $\eta > 0$ was arbitrary, this proves

$$\lim_{R\to\infty} \sup_k \int_{|\mathbf{x}|>R} \rho_{\mathbf{\Gamma}_k} = 0. \tag{163}$$

Choose a smooth real $h : [0,\infty) \to [0,\pi/2]$, equal to zero on $[0,1]$ and to $\pi/2$ on $[2,\infty)$. With $|\mathbf{X}|^2 = \sum_{n=1}^N |\mathbf{x}_n|^2$, define, for $\varepsilon > 0$,

$$\theta_\varepsilon(\mathbf{X}) = \cos h(\sqrt{\varepsilon}\,|\mathbf{X}|), \qquad \widetilde{\theta}_\varepsilon(\mathbf{X}) = \sin h(\sqrt{\varepsilon}\,|\mathbf{X}|).$$

Both multipliers are smooth and permutation invariant, and θ_ε equals 1 where $|\mathbf{X}| \leq \varepsilon^{-1/2}$ and vanishes where $|\mathbf{X}| \geq 2\varepsilon^{-1/2}$. They satisfy

$$\theta_\varepsilon^2 + \widetilde{\theta}_\varepsilon^2 = 1, \qquad \sum_{n=1}^N \big(|\boldsymbol{\nabla}_{\mathbf{x}_n}\theta_\varepsilon|^2 + |\boldsymbol{\nabla}_{\mathbf{x}_n}\widetilde{\theta}_\varepsilon|^2\big) \leq C\varepsilon.$$

Since the multipliers commute with the field and the interaction, the covariant IMS localization formula gives, for every $\Psi \in \mathcal{Q}_{\mathrm{PF}}$,

$$\begin{aligned} &\langle \theta_\varepsilon\Psi, H_\varepsilon^{0,0}\theta_\varepsilon\Psi\rangle + \langle \widetilde{\theta}_\varepsilon\Psi, H_\varepsilon^{0,0}\widetilde{\theta}_\varepsilon\Psi\rangle \\ &\qquad = \langle \Psi, H_\varepsilon^{0,0}\Psi\rangle + \frac{1}{2}\int_{\mathbb{R}^{3N}} \sum_{n=1}^N \big(|\boldsymbol{\nabla}_{\mathbf{x}_n}\theta_\varepsilon|^2 + |\boldsymbol{\nabla}_{\mathbf{x}_n}\widetilde{\theta}_\varepsilon|^2\big)\|\Psi(\mathbf{X})\|^2 \mathrm{d}\mathbf{X}. \end{aligned} \tag{164}$$

The identity follows first on a form core and then by form-norm approximation.

We now show that the $\mathbf{\Gamma}_k$ may be assumed to be supported where every $|\mathbf{x}_n| \leq 2\varepsilon_k^{-1/2}$. By (162),

$$(\rho_{\mathbf{\Gamma}_k}, \mathbf{j}^{\mathrm{c},\varepsilon_k}_{\mathbf{\Gamma}_k}) \rightharpoonup (\rho, \mathbf{j}^{\mathrm{c}}) \quad \text{in } X \times Y, \qquad \mathrm{Tr}\big(H_{\varepsilon_k}^{0,0}\mathbf{\Gamma}_k\big) \leq F_{\mathrm{PFL},\varepsilon_k}(\rho_k, \mathbf{j}_k^{\mathrm{c}}) + o(1), \tag{165}$$

and we check that both properties survive localization by θ_{ε_k} followed by normalization. If $|\mathbf{X}| > \varepsilon_k^{-1/2}$, then $|\mathbf{x}_n| > (N\varepsilon_k)^{-1/2}$ for some n. Hence (163) gives

$$0 \leq \mathrm{Tr}\Big(\widetilde{\theta}_{\varepsilon_k}^2\mathbf{\Gamma}_k\Big) \leq \int_{|\mathbf{x}|>(N\varepsilon_k)^{-1/2}} \rho_{\mathbf{\Gamma}_k}(\mathbf{x})\mathrm{d}\mathbf{x} \longrightarrow 0.$$

In particular, $\mathrm{Tr}\big(\theta_{\varepsilon_k}^2\mathbf{\Gamma}_k\big) = 1 - \mathrm{Tr}\Big(\widetilde{\theta}_{\varepsilon_k}^2\mathbf{\Gamma}_k\Big)$ is positive for all large k, and we discard the remaining indices. Positivity of the complementary localized form in (164) yields

$$\frac{\mathrm{Tr}\big(H_{\varepsilon_k}^{0,0}\theta_{\varepsilon_k}\mathbf{\Gamma}_k\theta_{\varepsilon_k}\big)}{\mathrm{Tr}\big(\theta_{\varepsilon_k}^2\mathbf{\Gamma}_k\big)} \leq \frac{\mathrm{Tr}\big(H_{\varepsilon_k}^{0,0}\mathbf{\Gamma}_k\big) + C\varepsilon_k}{\mathrm{Tr}\big(\theta_{\varepsilon_k}^2\mathbf{\Gamma}_k\big)} = \mathrm{Tr}\big(H_{\varepsilon_k}^{0,0}\mathbf{\Gamma}_k\big) + o(1),$$

since the energies are uniformly bounded. Combined with the energy bound in (165), this shows that the normalized localized density matrices satisfy that energy bound as well.

For the constraints, the density difference $\rho_{\mathbf{\Gamma}_k} - \rho_{\theta_{\varepsilon_k}\mathbf{\Gamma}_k\theta_{\varepsilon_k}}$ is nonnegative and has mass $N\operatorname{Tr}\left(\widetilde{\theta}^2_{\varepsilon_k}\mathbf{\Gamma}_k\right)$. For the current density, differentiation of the real multiplier θ_{ε_k} contributes a purely imaginary term, which disappears from its defining real part. Cauchy–Schwarz, including the state labels, thus gives

$$\begin{aligned}&\|\mathbf{j}^{\mathrm{c},\varepsilon_k}_{\mathbf{\Gamma}_k} - \mathbf{j}^{\mathrm{c},\varepsilon_k}_{\theta_{\varepsilon_k}\mathbf{\Gamma}_k\theta_{\varepsilon_k}}\|_1\\ &\qquad\le \left(N\operatorname{Tr}\left(\widetilde{\theta}^2_{\varepsilon_k}\mathbf{\Gamma}_k\right)\right)^{1/2}\left(\sum_{n=1}^{N}\operatorname{Tr}\left(\mathbf{D}^\dagger_{n,\varepsilon_k}\mathbf{D}_{n,\varepsilon_k}\mathbf{\Gamma}_k\right)\right)^{1/2} \longrightarrow 0.\end{aligned}$$

The trace in this display denotes the squared-derivative form trace. Division by $\operatorname{Tr}\left(\theta^2_{\varepsilon_k}\mathbf{\Gamma}_k\right)$ changes the density by another $N\operatorname{Tr}\left(\widetilde{\theta}^2_{\varepsilon_k}\mathbf{\Gamma}_k\right)$ in L^1 and the current density by $o(1)$ in L^1, by the energy bounds. The original and localized densities are uniformly bounded in L^3, and the corresponding current densities in $L^{3/2}$, by (159).

If $f_k \to 0$ in L^1 and (f_k) is bounded in L^p, $1 < p < \infty$, then $f_k \rightharpoonup 0$ in $L^1 \cap L^p$. Indeed, the L^∞ part of a dual test is controlled by L^1 convergence. For the $L^{p'}$ part, approximate it in that norm by bounded functions and use the uniform L^p bound. Applying this observation to the localization errors proves that they tend weakly to zero in $X \times Y$. Thus the normalized localized density matrices $\theta_{\varepsilon_k}\mathbf{\Gamma}_k\theta_{\varepsilon_k}/\operatorname{Tr}\left(\theta^2_{\varepsilon_k}\mathbf{\Gamma}_k\right)$ also satisfy (165), and they are supported where every $|\mathbf{x}_n| \le 2\varepsilon_k^{-1/2}$. Replacing $\mathbf{\Gamma}_k$ by them, we may assume that $\mathbf{\Gamma}_k$ has this support.

Apply (155) with $L = \varepsilon_k^{-1/2}$, so that $\varepsilon_k L = \sqrt{\varepsilon_k} \to 0$. Since the energies are uniformly bounded, this gives

$$\operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}_k) \le \operatorname{Tr}\left(H^{0,0}_{\varepsilon_k}\mathbf{\Gamma}_k\right) + o(1). \tag{166}$$

Similarly, (154) and (157) give

$$\|\mathbf{j}^{\mathrm{c},\varepsilon_k}_{\mathbf{\Gamma}_k} - \mathbf{j}^{\mathrm{c},\mathrm{d}}_{\mathbf{\Gamma}_k}\|_Y \longrightarrow 0.$$

Together with (165), this establishes

$$(\rho_{\mathbf{\Gamma}_k}, \mathbf{j}^{\mathrm{c},\mathrm{d}}_{\mathbf{\Gamma}_k}) \rightharpoonup (\rho, \mathbf{j}^{\mathrm{c}}) \quad \text{in } X \times Y.$$

The convex norm-lower-semicontinuous functional F_{d} is weakly lower semicontinuous. Hence, using (166) and the energy bound in (165),

$$\begin{aligned}F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}) &\le \liminf_k F_{\mathrm{d}}(\rho_{\mathbf{\Gamma}_k}, \mathbf{j}^{\mathrm{c},\mathrm{d}}_{\mathbf{\Gamma}_k}) \le \liminf_k \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}_k)\\ &\le \liminf_k \operatorname{Tr}\left(H^{0,0}_{\varepsilon_k}\mathbf{\Gamma}_k\right) \le \liminf_k F_{\mathrm{PFL},\varepsilon_k}(\rho_k, \mathbf{j}^{\mathrm{c}}_k).\end{aligned}$$

This proves (75).

Step 4. Recovery sequences converging in norm. Let $F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}) < \infty$. By (160), choose finite-rank density matrices $\mathbf{\Gamma}^m$ such that

$$\|\rho_{\mathbf{\Gamma}^m} - \rho\|_X + \|\mathbf{j}^{\mathrm{c},\mathrm{d}}_{\mathbf{\Gamma}^m} - \mathbf{j}^{\mathrm{c}}\|_Y \le m^{-1}, \qquad \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}^m) \le F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}) + m^{-1}.$$

Using (158), choose a strictly decreasing sequence $\delta_m \downarrow 0$ such that, for $0 < \varepsilon \le \delta_m$,

$$\|\mathbf{j}^{\mathrm{c},\varepsilon}_{\mathbf{\Gamma}^m} - \mathbf{j}^{\mathrm{c},\mathrm{d}}_{\mathbf{\Gamma}^m}\|_Y \le m^{-1}, \qquad |\operatorname{Tr}\left(H^{0,0}_{\varepsilon}\mathbf{\Gamma}^m\right) - \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}^m)| \le m^{-1}.$$

For $\delta_{m+1} < \varepsilon \le \delta_m$, put $(\rho_\varepsilon, \mathbf{j}^{\mathrm{c}}_\varepsilon) = (\rho_{\mathbf{\Gamma}^m}, \mathbf{j}^{\mathrm{c},\varepsilon}_{\mathbf{\Gamma}^m})$. Define $(\rho_\varepsilon, \mathbf{j}^{\mathrm{c}}_\varepsilon)$ arbitrarily for the remaining, larger parameters. Then $(\rho_\varepsilon, \mathbf{j}^{\mathrm{c}}_\varepsilon) \to (\rho, \mathbf{j}^{\mathrm{c}})$ in $X \times Y$, and (161) gives

$$\limsup_{\varepsilon \downarrow 0} F_{\mathrm{PFL},\varepsilon}(\rho_\varepsilon, \mathbf{j}^{\mathrm{c}}_\varepsilon) \le \limsup_{\varepsilon \downarrow 0} \mathrm{Tr}\Big(H^{0,0}_\varepsilon \mathbf{\Gamma}^{m(\varepsilon)}\Big) \le F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}).$$

If $F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c}}) = +\infty$, the constant sequence is a recovery sequence for the stated upper inequality. This proves (76). The lower bound of Step 3 applies in particular to norm-convergent sequences, so the result also implies norm-Gamma convergence. □

Proof of Proposition 4.20. Let $\Psi \in \mathcal{Q}_{\mathrm{PF}}$ be normalized, with U_{d} defined in (228). By Proposition A.10, $U_{\mathrm{d}}^\dagger \Psi$ has finite electronic kinetic energy, $\rho_{U_{\mathrm{d}}^\dagger \Psi} = \rho_\Psi$, and $\mathbf{j}^{\mathrm{p}}_{U_{\mathrm{d}}^\dagger \Psi} = \mathbf{j}^{\mathrm{c,d}}_\Psi$. The Coulomb multiplication form is unchanged. Hence the electronic marginal $\gamma = \mathrm{Tr}_{\mathrm{ph}} |U_{\mathrm{d}}^\dagger \Psi\rangle\langle U_{\mathrm{d}}^\dagger \Psi|$ satisfies

$$\begin{aligned} F_{\mathrm{VR}}(\rho_\Psi, \mathbf{j}^{\mathrm{c,d}}_\Psi) &\le \mathrm{Tr}\big(H^0_{\mathrm{el}} \gamma\big) \\ &= \frac{1}{2} \sum_{n=1}^N \|\mathbf{D}_{n,\mathrm{d}} \Psi\|^2 + \langle \Psi, W \Psi \rangle \le \langle \Psi, H_{\mathrm{d}} \Psi \rangle, \end{aligned} \tag{167}$$

where $W = \sum_{n<m} |\mathbf{x}_n - \mathbf{x}_m|^{-1}$. The equality uses (229), and the last inequality drops the nonnegative radiation energy $\|\sqrt{H_{\mathrm{rad}}} \Psi\|^2$.

Taking the pure constrained-search infimum in (167) gives $F_{\mathrm{VR}} \le F_{\mathrm{PFLL,d}}$. The electronic mixed-state functional is convex by mixing, and norm lower semicontinuous by the electronic compactness argument in the proof of Theorem 4.18. It is therefore bounded above by the norm-lower-semicontinuous convex envelope of $F_{\mathrm{PFLL,d}}$. By (74), this proves $F_{\mathrm{VR}} \le F_{\mathrm{d}}$.

For the upper bound, take any finite-energy electronic density matrix γ representing $(\rho, \mathbf{j}^{\mathrm{c,d}})$ and tensor it with the photon vacuum:

$$\mathbf{\Gamma} = \gamma \otimes |\Omega\rangle\langle\Omega|.$$

The vacuum field expectation vanishes, so $(\rho_{\mathbf{\Gamma}}, \mathbf{j}^{\mathrm{c,d}}_{\mathbf{\Gamma}}) = (\rho, \mathbf{j}^{\mathrm{c,d}})$. The cross terms in the covariant kinetic form also vanish. Since $\mathfrak{A}^\mu(0)\Omega = a^\dagger(G^\mu_0)\Omega$, (14) gives exactly

$$\mathrm{Tr}(H_{\mathrm{d}} \mathbf{\Gamma}) = \mathrm{Tr}\big(H^0_{\mathrm{el}} \gamma\big) + \frac{Ne^2}{2} \sum_{\mu=1}^3 \|G^\mu_0\|^2 = \mathrm{Tr}\big(H^0_{\mathrm{el}} \gamma\big) + \frac{Ne^2}{2} \|\widehat{\chi}\|^2. \tag{168}$$

In particular, $\mathbf{\Gamma}$ has finite energy, so it is a competitor in the mixed-state search (81) at $(\rho, \mathbf{j}^{\mathrm{c,d}})$. Hence Theorem 4.21 gives

$$F_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c,d}}) = \widetilde{F}_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c,d}}) \le \mathrm{Tr}(H_{\mathrm{d}} \mathbf{\Gamma}).$$

Taking the infimum over γ in (168) proves the upper inequality in (77). The two inequalities imply (78), and the hard-cutoff value follows from (11). □

Proof of Theorem 4.21. Fix a finite particle number $N \in \mathbb{N}$. First consider the mixed-state search (81). Factor the photon Fock space at $\omega = \kappa$, and write

$$\mathfrak{A}(0) = \mathfrak{A}_{\ge\kappa}(0) + \mathfrak{A}_{<\kappa}(0), \qquad H_{\mathrm{rad}} = H_{\mathrm{rad},\ge\kappa} + H_{\mathrm{rad},<\kappa}.$$

As in the paragraph preceding (228), Proposition A.6(iii) shows that the three components of each constant field strongly commute, and fields acting on the low- and high-frequency factors also commute. With $\mathbf{R} = \sum_{n=1}^{N} \mathbf{x}_n$, put

$$V_\kappa = \exp(-\mathrm{i}e\mathbf{R} \cdot \mathfrak{A}_{<\kappa}(0)), \qquad \mathbf{\Gamma}_\kappa = \big(\operatorname{Tr}_{<\kappa} V_\kappa \mathbf{\Gamma} V_\kappa^\dagger \big) \otimes |\Omega_{<\kappa}\rangle\langle\Omega_{<\kappa}|. \tag{169}$$

This is unitary conjugation followed by a partial trace and vacuum preparation, and hence defines a positive trace-preserving channel. The multiplier V_κ is permutation invariant, so this channel preserves the antisymmetric electronic space.

The weak-derivative argument used for (232) gives

$$(-\mathrm{i}\nabla_{\mathbf{x}_n} - e\mathfrak{A}_{\geq\kappa}(0))V_\kappa \Psi = V_\kappa \mathbf{D}_{n,\mathrm{d}} \Psi, \qquad 1 \leq n \leq N.$$

The high-mode radiation energy commutes with V_κ. Pointwise unitarity preserves the full electronic configuration density and hence the Coulomb energy. Taking the low-mode partial trace preserves the density and combined current density, while vacuum preparation adds the low-mode vacuum variance to each of the N kinetic terms. Writing $b_\kappa = \|\mathbb{1}_{\{\omega<\kappa\}}\widehat{\chi}\|$ and $E_{<\kappa}(\mathbf{\Gamma}) = \operatorname{Tr}(H_{\mathrm{rad},<\kappa}\mathbf{\Gamma})$, we obtain the exact identities

$$\begin{aligned} \rho_{\mathbf{\Gamma}_\kappa} = \rho_{\mathbf{\Gamma}}, \qquad \mathbf{j}^{\mathrm{c,d}}_{\mathbf{\Gamma}_\kappa} = \mathbf{j}^{\mathrm{c,d}}_{\mathbf{\Gamma}}, \\ \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}_\kappa) = \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}) - E_{<\kappa}(\mathbf{\Gamma}) + \frac{Ne^2}{2} b_\kappa^2. \end{aligned} \tag{170}$$

In particular the output has finite form energy. No low-mode radiation form bound on $V_\kappa\Psi$ is needed, since that factor is traced out. This observation avoids imposing any electronic position moment.

Let $m = \widetilde{F}_{\mathrm{d}}(\rho, \mathbf{j}^{\mathrm{c,d}}) < \infty$, and let $\mathbf{\Gamma}$ represent $(\rho, \mathbf{j}^{\mathrm{c,d}})$ with $\operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}) \leq m + \delta$. Since the channel preserves the density and combined current density, (170) implies, for every $t > 0$,

$$E_{<t}(\mathbf{\Gamma}) \leq \delta + \frac{Ne^2}{2} b_t^2.$$

The high-mode photon marginal is unchanged by the channel. Thus, for $0 < \kappa \leq 1$, integration of the one-photon energy measure against $\omega^{-1}\mathbb{1}_{\{\omega\geq\kappa\}}$ gives

$$\begin{aligned} \operatorname{Tr}(\mathcal{N}\mathbf{\Gamma}_\kappa) &= \operatorname{Tr}\big(\mathrm{d}\Gamma(\mathbb{1}_{\{\omega\geq\kappa\}})\mathbf{\Gamma}\big) \\ &\leq \operatorname{Tr}(H_{\mathrm{rad}}\mathbf{\Gamma}) + \int_\kappa^1 \frac{E_{<t}(\mathbf{\Gamma})}{t^2}\mathrm{d}t \\ &\leq \operatorname{Tr}(H_{\mathrm{d}}\mathbf{\Gamma}) + \frac{\delta}{\kappa} + \frac{Ne^2}{2}\left\| \frac{\mathbb{1}_{\{\omega<1\}}\widehat{\chi}}{\sqrt{\omega}} \right\|^2 . \end{aligned} \tag{171}$$

For the last step use Tonelli's theorem on $\int_0^1 b_t^2 t^{-2}\mathrm{d}t$.

Choose $\kappa_l \downarrow 0$ and almost minimizers with $\delta_l \leq \kappa_l$. Their images under (169) have the prescribed density and combined current density, uniformly bounded mean photon number, and energies at most $m + \delta_l + (Ne^2/2)b_{\kappa_l}^2 \to m$. The photon-loss compactness argument of Lemma 5.7 applies also to the constant coupling kernels G_0^μ. To check this directly, its form bounds and electronic localization are unchanged, and the kernel compactness step uses the singleton $\{G_0^\mu\}$ in place of $\{G_{\mathbf{x}}^\mu : |\mathbf{x}| \leq 2L\}$, so the same photon-localization error tends to zero. The uniform mean-number bound supplies its local-sector tightness condition. The fixed electronic density supplies electronic tightness. Consequently it produces a normalized

finite-energy density matrix with density ρ, combined current density $\mathbf{j}^{\mathrm{c,d}}$, and energy at most m. This proves attainment. The retained limit also has finite mean photon number by lower semicontinuity through the localized trace-norm limits.

The same argument proves norm lower semicontinuity. Given pairs $(\rho_l, \mathbf{j}_l^{\mathrm{c,d}})$ converging in $X \times Y$ with bounded mixed-state infima, choose an almost minimizer at each of them with error $\delta_l \le \kappa_l \to 0$ and apply the channel at κ_l. The output constraints are unchanged, the energies increase by at most $(Ne^2/2)b_{\kappa_l}^2 \to 0$, and (171) is uniform. Norm convergence of the densities gives electronic tightness, so the same compactness argument produces a density matrix at the limiting pair with energy at most the original liminf. Thus $\widetilde{F}_{\mathrm{d}}$ is norm lower semicontinuous. It is convex by mixing, and

$$F_{\mathrm{d}} \le \widetilde{F}_{\mathrm{d}} \le F_{\mathrm{PFLL,d}}.$$

The closed-convex-envelope identity (74) now gives $\widetilde{F}_{\mathrm{d}} = F_{\mathrm{d}}$.

It remains to compare pure-state and mixed-state infima. The dipole field leaves enough photon modes uncoupled to purify a density matrix at arbitrarily small energy. Indeed, in radial coordinates write

$$\mathfrak{H}_{\mathrm{ph}} = L^2((0,\infty), r^2\mathrm{d}r; L^2(S^2 \times \{1,2\})).$$

Let $p_{\mathrm{b}}(r)$ be the measurable orthogonal projection onto $\mathrm{Span}\{G_0^\mu(r,\cdot) : \mu = 1,2,3\}$, and set $\mathfrak{H}_{\mathrm{b}} = \mathrm{Ran}\, p_{\mathrm{b}}$ and $\mathfrak{H}_{\mathrm{d}} = \mathfrak{H}_{\mathrm{b}}^{\perp}$. Both spaces reduce multiplication by $\omega = r$, and every coupling kernel belongs to $\mathfrak{H}_{\mathrm{b}}$. Consequently, in the Fock factorization over $\mathfrak{H}_{\mathrm{b}} \oplus \mathfrak{H}_{\mathrm{d}}$, the field acts only on the first factor. Each angular fiber of $\mathfrak{H}_{\mathrm{d}}$ is infinite dimensional, because $p_{\mathrm{b}}(r)$ has rank at most three. Thus, for every $a > 0$, the dark subspace with $0 < \omega < a$ contains an orthonormal sequence (ξ_l).

Given a finite-energy density matrix, trace out its dark factor. This preserves its density and combined current density and can only decrease its energy. Write the resulting electronic–bright density matrix on $\mathfrak{H}_{\mathrm{el}}^N \otimes \mathcal{F}_s(\mathfrak{H}_{\mathrm{b}})$ spectrally as $\sum_l p_l |\Phi_l\rangle\langle\Phi_l|$ and purify it by

$$\Psi_a = \sum_l \sqrt{p_l}\, \Phi_l \otimes a^\dagger(\xi_l)\Omega_{\mathrm{d}}.$$

Each Φ_l is antisymmetric in the electronic variables, and so is Ψ_a. Orthogonality of the photon tags preserves the density, the combined current density, and the electronic interaction energy exactly. Their energies are at most a, so Ψ_a has form energy at most the original energy plus a. Letting $a \downarrow 0$ gives $F_{\mathrm{PFLL,d}} \le \widetilde{F}_{\mathrm{d}}$, and the reverse inequality follows by including rank-one density matrices. Therefore $F_{\mathrm{PFLL,d}} = \widetilde{F}_{\mathrm{d}} = F_{\mathrm{d}}$. The construction proves equality of the infima, without asserting that a pure minimizer exists. □

Proof of Corollary 4.22. **Step 1. The radiation-energy form.** Let U_{d} be the unitary (228). By Proposition A.10, $\Phi \mapsto \Psi = U_{\mathrm{d}}^\dagger \Phi$ maps $\mathcal{Q}_{\mathrm{PF}}$ bijectively onto the vectors Ψ with $U_{\mathrm{d}}\Psi \in \mathcal{Q}_{\mathrm{PF}}$, with $\rho_\Psi = \rho_\Phi$, $\mathbf{j}_\Psi^{\mathrm{p}} = \mathbf{j}_\Phi^{\mathrm{c,d}}$, and, by (229) and invariance of the Coulomb form, $\langle\Phi, H_{\mathrm{d}}\Phi\rangle = \langle\Psi, H_{\mathrm{el}}^0\Psi\rangle + \|\sqrt{H_{\mathrm{rad}}}U_{\mathrm{d}}\Psi\|^2$. The forms of H_{d}, $H^{0,0}$ and $H_{\mathrm{el}}^0 + H_{\mathrm{rad}}$ are all equivalent to the norm of $\mathcal{Q}_{\mathrm{PF}}$ ((27)), so the admissible set of (81) consists of the $\mathbf{\Gamma} \in \mathcal{D}$ with the prescribed density and combined current density. Applied to the eigenvectors of a density matrix, the above shows that $\mathbf{\Gamma} \mapsto U_{\mathrm{d}}^\dagger \mathbf{\Gamma} U_{\mathrm{d}}$ maps $\mathcal{D}$ bijectively onto the density matrices $\mathbf{\Gamma}$ with $U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^\dagger \in \mathcal{D}$. It

preserves the density, takes $\mathbf{j}^{\mathrm{c,d}}$ to $\mathbf{j}^{\mathrm{p}}$, and

$$\mathrm{Tr}\Big(H_{\mathrm{d}}U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^{\dagger}\Big)=\mathrm{Tr}\big(H_{\mathrm{el}}^{0}\mathbf{\Gamma}\big)+\mathrm{Tr}\Big(H_{\mathrm{rad}}U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^{\dagger}\Big). \tag{172}$$

By Theorem 4.21, $\widetilde{F}_{\mathrm{d}}=F_{\mathrm{d}}$, and every finite infimum in (81) is attained. Hence, for all $(\rho,\mathbf{j}^{\mathrm{c,d}})\in X\times Y$,

$$F_{\mathrm{d}}(\rho,\mathbf{j}^{\mathrm{c,d}})=\inf_{\substack{U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^{\dagger}\in\mathcal{D}\\ \rho_{\mathbf{\Gamma}}=\rho,\ \mathbf{j}_{\mathbf{\Gamma}}^{\mathrm{p}}=\mathbf{j}^{\mathrm{c,d}}}}\Big[\mathrm{Tr}\big(H_{\mathrm{el}}^{0}\mathbf{\Gamma}\big)+\mathrm{Tr}\Big(H_{\mathrm{rad}}U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^{\dagger}\Big)\Big], \tag{173}$$

and every finite infimum here is attained. This step uses neither $\sqrt{\omega}\,\widehat{\chi}\in L^{2}$ nor the moment assumption.

Step 2. Expansion of the radiation energy. Let $\mathbf{\Gamma}=\sum_{j}\lambda_{j}|\Psi_{j}\rangle\langle\Psi_{j}|$, with $\lambda_{j}>0$ and orthonormal Ψ_{j}, have density ρ. Since $|\mathbf{R}|^{2}\le N\sum_{n}|\mathbf{x}_{n}|^{2}$,

$$\sum_{j}\lambda_{j}\langle\Psi_{j},|\mathbf{R}|^{2}\Psi_{j}\rangle\le N\int_{\mathbb{R}^{3}}|\mathbf{x}|^{2}\rho<\infty.$$

At each electronic configuration take $h=e\sum_{\mu}R^{\mu}G_{0}^{\mu}$; then $\|\sqrt{\omega}h\|^{2}=e^{2}\mathbf{R}^{\top}\mathbf{M}\mathbf{R}\le e^{2}\|\mathbf{M}\|\mathbf{R}|^{2}$. The bound (212), applied with $\pm\mathrm{i}h$ and integrated, gives, for every Ψ with $\langle\Psi,|\mathbf{R}|^{2}\Psi\rangle<\infty$,

$$\|\sqrt{H_{\mathrm{rad}}}U_{\mathrm{d}}^{\pm1}\Psi\|^{2}\le2\|\sqrt{H_{\mathrm{rad}}}\Psi\|^{2}+2e^{2}\|\mathbf{M}\|\langle\Psi,|\mathbf{R}|^{2}\Psi\rangle.$$

Applying this to Ψ_{j} and to $U_{\mathrm{d}}\Psi_{j}$ shows that $U_{\mathrm{d}}\Psi_{j}\in D(\sqrt{H_{\mathrm{rad}}})$ if and only if $\Psi_{j}\in D(\sqrt{H_{\mathrm{rad}}})$. By Proposition A.10, applied also with $-e$ in place of e, $U_{\mathrm{d}}\Psi_{j}$ and Ψ_{j} have finite electronic kinetic energy together, so $U_{\mathrm{d}}\Psi_{j}\in\mathcal{Q}_{\mathrm{PF}}$ if and only if $\Psi_{j}\in\mathcal{Q}_{\mathrm{PF}}$. Summing the displayed bound over j and using (172) and the form-norm equivalence of Step 1 then shows that $U_{\mathrm{d}}\mathbf{\Gamma}U_{\mathrm{d}}^{\dagger}\in\mathcal{D}$ if and only if $\mathbf{\Gamma}\in\mathcal{D}$. Thus the admissible sets in (173) and (85) coincide. For each j, the Weyl shift (233) with $\eta=\Psi_{j}(\mathbf{X})$, integrated over $\mathbf{X}$, gives

$$\|\sqrt{H_{\mathrm{rad}}}U_{\mathrm{d}}\Psi_{j}\|^{2}=\langle\Psi_{j},\big[H_{\mathrm{rad}}-e\mathbf{R}\cdot\mathfrak{E}_{\perp}(0)+e^{2}\mathbf{R}^{\top}\mathbf{M}\mathbf{R}\big]\Psi_{j}\rangle,$$

where $e\sum_{\mu}R^{\mu}\Pi(\omega G_{0}^{\mu})=-e\mathbf{R}\cdot\mathfrak{E}_{\perp}(0)$ by (84). The bound on a_{ω} following (211) gives $|\Pi(\omega h)[\eta,\eta]|\le2\|\sqrt{\omega}h\|\,\|\sqrt{H_{\mathrm{rad}}}\eta\|\,\|\eta\|$, so by the Cauchy–Schwarz inequality the weighted sums over j of the three terms converge absolutely. Summing over j turns (173) into (85), and the attainment statement carries over. Restricting to rank-one $\mathbf{\Gamma}$ and using $F_{\mathrm{PFLL,d}}=F_{\mathrm{d}}$ from (82) gives the pure-state version. □

Appendix A. Transformation properties

We work in the solenoidal one-photon representation and, unless stated otherwise, specialize to the hard cutoff (10). Second quantization is understood whenever a one-photon unitary is applied to a Fock-space state. The displayed e,Λ labels on $\mathfrak{A}_{\Lambda}$, $H_{e,\Lambda}^{0,0}$, $(\mathbf{j}_{\Psi}^{\mathrm{c}})^{e,\Lambda}$, and $F^{e,\Lambda}$ record parameter dependence that was suppressed earlier. Here Λ abbreviates the form-factor label χ_{Λ}, so that, for instance, $F^{e,\Lambda}=F^{e,\chi_{\Lambda}}$. An unsuperscripted F carries the parameters shown in the surrounding formula. All state identities below apply to normalized vectors in the indicated form domains, and Hamiltonian identities are identities of self-adjoint operators established through their closed quadratic forms, unless explicitly stated only as form identities.

A.1. **Isometries.** The field momentum is the second quantization

$$\mathbf{P}_{\mathrm{ph}} = \mathrm{d}\Gamma(\mathbf{k}) = \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} \mathbf{k}\, a^\dagger(\mathbf{k},\lambda) a(\mathbf{k},\lambda) \mathrm{d}\mathbf{k}.$$

For $\mathbf{b} \in \mathbb{R}^3$, define the photon translation

$$(t_{\mathbf{b}}\mathbf{f})(\mathbf{k}) = e^{-\mathrm{i}\mathbf{b}\cdot\mathbf{k}}\mathbf{f}(\mathbf{k}), \qquad T_{\mathrm{ph}}(\mathbf{b}) = \Gamma(t_{\mathbf{b}}) = e^{-\mathrm{i}\mathbf{b}\cdot\mathbf{P}_{\mathrm{ph}}},$$

and the electron translation

$$(T_{\mathrm{el}}(\mathbf{b})\Phi)(\mathbf{x}_1,\dots,\mathbf{x}_N) = \Phi(\mathbf{x}_1-\mathbf{b},\dots,\mathbf{x}_N-\mathbf{b}).$$

The composite system is translated by

$$T(\mathbf{b}) = T_{\mathrm{el}}(\mathbf{b}) \otimes T_{\mathrm{ph}}(\mathbf{b}).$$

Proposition A.1. *$T(\mathbf{b})$ is a unitary preserving $\mathcal{Q}_{\mathrm{PF}}$, and*

$$T_{\mathrm{ph}}(\mathbf{b})^\dagger \mathfrak{A}_\Lambda(\mathbf{x}) T_{\mathrm{ph}}(\mathbf{b}) = \mathfrak{A}_\Lambda(\mathbf{x}-\mathbf{b}). \tag{174}$$

The internal Hamiltonian, density, and combined current density satisfy

$$\begin{gathered} T(\mathbf{b})^\dagger H^{0,0} T(\mathbf{b}) = H^{0,0}, \\ \rho_{T(\mathbf{b})\Psi}(\mathbf{x}) = \rho_\Psi(\mathbf{x}-\mathbf{b}), \qquad \mathbf{j}^{\mathrm{c}}_{T(\mathbf{b})\Psi}(\mathbf{x}) = \mathbf{j}^{\mathrm{c}}_\Psi(\mathbf{x}-\mathbf{b}). \end{gathered} \tag{175}$$

Consequently, for every $(\rho,\mathbf{j}^{\mathrm{c}}) \in X \times Y$ and $F \in \{F_{\mathrm{PFLL}}, F_{\mathrm{PFL}}\}$,

$$F(\rho(\,\cdot-\mathbf{b}), \mathbf{j}^{\mathrm{c}}(\,\cdot-\mathbf{b})) = F(\rho,\mathbf{j}^{\mathrm{c}}). \tag{176}$$

Proof. The solenoidal coupling functions in (13) obey $t_{\mathbf{b}}^\dagger \mathbf{G}^\mu_{\mathbf{x};\Lambda} = \mathbf{G}^\mu_{\mathbf{x}-\mathbf{b};\Lambda}$. Covariance of creation and annihilation operators under second quantization gives (174). Moreover, $t_{\mathbf{b}}$ commutes with ω, so $T_{\mathrm{ph}}(\mathbf{b})$ commutes with H_{rad}. Electronic translation preserves weak derivatives and all interparticle distances. Thus $T(\mathbf{b})$ preserves $\mathcal{Q}_{\mathrm{PF}}$, and the electronic and photon translations cancel in the field term:

$$T(\mathbf{b})^\dagger \mathfrak{A}_\Lambda(\mathbf{x}_n) T(\mathbf{b}) = \mathfrak{A}_\Lambda(\mathbf{x}_n), \qquad T(\mathbf{b})^\dagger \mathbf{D}_n T(\mathbf{b}) = \mathbf{D}_n.$$

These identities first hold on test vectors and extend by the field bound (20) and form-norm approximation. The kinetic, Coulomb, and radiation forms are therefore invariant. Changing the electronic integration variables in (33) and (36) gives the remaining identities in (175).

The inverse $T(-\mathbf{b})$ makes this an energy-preserving bijection between the corresponding constraint sets, proving (176) for F_{PFLL}, including empty constraint sets. Translation is a linear homeomorphism of $X \times Y$, so taking the norm-lower-semicontinuous convex envelope in (55) proves the identity for F_{PFL}. □

For $\mathbf{R} \in \mathrm{O}(3)$, define on $\mathfrak{H}_{\mathrm{sol}}$

$$(\Upsilon_{\mathbf{R}}\mathbf{f})(\mathbf{k}) = \mathbf{R}\mathbf{f}(\mathbf{R}^\top\mathbf{k}), \tag{177}$$

and on $\mathcal{H}_N$ define

$$(U_{\mathbf{R}}\Psi)(\mathbf{x}_1,\dots,\mathbf{x}_N) = \Upsilon_{\mathbf{R}}\Psi(\mathbf{R}^\top\mathbf{x}_1,\dots,\mathbf{R}^\top\mathbf{x}_N).$$

Proposition A.2. *These maps are unitary, and $U_{\mathbf{R}}$ preserves $\mathcal{Q}_{\mathrm{PF}}$. The creation, annihilation, and field operators transform according to*

$$\Upsilon_{\mathbf{R}} a^\#(\mathbf{f}) \Upsilon_{\mathbf{R}}^\dagger = a^\#(\Upsilon_{\mathbf{R}}\mathbf{f}), \tag{178}$$

$$\Upsilon_{\mathbf{R}}^\dagger \mathfrak{A}_\Lambda(\mathbf{x}) \Upsilon_{\mathbf{R}} = \mathbf{R}\mathfrak{A}_\Lambda(\mathbf{R}^\top\mathbf{x}). \tag{179}$$

The corresponding state identities are

$$U_{\mathbf{R}}^{\dagger} H^{0,0} U_{\mathbf{R}} = H^{0,0}, \tag{180}$$

$$\rho_{U_{\mathbf{R}}\Psi}(\mathbf{x}) = \rho_{\Psi}(\mathbf{R}^{\top}\mathbf{x}), \tag{181}$$

$$\mathbf{j}^{\mathrm{c}}_{U_{\mathbf{R}}\Psi}(\mathbf{x}) = \mathbf{R}\mathbf{j}^{\mathrm{c}}_{\Psi}(\mathbf{R}^{\top}\mathbf{x}). \tag{182}$$

Consequently, for every $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$ *and* $F \in \{F_{\mathrm{PFLL}}, F_{\mathrm{PFL}}\}$,

$$F(\rho \circ \mathbf{R}^{\top}, \mathbf{R}\mathbf{j}^{\mathrm{c}} \circ \mathbf{R}^{\top}) = F(\rho, \mathbf{j}^{\mathrm{c}}). \tag{183}$$

Proof. Orthogonal changes of variables preserve Lebesgue measure. For solenoidal $\mathbf{f}$, they also preserve transversality, since

$$\mathbf{k} \cdot \mathbf{R}\mathbf{f}(\mathbf{R}^{\top}\mathbf{k}) = (\mathbf{R}^{\top}\mathbf{k}) \cdot \mathbf{f}(\mathbf{R}^{\top}\mathbf{k}) = 0.$$

Thus $\Upsilon_{\mathbf{R}}$ is unitary on $\mathfrak{H}_{\mathrm{sol}}$ with inverse $\Upsilon_{\mathbf{R}^{\top}}$, and (178) is the second-quantization identity. By (8),

$$P_{\mathrm{sol}}(\mathbf{R}\mathbf{k}) = \mathbf{R} P_{\mathrm{sol}}(\mathbf{k}) \mathbf{R}^{\top}.$$

Using radiality of the hard cutoff in (13), we obtain

$$\Upsilon_{\mathbf{R}}^{\dagger} \mathbf{G}^{\mu}_{\mathbf{x};\Lambda} = \sum_{\nu=1}^{3} R^{\mu\nu} \mathbf{G}^{\nu}_{\mathbf{R}^{\top}\mathbf{x};\Lambda},$$

which proves (179). Radiality of ω also gives $\Upsilon_{\mathbf{R}}^{\dagger} H_{\mathrm{rad}} \Upsilon_{\mathbf{R}} = H_{\mathrm{rad}}$.

The electronic chain rule and (179) yield $U_{\mathbf{R}}^{\dagger} \mathbf{D}_n U_{\mathbf{R}} = \mathbf{R}\mathbf{D}_n$. Orthogonality preserves the squared covariant-derivative norms and the Coulomb interaction. These facts prove form-domain preservation and (180), first on test vectors and then by form approximation. Changing variables in the partial inner products gives (181) and (182). Finally, $U_{\mathbf{R}^{\top}}$ is the inverse map on constraint sets, so (183) holds for F_{PFLL}. The induced map on $X \times Y$ is a linear homeomorphism, so (55) proves the result for F_{PFL}. □

A.2. **Dilations.**

Proposition A.3 (Dilation identities)**.** *For* $\lambda > 0$*, define on* $\mathfrak{H}_{\mathrm{sol}}$

$$(\Upsilon_{\lambda}\mathbf{f})(\mathbf{k}) = \lambda^{3/2}\mathbf{f}(\lambda\mathbf{k}).$$

This is unitary, and

$$\Upsilon_{\lambda} a^{\#}(\mathbf{f}) \Upsilon_{\lambda}^{\dagger} = a^{\#}(\Upsilon_{\lambda}\mathbf{f}), \tag{184}$$

$$\Upsilon_{\lambda} H_{\mathrm{rad}} \Upsilon_{\lambda}^{\dagger} = \lambda H_{\mathrm{rad}}, \tag{185}$$

$$\Upsilon_{\lambda} \mathfrak{A}_{\Lambda}(\mathbf{x}) \Upsilon_{\lambda}^{\dagger} = \lambda \mathfrak{A}_{\Lambda/\lambda}(\lambda\mathbf{x}). \tag{186}$$

Let

$$(S_{\lambda}\Phi)(\mathbf{X}) = \lambda^{3N/2}\Phi(\lambda\mathbf{X}), \qquad V_{\lambda} = S_{\lambda} \otimes \Upsilon_{\lambda}^{\dagger}, \qquad \Psi_{\lambda} = V_{\lambda}\Psi.$$

The map V_{λ} *is unitary on* $\mathcal{H}_N$ *and maps* $Q(H^{0,0}_{e,\Lambda/\lambda})$ *bijectively onto* $Q(H^{0,0}_{e,\Lambda})$*. The density and current density satisfy*

$$\rho_{\Psi_{\lambda}}(\mathbf{x}) = \lambda^3 \rho_{\Psi}(\lambda\mathbf{x}), \tag{187}$$

$$(\mathbf{j}^{\mathrm{c}}_{\Psi_{\lambda}})^{e,\Lambda}(\mathbf{x}) = \lambda^4 (\mathbf{j}^{\mathrm{c}}_{\Psi})^{e,\Lambda/\lambda}(\lambda\mathbf{x}). \tag{188}$$

The internal Hamiltonian satisfies the operator identity

$$V_\lambda^\dagger H_{e,\Lambda}^{0,0} V_\lambda = \frac{\lambda^2}{2}\sum_{n=1}^{N}\big(-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} - e\mathfrak{A}_{\Lambda/\lambda}(\mathbf{x}_n)\big)^2 + \lambda\sum_{1\le n<m\le N}\frac{1}{|\mathbf{x}_n-\mathbf{x}_m|} + \lambda H_{\mathrm{rad}}. \tag{189}$$

The right-hand side denotes the self-adjoint operator associated with the displayed sum of nonnegative forms on $\mathcal{Q}_{\mathrm{PF}}$.

Proof. A change of momentum variables proves unitarity of Υ_λ, and transversality is preserved because $\mathbf{k}\cdot\mathbf{f}(\lambda\mathbf{k}) = \lambda^{-1}(\lambda\mathbf{k})\cdot\mathbf{f}(\lambda\mathbf{k})$. Second quantization gives (184), while $\Upsilon_\lambda\omega\Upsilon_\lambda^\dagger = \lambda\omega$ gives (185). The hard cutoff obeys

$$P_{\mathrm{sol}}(\lambda\mathbf{k}) = P_{\mathrm{sol}}(\mathbf{k}), \qquad \widehat{\chi}_\Lambda(\lambda\mathbf{k}) = \lambda^{-1/2}\widehat{\chi}_{\Lambda/\lambda}(\mathbf{k}).$$

Consequently, (13) gives $\Upsilon_\lambda \mathbf{G}^\mu_{\mathbf{x};\Lambda} = \lambda\mathbf{G}^\mu_{\lambda\mathbf{x};\Lambda/\lambda}$, which proves (186).

The electronic chain rule and (186) imply

$$\mathbf{D}_n^{e,\Lambda} V_\lambda \Psi = \lambda V_\lambda \mathbf{D}_n^{e,\Lambda/\lambda}\Psi.$$

The electronic derivatives scale by λ, the radiation form by λ, and $V_\lambda^{-1} = V_{1/\lambda}$. Thus the reference domain (23) is preserved in both directions. A change of electronic variables gives (187) and (188), with the extra factor in the current density coming from the covariant derivative. The Coulomb interaction scales by λ, so the squared-derivative identity gives equality of the quadratic forms on the two sides of (189). The calculation extends from test vectors to $\mathcal{Q}_{\mathrm{PF}}$ by (27). Since $\lambda > 0$, the form on the right is closed on this domain, with a norm equivalent to the reference form norm. Polarization and uniqueness in the representation theorem for closed forms therefore give the asserted equality of self-adjoint operators. □

The covariant kinetic term scales quadratically. The Coulomb and photon terms scale linearly.

A.3. **Time reversal.** Time reversal needs only (9), not the hard cutoff. In the solenoidal representation, recall the conjugation $(J\mathbf{f})(\mathbf{k}) = \overline{\mathbf{f}(-\mathbf{k})}$. This is an antiunitary involution commuting with ω and with the rotations (177), and (9) gives $J\mathbf{G}^\mu_{\mathbf{x}} = \mathbf{G}^\mu_{\mathbf{x}}$. Let $\mathcal{C}_J$ be the induced antiunitary involution of $\mathcal{F}_{\mathrm{ph}}$, characterized by $\mathcal{C}_J a^\#(\mathbf{f})\mathcal{C}_J = a^\#(J\mathbf{f})$, and define the time reversal

$$(\Theta\Psi)(\mathbf{X}) = (-1)^{\mathcal{N}}\mathcal{C}_J\big(\Psi(\mathbf{X})\big), \tag{190}$$

where $(-1)^{\mathcal{N}} = \Gamma(-\mathbb{1}) = e^{\mathrm{i}\pi\mathcal{N}}$ multiplies the m-photon component by $(-1)^m$. Equivalently, $\Theta = C\otimes\Gamma(-J)$, where C is complex conjugation of electronic wave functions.

Proposition A.4 (Time reversal)**.** *Θ is an antiunitary involution of $\mathcal{H}_N$ that preserves $\mathcal{Q}_{\mathrm{PF}}$ and commutes with every $U_{\mathbf{R}}$ of Proposition A.2. The field and the covariant derivatives are odd and the radiation energy is even:*

$$\Theta\mathfrak{A}(\mathbf{x})\Theta^{-1} = -\mathfrak{A}(\mathbf{x}), \qquad \Theta\mathbf{D}_n\Theta^{-1} = -\mathbf{D}_n, \qquad \Theta H_{\mathrm{rad}}\Theta^{-1} = H_{\mathrm{rad}}. \tag{191}$$

Consequently, $\mathfrak{E}_\perp$ is even and $\mathfrak{B}$ is odd, and for external potentials in (29),

$$\Theta H^{v,\mathbf{A}}\Theta^{-1} = H^{v,-\mathbf{A}}. \tag{192}$$

The corresponding state identities are

$$\rho_{\Theta\Psi} = \rho_\Psi, \qquad \mathbf{j}^{\mathrm{c}}_{\Theta\Psi} = -\mathbf{j}^{\mathrm{c}}_{\Psi}, \qquad \langle \Theta\Psi, H^{0,0}\Theta\Psi\rangle = \langle \Psi, H^{0,0}\Psi\rangle. \tag{193}$$

Consequently, for every $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$ *and* $F \in \{F_{\mathrm{PFLL}}, F_{\mathrm{PFL}}\}$,

$$F(\rho, -\mathbf{j}^{\mathrm{c}}) = F(\rho, \mathbf{j}^{\mathrm{c}}). \tag{194}$$

Proof. Second quantization of $J\mathbf{G}^\mu_{\mathbf{x}} = \mathbf{G}^\mu_{\mathbf{x}}$ and $J\omega = \omega J$ gives $\mathcal{C}_J \mathfrak{A}(\mathbf{x}) \mathcal{C}_J = \mathfrak{A}(\mathbf{x})$ and $\mathcal{C}_J H_{\mathrm{rad}} \mathcal{C}_J = H_{\mathrm{rad}}$, while $(-1)^{\mathcal{N}} a^\#(\mathbf{f})(-1)^{\mathcal{N}} = -a^\#(\mathbf{f})$. Applied pointwise in $\mathbf{X}$, the antilinear map $\mathcal{C}_J$ also conjugates the electronic dependence, so $-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n}$ changes sign. This proves (191) on test vectors. The field bound (20) and form-norm approximation extend it, and show that Θ preserves $\mathcal{Q}_{\mathrm{PF}}$. Since $\mathcal{C}_J^2 = \mathbb{1}$ and $(-1)^{\mathcal{N}}$ commutes with $\mathcal{C}_J$, $\Theta^2 = \mathbb{1}$. The pointwise action preserves fermionic antisymmetry. Because J commutes with the one-photon rotations, $\mathcal{C}_J$ and $(-1)^{\mathcal{N}}$ commute with their second quantizations, so $\Theta U_{\mathbf{R}} = U_{\mathbf{R}}\Theta$.

As Θ is antilinear, $\mathfrak{E}_\perp = -\mathrm{i}[H_{\mathrm{rad}}, \mathfrak{A}]$ is even, and $\mathfrak{B} = \boldsymbol{\nabla} \times \mathfrak{A}$ is odd. The real multiplication operators v, $\mathbf{A}(\mathbf{x}_n)$, and the Coulomb interaction commute with Θ, which gives (192) as an identity of closed forms. Pointwise antiunitarity gives $\rho_{\Theta\Psi} = \rho_\Psi$ and, by (191),

$$\mathbf{j}^{\mathrm{c}}_{\Theta\Psi}(\mathbf{x}) = N \operatorname{Re}\langle \Theta\Psi, \mathbf{D}_1 \Theta\Psi\rangle_{\mathbf{x}} = -N \operatorname{Re}\overline{\langle \Psi, \mathbf{D}_1 \Psi\rangle_{\mathbf{x}}} = -\mathbf{j}^{\mathrm{c}}_{\Psi}(\mathbf{x}).$$

The energy identity is (192) with $v = 0$ and $\mathbf{A} = 0$. Finally, Θ is an energy-preserving bijection between the pure constraint sets at $(\rho, \mathbf{j}^{\mathrm{c}})$ and $(\rho, -\mathbf{j}^{\mathrm{c}})$, which proves (194) for F_{PFLL}. The map $(\rho, \mathbf{j}^{\mathrm{c}}) \mapsto (\rho, -\mathbf{j}^{\mathrm{c}})$ is a linear homeomorphism of $X \times Y$, so (55) gives the identity for F_{PFL}. □

A.4. **Gauge covariance.**

Proposition A.5 (Gauge covariance)**.** *Let* $g \in W^{1,1}_{\mathrm{loc}}(\mathbb{R}^3, \mathbb{R})$ *satisfy*

$$\boldsymbol{\nabla} g \in L^3(\mathbb{R}^3, \mathbb{R}^3) + L^\infty(\mathbb{R}^3, \mathbb{R}^3),$$

and define

$$(U_g \Psi)(\mathbf{X}) = e^{\mathrm{i}\sum_{n=1}^N g(\mathbf{x}_n)} \Psi(\mathbf{X}). \tag{195}$$

Then U_g *is unitary and preserves* $\mathcal{Q}_{\mathrm{PF}}$*. For external potentials in* (29)*,*

$$H^{v,\mathbf{A}-\boldsymbol{\nabla} g} = U_g H^{v,\mathbf{A}} U_g^\dagger, \tag{196}$$

$$\rho_{U_g\Psi} = \rho_\Psi, \qquad \mathbf{j}^{\mathrm{c}}_{U_g\Psi} = \mathbf{j}^{\mathrm{c}}_{\Psi} + \rho_\Psi \boldsymbol{\nabla} g. \tag{197}$$

In particular, the physical current density $\mathbf{j}^{\mathrm{c}}_{\Psi} + \rho_\Psi \mathbf{A}$ *is invariant under the simultaneous transformation* $(\Psi, \mathbf{A}) \mapsto (U_g\Psi, \mathbf{A} - \boldsymbol{\nabla} g)$*. The internal energy satisfies*

$$\langle U_g\Psi, H^{0,0} U_g \Psi\rangle = \langle \Psi, H^{0,0}\Psi\rangle + \int_{\mathbb{R}^3} \boldsymbol{\nabla} g \cdot \mathbf{j}^{\mathrm{c}}_{\Psi} + \frac{1}{2}\int_{\mathbb{R}^3} \rho_\Psi |\boldsymbol{\nabla} g|^2. \tag{198}$$

For every $(\rho, \mathbf{j}^{\mathrm{c}}) \in X \times Y$ *and* $F \in \{F_{\mathrm{PFLL}}, F_{\mathrm{PFL}}\}$,

$$F(\rho, \mathbf{j}^{\mathrm{c}} + \rho \boldsymbol{\nabla} g) = F(\rho, \mathbf{j}^{\mathrm{c}}) + \int_{\mathbb{R}^3} \boldsymbol{\nabla} g \cdot \mathbf{j}^{\mathrm{c}} + \frac{1}{2}\int_{\mathbb{R}^3} \rho |\boldsymbol{\nabla} g|^2. \tag{199}$$

Proof. The Sobolev chain and product rules give

$$\mathbf{D}_n U_g \Psi = U_g\big(\mathbf{D}_n + (\boldsymbol{\nabla} g)(\mathbf{x}_n)\big)\Psi.$$

By the vector-valued Sobolev inequality, multiplication by $(\boldsymbol{\nabla} g)(\mathbf{x}_n)$ is bounded from $\mathcal{Q}_{\mathrm{PF}}$ to $\mathcal{H}_N$, so this identity is valid for every $\Psi \in \mathcal{Q}_{\mathrm{PF}}$. The phase commutes with H_{rad}, and its inverse is U_{-g}, so it preserves the form domain in both directions.

Adding $\mathbf{A}(\mathbf{x}_n) - (\boldsymbol{\nabla} g)(\mathbf{x}_n)$ to the transformed derivative proves (196) as a closed-form identity. Pointwise unitarity and the same derivative formula give (197) and the asserted physical-current invariance.

Expanding the squared covariant-derivative norms, the cross term is

$$\sum_{n=1}^{N} \mathrm{Re}\langle \mathbf{D}_n \Psi, (\boldsymbol{\nabla} g)(\mathbf{x}_n)\Psi\rangle = \int_{\mathbb{R}^3} \boldsymbol{\nabla} g \cdot \mathbf{j}^{\mathrm{c}}_{\Psi},$$

and the quadratic term is $\frac{1}{2}\int_{\mathbb{R}^3} \rho_\Psi |\boldsymbol{\nabla} g|^2$. The Coulomb and radiation terms are unchanged, proving (198). The bijection U_g between the two constraint sets therefore proves (199) for F_{PFLL}.

For F_{PFL} the argument is the same, applied to density matrices. By (197) and (198), applied to spectral decompositions, $\boldsymbol{\Gamma} \mapsto U_g \boldsymbol{\Gamma} U_g^\dagger$ is a bijection of $\mathcal{D}$ onto itself that maps the constraint set of (56) at $(\rho, \mathbf{j}^{\mathrm{c}})$ onto the one at $(\rho, \mathbf{j}^{\mathrm{c}} + \rho \boldsymbol{\nabla} g)$ and shifts the energy by the last two terms in (199). This proves (199) for $\widetilde{F}_{\mathrm{PFL}}$, and hence for F_{PFL} by (58). □

A.5. **Weyl displacement operators.** We collect the displacement identities used throughout the paper. The algebraic statements hold on the bosonic Fock space over any complex one-particle space $\mathfrak{H}$. Define the exponential vector and the Weyl operator by

$$\boxed{\mathcal{E}(f) := \bigoplus_{n=0}^{\infty} \frac{f^{\otimes n}}{\sqrt{n!}}, \qquad W(f) := \exp\bigl(-\mathrm{i}\Phi(\mathrm{i}f)\bigr) = \exp\bigl(a^\dagger(f) - a(f)\bigr).} \tag{200}$$

The exponential is defined through the self-adjoint Segal field $\Phi(\mathrm{i}f)$. This convention gives $W(\mathrm{i}f) = \exp(\mathrm{i}\Phi(f))$.

Proposition A.6 (Weyl relations and field shifts)**.** *For $f, g, h \in \mathfrak{H}$, the following properties hold true.*

(i) The Weyl operators act on exponential vectors and compose according to

$$W(f)\mathcal{E}(g) = e^{-\|f\|^2/2 - \langle f,g\rangle}\mathcal{E}(f+g), \tag{201}$$

$$W(f)^\dagger = W(-f), \qquad W(f)W(g) = e^{-\mathrm{i}\,\mathrm{Im}\langle f,g\rangle} W(f+g). \tag{202}$$

(ii) The map $f \mapsto W(f)$ is strongly continuous. On the linear span of exponential vectors, $W(f)$ has the normally ordered expression

$$W(f) = e^{-\|f\|^2/2} e^{a^\dagger(f)} e^{-a(f)}.$$

Here the two normally ordered exponentials act by their convergent power series on exponential vectors.

(iii) The closed creation and annihilation operators and the Segal fields satisfy

$$W(f)^\dagger a(h) W(f) = a(h) + \langle h, f\rangle \mathbb{1}, \tag{203}$$

$$W(f)^\dagger a^\dagger(h) W(f) = a^\dagger(h) + \langle f, h\rangle \mathbb{1}, \tag{204}$$

$$W(f)^\dagger \Phi(h) W(f) = \Phi(h) + 2\,\mathrm{Re}\langle h, f\rangle \mathbb{1}, \tag{205}$$

$$W(f)^\dagger \Pi(h) W(f) = \Pi(h) + 2\,\mathrm{Im}\langle h, f\rangle \mathbb{1}. \tag{206}$$

Each identity includes invariance of the domain of the operator being conjugated. If $\mathrm{Im}\langle h, g\rangle = 0$, then $\Phi(h)$ and $\Phi(g)$ strongly commute.

(iv) For any unitary T on $\mathfrak{H}$,

$$\Gamma(T)W(f)\Gamma(T)^\dagger = W(Tf). \tag{207}$$

(v) Under the canonical Fock-space factorization over $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$,

$$W(f_1 \oplus f_2) = W(f_1) \otimes W(f_2). \tag{208}$$

Proof. (i) The defining series gives $\langle \mathcal{E}(g), \mathcal{E}(h)\rangle = e^{\langle g,h\rangle}$, and exponential vectors are eigenvectors of the annihilation operators:

$$a(f)\mathcal{E}(g) = \langle f, g\rangle \mathcal{E}(g). \tag{209}$$

Exponential vectors have dense linear span. Indeed, if $\Psi = (\psi^{(n)})_{n\geq 0}$ is orthogonal to every $\mathcal{E}(tg)$, $t \in \mathbb{R}$, then the power series $\sum_n t^n \langle g^{\otimes n}, \psi^{(n)}\rangle/\sqrt{n!}$ vanishes identically, so $\langle g^{\otimes n}, \psi^{(n)}\rangle = 0$ for all g and n. The polarization identity

$$\mathrm{Sym}(g_1 \otimes \cdots \otimes g_n) = \frac{1}{2^n n!} \sum_{\varepsilon \in \{\pm 1\}^n} \varepsilon_1 \cdots \varepsilon_n (\varepsilon_1 g_1 + \cdots + \varepsilon_n g_n)^{\otimes n},$$

where Sym averages over permutations of the factors, then gives $\langle \mathrm{Sym}(g_1 \otimes \cdots \otimes g_n), \psi^{(n)}\rangle = 0$. These symmetrizations span a dense subspace of the n-particle sector, so $\psi^{(n)} = 0$. The right-hand side of (201) preserves inner products of exponential vectors. Its inverse is the same formula with $-f$, so it defines a unitary. Composing the formulas gives (202), and norm continuity on exponential vectors, followed by density, gives strong continuity in f. In particular, $t \mapsto W(tf)$ is a strongly continuous one-parameter unitary group. Differentiating at $t = 0$ gives $a^\dagger(f) - a(f) = -\mathrm{i}\Phi(\mathrm{i}f)$ as its generator. The exponential span is a core for this Segal field, so this unitary is precisely (200).

(ii) Strong continuity was shown in (i). The normally ordered formula follows from (209) and $e^{a^\dagger(f)}\mathcal{E}(g) = \mathcal{E}(f+g)$.

(iii) The eigenvector identity (209) proves (203) on the exponential span. This span is an operator core for $a(h)$ and $a^\dagger(h)$: finite symmetric tensors are obtained by differentiating exponential vectors in their graph norms, and finite-particle truncation gives a core for the closed operators. Since $W(f)$ and $W(-f)$ map the exponential span onto itself, closure gives (203) with equality of domains. Taking adjoints gives (204). Applying (202) to $W(\mathrm{i}th) = e^{\mathrm{i}t\Phi(h)}$ and using uniqueness of the self-adjoint generator proves (205). Replacing h by $\mathrm{i}h$ gives (206). When $\mathrm{Im}\langle h, g\rangle = 0$, the Weyl relations make the two unitary groups $e^{\mathrm{i}t\Phi(h)}$ and $e^{\mathrm{i}s\Phi(g)}$ commute for all $s, t \in \mathbb{R}$, which is strong commutation of their generators.

(iv) The identity $\Gamma(T)\mathcal{E}(g) = \mathcal{E}(Tg)$ and (201) prove (207) on exponential vectors, and density extends it.

(v) The canonical factorization sends $\mathcal{E}(g_1 \oplus g_2)$ to $\mathcal{E}(g_1) \otimes \mathcal{E}(g_2)$, and applying (201) proves (208). □

The radiation form is expressed through the annihilation operators. The sector-wise annihilation formulas define a closed map

$$(\mathcal{T}\eta)(\mathbf{k}, \lambda) := \sqrt{\omega(\mathbf{k})}\, a(\mathbf{k}, \lambda)\eta, \qquad \|\mathcal{T}\eta\| = \|\sqrt{H_{\mathrm{rad}}}\eta\|,$$

from $D(\sqrt{H_{\mathrm{rad}}})$ to $L^2(\mathbb{R}^3 \times \{1, 2\}; \mathcal{F}_{\mathrm{ph}})$. It lets us extend the annihilation operator to kernels that are not square integrable. This is needed below for $g = \omega f$ with

only $f \in D(\sqrt{\omega})$, in which case g need not lie in $\mathfrak{H}_{\mathrm{ph}}$ and $a(g)$ is not defined. For a measurable kernel g with $g/\sqrt{\omega} \in \mathfrak{H}_{\mathrm{ph}}$ and $\eta, \zeta \in D(\sqrt{H_{\mathrm{rad}}})$, define

$$a_\omega(g)\eta := \sum_{\lambda=1}^{2} \int_{\mathbb{R}^3} \frac{\overline{g(\mathbf{k},\lambda)}}{\sqrt{\omega(\mathbf{k})}} \, (\mathcal{T}\eta)(\mathbf{k},\lambda)\, \mathrm{d}\mathbf{k}, \tag{210}$$

$$\Phi_\omega(g)[\eta,\zeta] := \langle a_\omega(g)\eta, \zeta\rangle + \langle \eta, a_\omega(g)\zeta\rangle. \tag{211}$$

The integrand pairs two square-integrable factors, so the Cauchy–Schwarz inequality gives

$$\|a_\omega(g)\eta\| \le \|g/\sqrt{\omega}\| \, \|\sqrt{H_{\mathrm{rad}}}\eta\|.$$

Thus $a_\omega(g)$ is a bounded operator from the radiation form domain to $\mathcal{F}_{\mathrm{ph}}$, and $\Phi_\omega(g)$ is a continuous symmetric form on that domain. If also $g \in \mathfrak{H}_{\mathrm{ph}}$, then $a_\omega(g) = a(g)$ on $D(\sqrt{H_{\mathrm{rad}}})$, and $\Phi_\omega(g)$ is the form of $\Phi(g)$ there.

Proposition A.7 (Radiation energy and photon number under displacement)**.** *On $\mathcal{F}_{\mathrm{ph}}$, let $f \in \mathfrak{H}_{\mathrm{ph}}$. The following hold.*

(i) If $f \in D(\sqrt{\omega})$, then $W(f)$ maps $D(\sqrt{H_{\mathrm{rad}}})$ bijectively onto itself, and

$$\|\sqrt{H_{\mathrm{rad}}} W(f)\eta\| \le \|\sqrt{H_{\mathrm{rad}}}\eta\| + \|\sqrt{\omega} f\| \, \|\eta\|. \tag{212}$$

(ii) If $f \in D(\sqrt{\omega})$, the radiation form shifts exactly: for all $\eta, \zeta \in D(\sqrt{H_{\mathrm{rad}}})$,

$$\langle W(f)\eta, H_{\mathrm{rad}} W(f)\zeta\rangle = \langle \eta, H_{\mathrm{rad}}\zeta\rangle + \Phi_\omega(\omega f)[\eta,\zeta] + \|\sqrt{\omega} f\|^2 \langle \eta, \zeta\rangle, \tag{213}$$

where $\langle \eta, H_{\mathrm{rad}}\zeta\rangle = \langle \sqrt{H_{\mathrm{rad}}}\eta, \sqrt{H_{\mathrm{rad}}}\zeta\rangle$ is the radiation form.

(iii) If $f \in D(\omega)$, then $W(f)$ preserves $D(H_{\mathrm{rad}})$, and the operator identity on this domain is

$$W(f)^\dagger H_{\mathrm{rad}} W(f) = H_{\mathrm{rad}} + \Phi(\omega f) + \|\sqrt{\omega} f\|^2 \mathbb{1}. \tag{214}$$

(iv) The photon number satisfies

$$W(f) D(\sqrt{\mathcal{N}}) = D(\sqrt{\mathcal{N}}), \qquad \|\sqrt{\mathcal{N}} W(f)\eta\| \le \|\sqrt{\mathcal{N}}\eta\| + \|f\| \, \|\eta\|. \tag{215}$$

(v) The normalized coherent vector $W(f)\Omega$ satisfies

$$\langle W(f)\Omega, \mathcal{N} W(f)\Omega\rangle = \|f\|^2, \qquad \langle W(f)\Omega, H_{\mathrm{rad}} W(f)\Omega\rangle = \|\sqrt{\omega} f\|^2. \tag{216}$$

The second equality allows the value $+\infty$. Thus $f \in D(\sqrt{\omega})$ is also necessary for preservation of the radiation form domain.

Proof. We use the closed map $\mathcal{T}$ defined before the proposition. For $h \in D(\sqrt{\omega})$, (201) gives, first on $\eta = \mathcal{E}(h)$,

$$\mathcal{T} W(f)\eta = (\mathbb{1} \otimes W(f))\big(\mathcal{T}\eta + \sqrt{\omega} f \otimes \eta\big). \tag{217}$$

The span of these exponential vectors is a radiation form core. Indeed, finite symmetric tensors with factors in $D(\sqrt{\omega})$ form such a core by particle truncation and one-particle spectral truncation. They are in turn limits, in the form norm, of finite differences of exponential vectors, obtained by polarizing and differentiating their defining series.

The triangle inequality in (217) proves (212) on this core. For a form-convergent sequence, the right-hand side of (217) converges and $W(f)\eta_n$ converges in Fock space. Closedness of $\mathcal{T}$ extends the identity and the bound to the full form domain. Applying the same argument to $-f$ proves invariance in both directions.

Taking the inner product of the two sides of (217), for η and ζ, and using (210) with $g = \omega f$, so that $g/\sqrt{\omega} = \sqrt{\omega} f$, gives (213). For $f \in D(\omega)$ and $\zeta \in D(H_{\mathrm{rad}})$,

the right-hand side of (213) is represented by the vector $(H_{\mathrm{rad}}+\Phi(\omega f)+\|\sqrt{\omega}f\|^2)\zeta$. The representation theorem for closed forms therefore gives $W(f)\zeta \in D(H_{\mathrm{rad}})$ and (214). Repeating this with $-f$ proves equality of the operator domains.

The same proof with weight 1 in place of ω proves (215). Applying the identities to Ω proves (216) when the right-hand side is finite. In general the coherent annihilation formula $a(\mathbf{k},\lambda)W(f)\Omega = f(\mathbf{k},\lambda)W(f)\Omega$ gives the energy equality as a nonnegative integral, including the value $+\infty$. □

Corollary A.8 (Displacement of density, current, and energy)**.** *Assume* (9)*, let* $f \in D(\sqrt{\omega})$*, and set*

$$c_f^\mu(\mathbf{x}) = 2\,\mathrm{Re}\langle G_{\mathbf{x}}^\mu, f\rangle. \tag{218}$$

The field $\mathbf{c}_f$ *is real, bounded, continuous, and divergence-free. The photon unitary* $W(tf)$ *preserves* $\mathcal{Q}_{\mathrm{PF}}$ *for every* $t \in \mathbb{R}$*. For* $\boldsymbol{\Gamma} \in \mathcal{D}$*, let*

$$\boxed{\boldsymbol{\Gamma}_t = W(tf)\boldsymbol{\Gamma}W(tf)^\dagger,}$$

with the electronic identity suppressed. Then the following hold.

(i) $\boldsymbol{\Gamma}_t \in \mathcal{D}$*, its electronic reduced state is unchanged, and*

$$\rho_{\boldsymbol{\Gamma}_t} = \rho_{\boldsymbol{\Gamma}}, \qquad \mathbf{j}^{\mathrm{p}}_{\boldsymbol{\Gamma}_t} = \mathbf{j}^{\mathrm{p}}_{\boldsymbol{\Gamma}}, \qquad \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}_t} = \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} - et\rho_{\boldsymbol{\Gamma}}\mathbf{c}_f. \tag{219}$$

(ii) For admissible external potentials, the exact energy change is

$$\begin{aligned}\mathrm{Tr}\big(H^{v,\mathbf{A}}\boldsymbol{\Gamma}_t\big) = \mathrm{Tr}\big(H^{v,\mathbf{A}}\boldsymbol{\Gamma}\big) &\\ + t\left[\mathrm{Tr}\big(\Phi_\omega(\omega f)\boldsymbol{\Gamma}\big) - e\int \mathbf{c}_f\cdot\big(\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} + \rho_{\boldsymbol{\Gamma}}\mathbf{A}\big)\right] &\\ + t^2\left[\|\sqrt{\omega}f\|^2 + \frac{e^2}{2}\int \rho_{\boldsymbol{\Gamma}}|\mathbf{c}_f|^2\right].&\end{aligned} \tag{220}$$

Here the trace of the weighted field is the sum of its forms over any spectral decomposition of $\boldsymbol{\Gamma}$*. It is finite, with*

$$\big|\mathrm{Tr}\big(\Phi_\omega(\omega f)\boldsymbol{\Gamma}\big)\big| \le 2\|\sqrt{\omega}f\|\big(\mathrm{Tr}(H_{\mathrm{rad}}\boldsymbol{\Gamma})\big)^{1/2}. \tag{221}$$

For $f \in D(\omega)$*, this trace equals* $2\,\mathrm{Re}\,\mathrm{Tr}(a(\omega f)\boldsymbol{\Gamma})$.

Proof. The continuity and uniform bounds of $G_{\mathbf{x}}^\mu$ give $\|\mathbf{c}_f\|_\infty \le 2\|\widehat{\chi}\|\|f\|$ and continuity. The weak Coulomb-gauge identity gives $\mathrm{div}\,\mathbf{c}_f = 0$. Since $W(tf)$ acts independently of the electronic positions, it commutes with electronic weak derivatives. Proposition A.7 then gives preservation of $\mathcal{Q}_{\mathrm{PF}}$. Partial trace over photons is unchanged by a photon unitary, so the density and paramagnetic current density are unchanged. By (205),

$$W(tf)^\dagger\mathfrak{A}(\mathbf{x})W(tf) = \mathfrak{A}(\mathbf{x}) + t\mathbf{c}_f(\mathbf{x}).$$

The definitions of $\mathbf{j}^{\mathrm{ph}}$ and $\mathbf{j}^{\mathrm{c}}$ now give (219). Expanding the kinetic form replaces $\mathbf{D}_n + \mathbf{A}$ by $\mathbf{D}_n + \mathbf{A} - et\mathbf{c}_f$. Its linear term is $-et\int \mathbf{c}_f\cdot(\mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} + \rho_{\boldsymbol{\Gamma}}\mathbf{A})$ and its quadratic term is $\frac{1}{2}e^2t^2\int \rho_{\boldsymbol{\Gamma}}|\mathbf{c}_f|^2$. The scalar and Coulomb forms are unchanged. Adding (213) proves (220), first for pure states. The weighted annihilation bound and Cauchy–Schwarz in a spectral decomposition prove (221) and justify summing the identities for density matrices. For independence of the spectral decomposition, put $K = (1 + H_{\mathrm{rad}})^{1/2}$ and let B_f be the bounded operator with

$$\langle \eta, B_f\zeta\rangle = \Phi_\omega(\omega f)[K^{-1}\eta, K^{-1}\zeta].$$

The form trace equals $\operatorname{Tr}(B_f K\mathbf{\Gamma}K)$, where $K\mathbf{\Gamma}K$ is the positive trace-class operator defined by the finite radiation energy. Hence it does not depend on the chosen decomposition. All remaining terms are integrable since $\mathbf{c}_f$ is bounded and $\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}}, \rho_{\mathbf{\Gamma}}\mathbf{A} \in L^1$. □

In particular, for real $\mathbf{u} \in C^\infty_c(\mathbb{R}^3;\mathbb{R}^3)$ and $g_{\mathbf{u}} = \sum_\mu \int u^\mu(\mathbf{x}) G^\mu_{\mathbf{x}} \mathrm{d}\mathbf{x}$, symmetry of the form factor gives $\langle G^\mu_{\mathbf{x}}, g_{\mathbf{u}}\rangle \in \mathbb{R}$. Consequently,

$$\mathbf{c}_{\mathrm{i}g_{\mathbf{u}}} = 0, \qquad \Phi(\mathrm{i}\omega g_{\mathbf{u}}) = -\int \mathbf{u}\cdot\mathfrak{E}_\perp.$$

These are the displacements preserving both constraints in the proof of Proposition 4.13. General displacements instead give the current change in (219).

Proposition A.9 (Coherent vectors and position-dependent displacements)**.** *Let $\mathcal{O} \subset \mathbb{R}^m$ be open. The following hold.*

(i) For $f, g, h \in \mathfrak{H}$, the normalized coherent vectors satisfy

$$W(f)\Omega = e^{-\|f\|^2/2}\mathcal{E}(f), \qquad a(h)W(f)\Omega = \langle h, f\rangle W(f)\Omega, \tag{222}$$

$$\langle W(f)\Omega, W(g)\Omega\rangle = \exp\Big(-\frac{1}{2}\|f-g\|^2 + \mathrm{i}\operatorname{Im}\langle f, g\rangle\Big). \tag{223}$$

(ii) As a map of real Hilbert spaces, $f \mapsto W(f)\Omega$ is smooth. Its derivative at f in the direction h is

$$\frac{\mathrm{d}}{\mathrm{d}s} W(f+sh)\Omega\Big|_{s=0} = \big(a^\dagger(h) - \operatorname{Re}\langle f, h\rangle\big)W(f)\Omega, \tag{224}$$

and this vector satisfies

$$\begin{aligned} \langle W(f)\Omega, \big(a^\dagger(h) - \operatorname{Re}\langle f,h\rangle\big)W(f)\Omega\rangle &= \mathrm{i}\operatorname{Im}\langle f, h\rangle, \\ \big\|\big(a^\dagger(h) - \operatorname{Re}\langle f,h\rangle\big)W(f)\Omega\big\|^2 &= \|h\|^2 + \big(\operatorname{Im}\langle f,h\rangle\big)^2. \end{aligned} \tag{225}$$

(iii) Let $f \in H^1_{\mathrm{loc}}(\mathcal{O};\mathfrak{H})$ and $S \in H^1_{\mathrm{loc}}(\mathcal{O};\mathbb{R})$. Then $e^{\mathrm{i}S}W(f)\Omega \in W^{1,1}_{\mathrm{loc}}$ and, almost everywhere,

$$\begin{aligned} \operatorname{Im}\langle e^{\mathrm{i}S}W(f)\Omega, \partial_j\big(e^{\mathrm{i}S}W(f)\Omega\big)\rangle &= \partial_j S + \operatorname{Im}\langle f, \partial_j f\rangle, \\ \big\|\partial_j\big(e^{\mathrm{i}S}W(f)\Omega\big)\big\|^2 &= \|\partial_j f\|^2 + \big|\partial_j S + \operatorname{Im}\langle f, \partial_j f\rangle\big|^2. \end{aligned} \tag{226}$$

In particular, $e^{\mathrm{i}S}W(f)\Omega \in H^1_{\mathrm{loc}}$ if $\boldsymbol{\nabla}S + \operatorname{Im}\langle f, \boldsymbol{\nabla} f\rangle \in L^2_{\mathrm{loc}}$.

(iv) If J is a conjugation on $\mathfrak{H}$, the map $f \mapsto W(f)\Omega$ is globally Lipschitz on $\mathfrak{H}_J := \{f : Jf = f\}$:

$$\|W(f)\Omega - W(g)\Omega\|^2 = 2\big(1 - e^{-\|f-g\|^2/2}\big) \le \|f-g\|^2 \qquad (f, g \in \mathfrak{H}_J). \tag{227}$$

Thus for $f \in H^1_{\mathrm{loc}}(\mathcal{O};\mathfrak{H}_J)$, $W(f)\Omega \in H^1_{\mathrm{loc}}$ and

$$\langle W(f)\Omega, \partial_j\big(W(f)\Omega\big)\rangle = 0, \qquad \|\partial_j\big(W(f)\Omega\big)\|^2 = \|\partial_j f\|^2.$$

Proof. (201) applied to the vacuum gives (222), and the exponential-vector inner product gives (223). The norm-convergent exponential series and its derivatives converge uniformly on bounded sets of f, so differentiating gives (224). The eigenvector identity (209) and the CCR yield

$$\langle W(f)\Omega, a^\dagger(h)W(f)\Omega\rangle = \langle f, h\rangle, \qquad \|a^\dagger(h)W(f)\Omega\|^2 = \|h\|^2 + |\langle h, f\rangle|^2.$$

Substitution proves (225). Differentiating the scalar phase then proves (226) for smooth f, S.

For the stated Sobolev regularity, first compose the map $g \mapsto W(g)\Omega$ with smooth radial truncations of f. On bounded sets its derivative is bounded, and (225) gives the global estimate

$$\big\| \big(a^\dagger(h) - \mathrm{Re}\langle f, h\rangle\big) W(f)\Omega \big\| \leq (1 + \|f\|)\|h\|.$$

Since $(1 + \|f\|)\|\boldsymbol{\nabla} f\|$ is locally integrable, the truncated chain rules pass to the limit in $W^{1,1}_{\mathrm{loc}}$. The product rule with $e^{\mathrm{i}S}$ proves the displayed identities almost everywhere. Their right-hand sides give square-integrable derivatives when $\boldsymbol{\nabla} S + \mathrm{Im}\langle f, \boldsymbol{\nabla} f\rangle \in L^2_{\mathrm{loc}}$. Finally, scalar products of J-real vectors are real, so (223) gives (227). In this case $\mathrm{Im}\langle f, \partial_j f\rangle = 0$, and the last assertions follow from the same derivative identities with $S = 0$. □

These formulas imply (96) and apply to the tags in Lemma C.3. The distinction between $W^{1,1}_{\mathrm{loc}}$ and H^1_{loc} matters for complex displacements: $f \in H^1_{\mathrm{loc}}$ alone does not control the square of $\mathrm{Im}\langle f, \boldsymbol{\nabla} f\rangle$.

A.6. **Length-gauge transformation.** In this subsection the form factor need only satisfy (9). The additional ultraviolet moment needed to expand the transformed radiation form will be stated separately. Put $\mathbf{R} = \sum_{n=1}^N \mathbf{x}_n$, and let H_{d} be the dipole Hamiltonian in (79).

Note first that by (8) and (12),

$$\langle G_0^\mu, G_0^\nu\rangle = \frac{1}{2}\int_{\mathbb{R}^3} |\widehat{\chi}(\mathbf{k})|^2 \left(\delta^{\mu\nu} - \frac{k^\mu k^\nu}{|\mathbf{k}|^2}\right) \mathrm{d}\mathbf{k} \in \mathbb{R}.$$

Since $\mathfrak{A}^\mu(0) = \Phi(G_0^\mu)$, Proposition A.6(iii) shows that the components of $\mathfrak{A}(0)$ strongly commute. At each electronic configuration $\mathbf{X}$, the operator $e\mathbf{R}\cdot\mathfrak{A}(0)$ is the Segal field $\Phi\big(e\sum_{\mu=1}^3 R^\mu G_0^\mu\big)$. We define the multiplication operator

$$U_{\mathrm{d}} := \exp(\mathrm{i}e\mathbf{R}\cdot\mathfrak{A}(0)), \qquad \text{that is,} \qquad U_{\mathrm{d}}(\mathbf{X}) = W\big(\mathrm{i}e\textstyle\sum_{\mu=1}^3 R^\mu G_0^\mu\big). \tag{228}$$

Proposition A.10 (Length-gauge transformation)**.** *Let $\mathcal{Q}_{\mathrm{d}} := U_{\mathrm{d}}^\dagger \mathcal{Q}_{\mathrm{PF}}$ be the transported form domain. The following hold.*

(i) U_{d} is unitary on $\mathcal{H}_N$.

(ii) Every $\Psi \in \mathcal{Q}_{\mathrm{d}}$ has finite ordinary electronic kinetic energy, and on $\mathcal{Q}_{\mathrm{d}}$

$$U_{\mathrm{d}}^\dagger \mathbf{D}_{n,\mathrm{d}} U_{\mathrm{d}} = -\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n}, \qquad 1 \leq n \leq N. \tag{229}$$

(iii) For $\Psi \in \mathcal{Q}_{\mathrm{d}}$, the density and current density satisfy

$$\rho_\Psi = \rho_{U_{\mathrm{d}}\Psi}, \qquad \mathbf{j}^{\mathrm{p}}_\Psi = \mathbf{j}^{\mathrm{c,d}}_{U_{\mathrm{d}}\Psi}. \tag{230}$$

(iv) If $\sqrt{\omega}\,\widehat{\chi} \in L^2(\mathbb{R}^3)$, then $\mathscr{C}_{\mathrm{PF}} \subset \mathcal{Q}_{\mathrm{d}}$, and on this algebraic test space the following identity holds in the quadratic-form sense:

$$U_{\mathrm{d}}^\dagger H_{\mathrm{d}} U_{\mathrm{d}} = H^0_{\mathrm{el}} + H_{\mathrm{rad}} + e\sum_{\mu=1}^3 R^\mu \Pi(\omega G_0^\mu) + e^2 \mathbf{R}^\top \mathbf{M}\mathbf{R}, \tag{231}$$

where $\mathbf{M}$ is the matrix (83). For $f/\sqrt{\omega} \in \mathfrak{H}_{\mathrm{ph}}$, $\Pi(f)$ denotes the form $\Phi_\omega(\mathrm{i}f)$ of (211) on $D(\sqrt{H_{\mathrm{rad}}})$. Since $\Pi(f) = \Phi(\mathrm{i}f)$, this extends the conjugate Segal field (1). An interpretation as a Segal operator requires $f \in \mathfrak{H}_{\mathrm{ph}}$.

Proof. By (228), U_{d} acts at each electronic configuration by a Weyl operator, which is unitary and, by Proposition A.6(ii), strongly continuous in $\mathbf{X}$. Its dependence on $\mathbf{X}$ is permutation invariant, and hence it preserves fermionic antisymmetry.

For $\Psi \in \mathscr{C}_{\mathrm{PF}}$, differentiation of this multiplier gives

$$-\mathrm{i}\boldsymbol{\nabla}_{\mathbf{x}_n} U_{\mathrm{d}}^{\dagger}\Psi = U_{\mathrm{d}}^{\dagger}\mathbf{D}_{n,\mathrm{d}}\Psi, \qquad 1 \le n \le N. \tag{232}$$

Here the photon factors in the core belong to the domains of all three field components, and their strong commutation justifies differentiation of the corresponding unitary groups. For general $\Psi \in \mathcal{Q}_{\mathrm{PF}}$, approximate by $\mathscr{C}_{\mathrm{PF}}$ in the common form norm. The field bound (20) makes $\mathbf{D}_{n,\mathrm{d}} : \mathcal{Q}_{\mathrm{PF}} \to \mathcal{H}_N^3$ continuous. Unitarity and closedness of the electronic weak derivative then extend (232) to the limit. This proves both the finite kinetic energy of every vector in $\mathcal{Q}_{\mathrm{d}}$ and (229), but not that $\mathcal{Q}_{\mathrm{d}} \subset \mathcal{Q}_{\mathrm{PF}}$.

Pointwise unitarity preserves the electronic configuration density, and (232) preserves the local pairings that define the current density. Integrating over the remaining electronic variables gives (230).

It remains to prove (iv), so assume $\sqrt{\omega}\,\widehat{\chi} \in L^2(\mathbb{R}^3)$. Then $G_0^{\mu} \in D(\sqrt{\omega})$ by (12), and the linear term in (231) is defined, since $\omega G_0^{\mu}/\sqrt{\omega} = \sqrt{\omega}\,G_0^{\mu} \in \mathfrak{H}_{\mathrm{ph}}$. For $h \in D(\sqrt{\omega})$, Proposition A.7(i) with $f = \mathrm{i}h$ shows that $W(\mathrm{i}h)$ maps $D(\sqrt{H_{\mathrm{rad}}})$ bijectively onto itself, and Proposition A.7(ii) gives, for $\eta \in D(\sqrt{H_{\mathrm{rad}}})$,

$$\|\sqrt{H_{\mathrm{rad}}}W(\mathrm{i}h)\eta\|^2 = \|\sqrt{H_{\mathrm{rad}}}\eta\|^2 + \Pi(\omega h)[\eta,\eta] + \|\sqrt{\omega}h\|^2\|\eta\|^2. \tag{233}$$

At each electronic configuration take $h = e\sum_{\mu} R^{\mu}G_0^{\mu}$, so that $U_{\mathrm{d}}(\mathbf{X}) = W(\mathrm{i}h)$, $\Pi(\omega h) = e\sum_{\mu} R^{\mu}\Pi(\omega G_0^{\mu})$, and $\|\sqrt{\omega}h\|^2 = e^2\mathbf{R}^{\top}\mathbf{M}\mathbf{R}$. For $\Phi \in \mathscr{C}_{\mathrm{PF}}$ the electronic support is compact, so (212) gives finite radiation energy of $U_{\mathrm{d}}\Phi$. Differentiation of the unitary multiplier and its commutation with $\mathfrak{A}(0)$ give finite electronic kinetic energy as well. Thus $U_{\mathrm{d}}\Phi \in \mathcal{Q}_{\mathrm{PF}}$, that is, $\Phi \in \mathcal{Q}_{\mathrm{d}}$. By (229) and invariance of the Coulomb multiplication form, the kinetic and Coulomb parts of $\langle \Phi, U_{\mathrm{d}}^{\dagger}H_{\mathrm{d}}U_{\mathrm{d}}\Phi\rangle$ equal $\langle \Phi, H_{\mathrm{el}}^0\Phi\rangle$. Integrating (233) over $\mathbf{X}$ gives the radiation part and proves (231). □

The integral form of the matrix (83) follows from (8) and (12). For the hard cutoff (10), the radial weight in this integral is the indicator of the ball of radius Λ. Since $\int_{\mathbb{S}^2}(\delta^{\mu\nu} - \theta^{\mu}\theta^{\nu})\,\mathrm{d}\theta = (8\pi/3)\delta^{\mu\nu}$ and $\int_0^{\Lambda} r^2\,\mathrm{d}r = \Lambda^3/3$, it follows that

$$\mathbf{M} = \frac{4\pi\Lambda^3}{9}\mathbb{1}.$$

The last term in (231) is the dipole self-polarization energy and is part of the unitary transformation. Its role in stability is discussed in [44]. The expanded formula is asserted on the stated test space. On the full transported domain $\mathcal{Q}_{\mathrm{d}}$, the radiation energy is $\|\sqrt{H_{\mathrm{rad}}}U_{\mathrm{d}}\Psi\|^2$, which is nonnegative and requires neither the separate terms in the expansion to be finite nor an electronic position moment.

Even though $\mathfrak{A}(0)$ is spatially uniform, its conditional expectation in an entangled state can depend on $\mathbf{x}$. Thus the field-induced current density need not equal $\rho(\mathbf{x})$ times the unconditional field expectation. Moreover, this limit keeps the photon continuum: the span of the three G_0^{μ} is generally not invariant under ω. The coupled one-photon space is the closed span of $f(\omega)G_0^{\mu}$, with f bounded Borel. A finite-mode model requires a further approximation. Likewise, fixing photon

displacement expectations as additional density variables would define a different constrained-search functional.

Appendix B. Symmetric tensor lifts

In this appendix we construct the permutation-invariant multipliers used in Appendix C and in the proof of Theorem 4.6. We use the following notation. For a separable complex Hilbert space $\mathcal{V}$, the permutation group $\mathscr{S}_N$ acts on configurations $\mathbf{X} = (\mathbf{x}_1, \dots, \mathbf{x}_N) \in (\mathbb{R}^3)^N$ and on $\mathcal{V}^{\otimes N}$ by

$$(\pi\mathbf{X})^i = \mathbf{x}^{\pi^{-1}(i)}, \qquad R_\pi(z_1 \otimes \cdots \otimes z_N) = z_{\pi^{-1}(1)} \otimes \cdots \otimes z_{\pi^{-1}(N)},$$

and $\Pi_N = \frac{1}{N!}\sum_{\pi\in\mathscr{S}_N} R_\pi$ is the projection onto the fully symmetric tensors. Let $\mathcal{D}_N \subset (\mathbb{R}^3)^N$ be the open set of configurations with pairwise distinct points. For $t : \mathbb{R}^3 \to \mathcal{V}$ put

$$T(\mathbf{X}) = \bigotimes_{i=1}^{N} t(\mathbf{x}_i),$$

so that $T(\pi\mathbf{X}) = R_\pi T(\mathbf{X})$. For a map F on $\mathcal{D}_N$, $\mathrm{d}F = \sum_{i,\mu} \partial_{x_i^\mu} F \, \mathrm{d}x_i^\mu$ denotes its differential in $\mathbf{X}$.

The product T has the connection and derivatives we need, but it is not permutation invariant. The next lemma provides isometries $U_N(\mathbf{X})$ that absorb the permutations, so that $U_N T$ is invariant. The flatness condition $U_N^\dagger \mathrm{d}U_N = 0$ ensures that composition with U_N leaves the connection of T unchanged. The construction glues local maps with a partition of unity whose gradients blow up when all electrons come together. There T is almost fully symmetric, which is why the fully symmetric part is kept fixed. The resulting derivative bound is uniform when t is Lipschitz, even when electron coordinates coincide. For general t it is controlled by the inverse squared pair distances, which are integrable against finite-energy states by Hardy's inequality.

Lemma B.1 (Flat symmetric isometries)**.** *For every $N \in \mathbb{N}$ and every separable complex Hilbert space $\mathcal{V}$, there are a separable complex Hilbert space $\mathcal{K}_N$, finite-dimensional if $\mathcal{V}$ is, a smooth map U_N from $\mathcal{D}_N$ to the isometries $\mathcal{V}^{\otimes N} \to \mathcal{K}_N$, and a constant b_N depending only on N with the following properties. For $\mathbf{X} \in \mathcal{D}_N$ and $\pi \in \mathscr{S}_N$,*

$$U_N(\pi\mathbf{X})R_\pi = U_N(\mathbf{X}), \qquad U_N^\dagger \mathrm{d}U_N = 0, \qquad U_N(\mathbf{X})\Pi_N \text{ is independent of } \mathbf{X}, \tag{234}$$

and for every map $t : \mathbb{R}^3 \to \mathcal{V}$ with $\|t(\mathbf{x})\| = 1$,

$$\sum_{i=1}^{N}\sum_{\mu=1}^{3} \|(\partial_{x_i^\mu} U_N(\mathbf{X}))T(\mathbf{X})\|^2 \le b_N \min\Big\{ \sum_{i<j} \frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^2},\ \|\boldsymbol{\nabla} t\|_\infty^2 \Big\}, \tag{235}$$

where $\|\boldsymbol{\nabla} t\|_\infty = \infty$ unless t is Lipschitz.

Proof. We argue by induction on N. For $N = 1$ take $\mathcal{K}_1 = \mathcal{V}$, $U_1 = \mathbb{1}$, and $b_1 = 0$. Let $N \ge 2$ and suppose that $\mathcal{K}_{N'}$, $U_{N'}$, and $b_{N'}$ have been constructed for all $N' < N$.

Step 1. An invariant partition of unity. Put

$$\bar{\mathbf{x}} = \frac{1}{N}\sum_i \mathbf{x}_i, \qquad r(\mathbf{X}) = \Big(\sum_i |\mathbf{x}_i - \bar{\mathbf{x}}|^2\Big)^{1/2}, \qquad s(\mathbf{X}) = \frac{(\mathbf{x}_1 - \bar{\mathbf{x}}, \dots, \mathbf{x}_N - \bar{\mathbf{x}})}{r(\mathbf{X})}.$$

Since $N \geq 2$, $r > 0$ on $\mathcal{D}_N$, and s is smooth there with values in the compact centered unit sphere

$$\mathbb{S}_N = \Big\{ \mathbf{Y} \in (\mathbb{R}^3)^N : \sum_i \mathbf{y}_i = 0,\ \sum_i |\mathbf{y}_i|^2 = 1 \Big\}.$$

Moreover $r(\pi\mathbf{X}) = r(\mathbf{X})$ and $s(\pi\mathbf{X}) = \pi s(\mathbf{X})$. The stabilizer of a point $\mathbf{Y} \in \mathbb{S}_N$ is the product of the permutation groups of the blocks of indices i with equal $\mathbf{y}_i$. Every block has fewer than N elements, because $\mathbb{S}_N$ excludes total coincidence. Choose a ball O in $\mathbb{S}_N$ centered at $\mathbf{Y}$, so small that $\pi O \cap O = \emptyset$ for every π outside the stabilizer. Since permutations act isometrically, O is invariant under the stabilizer, and any two translates πO, $\pi' O$ are either equal or disjoint. By compactness, finitely many such balls O_a, with blocks $I_{a,j}$, cover $\mathbb{S}_N$. Take smooth bump functions supported in the O_a whose positivity sets still cover $\mathbb{S}_N$, average each over the stabilizer of O_a, extend it to the translates πO_a by invariance, and normalize by the square root of the sum of their squares. This gives smooth permutation-invariant functions χ_a on $\mathbb{S}_N$, supported compactly inside $\bigcup_\pi \pi O_a$, with $\sum_a \chi_a^2 = 1$. We write χ_a also for $\chi_a \circ s$. Then $\sum_a \chi_a \mathrm{d}\chi_a = 0$, and since the derivatives of s are $O(r^{-1})$,

$$\sum_{a,i,\mu} |\partial_{x_i^\mu} \chi_a(\mathbf{X})|^2 \leq A_N r(\mathbf{X})^{-2},$$

where $A_N < \infty$ depends only on the chosen atlas, hence only on N.

Step 2. Local maps. Fix a chart a. For $\mathbf{X} \in \mathcal{D}_N$ with $s(\mathbf{X}) \in O_a$ put

$$V_a(\mathbf{X}) = \bigotimes_j U_{|I_{a,j}|}(\mathbf{X}_{I_{a,j}}), \qquad \mathbf{X}_I = (\mathbf{x}_i)_{i \in I},$$

where $\mathcal{V}^{\otimes N}$ is identified with $\bigotimes_j \mathcal{V}^{\otimes I_{a,j}}$ by a fixed reordering of the tensor factors. By the inductive hypothesis, V_a is a smooth isometry into the separable space $\mathcal{K}^{(a)} = \bigotimes_j \mathcal{K}_{|I_{a,j}|}$, it satisfies $V_a(\tau\mathbf{X}) R_\tau = V_a(\mathbf{X})$ for τ in the stabilizer of O_a, and $V_a^\dagger \mathrm{d}V_a = 0$ by the product rule. Moreover, $V_a \Pi_N$ is constant: a fully symmetric tensor is symmetric within each block, so $\Pi_N = (\bigotimes_j \Pi_{|I_{a,j}|})\Pi_N$, and each $U_{|I_{a,j}|}\Pi_{|I_{a,j}|}$ is constant. Extend V_a to the translates by

$$\widetilde{V}_a(\mathbf{X}) = V_a(\pi^{-1}\mathbf{X}) R_{\pi^{-1}}, \qquad s(\mathbf{X}) \in \pi O_a.$$

If $\pi O_a = \pi' O_a$, then $\pi^{-1}\pi'$ lies in the stabilizer of O_a, and the invariance of V_a under the stabilizer shows that $\widetilde{V}_a$ does not depend on the choice of π. By construction, $\widetilde{V}_a(\pi\mathbf{X}) R_\pi = \widetilde{V}_a(\mathbf{X})$. The map $\widetilde{V}_a$ inherits $\widetilde{V}_a^\dagger \mathrm{d}\widetilde{V}_a = 0$, and $\widetilde{V}_a \Pi_N$ is constant because $R_{\pi^{-1}} \Pi_N = \Pi_N$.

Step 3. Definition of U_N. Let $\mathcal{K}_N = \operatorname{Ran} \Pi_N \oplus \bigoplus_a \mathcal{K}^{(a)}$, an orthogonal direct sum, and define

$$U_N(\mathbf{X}) u = \Pi_N u \ \oplus \ \bigoplus_a \chi_a(\mathbf{X}) \widetilde{V}_a(\mathbf{X}) (\mathbb{1} - \Pi_N) u,$$

where each term is extended by zero outside the support of χ_a. Since $\sum_a \chi_a^2 = 1$ and each $\widetilde{V}_a$ is an isometry, $\|U_N(\mathbf{X})u\|^2 = \|\Pi_N u\|^2 + \|(\mathbb{1} - \Pi_N)u\|^2 = \|u\|^2$. The first identity in (234) follows from the invariance of χ_a and $\widetilde{V}_a$ and from $R_\pi \Pi_N = \Pi_N R_\pi = \Pi_N$. The third holds because $U_N(\mathbf{X}) \Pi_N u = \Pi_N u \oplus 0$. For the second,

$$U_N^\dagger \mathrm{d}U_N = (\mathbb{1} - \Pi_N) \Big(\sum_a \chi_a \mathrm{d}\chi_a \, \widetilde{V}_a^\dagger \widetilde{V}_a + \sum_a \chi_a^2 \, \widetilde{V}_a^\dagger \mathrm{d}\widetilde{V}_a \Big) (\mathbb{1} - \Pi_N) = 0.$$

Step 4. The derivative bound. Let t be as in (235), and let $m(\mathbf{X})$ denote the minimum on its right-hand side, without the factor b_N. Since T is a unit vector, $\|(\mathbb{1}-\Pi_N)T\| \le 1$. If t is Lipschitz, then, since $t(\bar{\mathbf{x}})^{\otimes N} \in \operatorname{Ran}\Pi_N$ and all $t(\mathbf{x}_i)$ are unit vectors, telescoping the tensor product gives

$$\|(\mathbb{1}-\Pi_N)T\| \le \|T - t(\bar{\mathbf{x}})^{\otimes N}\| \le \sum_i \|t(\mathbf{x}_i) - t(\bar{\mathbf{x}})\| \le \sqrt{N}\, r(\mathbf{X}) \|\boldsymbol{\nabla} t\|_\infty.$$

Moreover, $r^2 = N^{-1}\sum_{i<j}|\mathbf{x}_i - \mathbf{x}_j|^2$, so $r^{-2} \le N|\mathbf{x}_k - \mathbf{x}_l|^{-2}$ for every pair $k<l$. Using $\|(\mathbb{1}-\Pi_N)T\| \le 1$ with this for the first entry of the minimum, and the telescoping bound for the second,

$$r(\mathbf{X})^{-2}\|(\mathbb{1}-\Pi_N)T(\mathbf{X})\|^2 \le N\, m(\mathbf{X}). \tag{236}$$

Since $\widetilde{V}_a\Pi_N$ is constant, $(\partial\widetilde{V}_a)(\mathbb{1}-\Pi_N)T = (\partial\widetilde{V}_a)T$ for $\partial = \partial_{x_i^\mu}$, and therefore

$$(\partial U_N)T = 0 \oplus \bigoplus_a \Big((\partial\chi_a)\widetilde{V}_a(\mathbb{1}-\Pi_N)T + \chi_a(\partial\widetilde{V}_a)T \Big).$$

The cross terms in the squared norm vanish by $\widetilde{V}_a^\dagger \partial\widetilde{V}_a = 0$, so

$$\sum_{i,\mu}\|(\partial_{x_i^\mu}U_N)T\|^2 = \sum_{a,i,\mu}|\partial_{x_i^\mu}\chi_a|^2\|(\mathbb{1}-\Pi_N)T\|^2 + \sum_a \chi_a^2 \sum_{i,\mu}\|(\partial_{x_i^\mu}\widetilde{V}_a)T\|^2.$$

By Step 1 and (236), the first sum is at most $NA_N m(\mathbf{X})$. For the second, let $s(\mathbf{X}) \in \pi O_a$ and $\mathbf{Y} = \pi^{-1}\mathbf{X}$. Since $R_{\pi^{-1}}T(\mathbf{X}) = T(\mathbf{Y})$ and the sum over i,μ is invariant under relabeling the particles,

$$\sum_{i,\mu}\|(\partial_{x_i^\mu}\widetilde{V}_a)(\mathbf{X})T(\mathbf{X})\|^2 = \sum_{i,\mu}\|(\partial_{y_i^\mu}V_a)(\mathbf{Y})T(\mathbf{Y})\|^2.$$

The vector $V_a(\mathbf{Y})T(\mathbf{Y})$ is the tensor product over j of the unit vectors

$$U_{|I_{a,j}|}(\mathbf{Y}_{I_{a,j}})\, T(\mathbf{Y}_{I_{a,j}}),$$

and a derivative in a coordinate from block $I_{a,j}$ acts only on the jth factor. The inductive bound therefore estimates the right-hand side by $\sum_j b_{|I_{a,j}|}m(\mathbf{X})$, since the pairs within a block are among all pairs and the sum over all pairs is permutation invariant. Hence (235) holds with

$$b_N = NA_N + \max_a \sum_j b_{|I_{a,j}|},$$

which depends only on N. This completes the induction. □

Lemma B.2 (A symmetric tensor lift with controlled derivatives)**.** *Let $N \in \mathbb{N}$, let $\mathcal{V}$ be a separable complex Hilbert space, and let $\mathcal{K}_N$ and b_N be as in Lemma B.1. If $t \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathcal{V})$ and $\|t(\mathbf{x})\| = 1$, there is a permutation-invariant map $K \in H^1_{\mathrm{loc}}((\mathbb{R}^3)^N;\mathcal{K}_N)$ such that, almost everywhere,*

$$\|K(\mathbf{X})\|^2 = 1, \qquad \langle K(\mathbf{X}), \partial_{x_i^\mu}K(\mathbf{X})\rangle = \langle t(\mathbf{x}_i), \partial_\mu t(\mathbf{x}_i)\rangle, \tag{237}$$

$$\sum_{i=1}^N\sum_{\mu=1}^3\|\partial_{x_i^\mu}K(\mathbf{X})\|^2 \le \sum_{i=1}^N\|\boldsymbol{\nabla}t(\mathbf{x}_i)\|^2 + b_N \min\Big\{\sum_{i<j}\frac{1}{|\mathbf{x}_i-\mathbf{x}_j|^2},\ \|\boldsymbol{\nabla}t\|_\infty^2\Big\}. \tag{238}$$

If $t \in W^{1,\infty}(\mathbb{R}^3;\mathcal{V})$, then $K \in W^{1,\infty}((\mathbb{R}^3)^N;\mathcal{K}_N)$, and the right-hand side of (238) is at most $C_N\|\boldsymbol{\nabla}t\|_\infty^2$ with $C_N = N + b_N$. Here $\mathbf{X} = (\mathbf{x}_1,\dots,\mathbf{x}_N)$ and the inner product is linear in its second argument.

Proof. Let U_N be as in Lemma B.1, take the Lipschitz representative of t if t is Lipschitz, and set $K(\mathbf{X}) = U_N(\mathbf{X})T(\mathbf{X})$ on $\mathcal{D}_N$. Because t is bounded and in H^1_{loc}, so is T. Since $T(\pi\mathbf{X}) = R_\pi T(\mathbf{X})$, the first identity in (234) makes K permutation invariant, and $\|K\| = \|T\| = 1$. For $\partial = \partial_{x_i^\mu}$,

$$\partial K = (\partial U_N)T + U_N \partial T$$

almost everywhere. Flatness gives $\langle K, (\partial U_N)T\rangle = \langle T, U_N^\dagger(\partial U_N)T\rangle = 0$. Since U_N is an isometry and the other factors of T are unit vectors,

$$\langle K, \partial K\rangle = \langle T, \partial T\rangle = \langle t(\mathbf{x}_i), \partial_\mu t(\mathbf{x}_i)\rangle,$$

which is (237). Flatness also removes the cross term in $\|\partial K\|^2$, so

$$\sum_{i,\mu} \|\partial_{x_i^\mu} K\|^2 = \sum_i \|\boldsymbol{\nabla} t(\mathbf{x}_i)\|^2 + \sum_{i,\mu} \|(\partial_{x_i^\mu} U_N)T\|^2,$$

and (235) gives (238) on $\mathcal{D}_N$. The collision diagonals have codimension three, so $|\mathbf{x}_i - \mathbf{x}_j|^{-2}$ is locally integrable and the right-hand side of (238) lies in $L^1_{\mathrm{loc}}((\mathbb{R}^3)^N)$. Almost every line parallel to a coordinate axis misses the diagonals, so the absolute-continuity criterion on coordinate lines extends K to $H^1_{\mathrm{loc}}((\mathbb{R}^3)^N; \mathcal{K}_N)$, and to $W^{1,\infty}((\mathbb{R}^3)^N; \mathcal{K}_N)$ when t is Lipschitz, since the bound is then uniform. The extension remains permutation invariant and has norm one. In the Lipschitz case, the right-hand side of (238) is at most $(N + b_N)\|\boldsymbol{\nabla} t\|^2_\infty$. □

Appendix C. Paramagnetic current density shift

The next lemma shifts the paramagnetic (and hence the combined) current density by combining six contributions to the mixed state, corresponding to momentum kicks in the positive and negative coordinate directions. Their position-dependent weights make the average kick equal to the prescribed velocity shift $\mathbf{v}$, while preserving the electronic density and photon reduced state.

Lemma C.1 (Exact current shift for one electron)**.** *Let $N = 1$, $\boldsymbol{\Gamma} \in \mathcal{D}$, and $\mathbf{v} \in W^{1,\infty}(\mathbb{R}^3, \mathbb{R}^3)$ with $\mathbf{v} \neq 0$. There is a finite mixture $\boldsymbol{\Gamma}_\mathbf{v} \in \mathcal{D}$ with*

$$\rho_{\boldsymbol{\Gamma}_\mathbf{v}} = \rho_{\boldsymbol{\Gamma}}, \qquad \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}_\mathbf{v}} = \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} + \rho_{\boldsymbol{\Gamma}}\mathbf{v}, \qquad \mathrm{Tr}_{\mathrm{el}}\, \boldsymbol{\Gamma}_\mathbf{v} = \mathrm{Tr}_{\mathrm{el}}\, \boldsymbol{\Gamma}, \tag{239}$$

and

$$\mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}_\mathbf{v}\big) \leq \mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}\big) + \int_{\mathbb{R}^3} \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} \cdot \mathbf{v} + 36\|\mathbf{v}\|^2_\infty + \left(\int_{\mathbb{R}^3} \rho_{\boldsymbol{\Gamma}} |\boldsymbol{\nabla}\mathbf{v}|^2\right)^{1/2}.$$

Proof. For $q > 3\|\mathbf{v}\|_\infty$, let $K_{\mu,\sigma}$ be electronic multiplication by

$$K_{\mu,\sigma}(\mathbf{x}) = \frac{1}{\sqrt{6}} \sqrt{1 + \frac{3\sigma v^\mu(\mathbf{x})}{q}}\, e^{\mathrm{i}\sigma q x^\mu}, \qquad \mu = 1, 2, 3, \quad \sigma \in \{-1, 1\},$$

and set

$$\boldsymbol{\Gamma}_{\mathbf{v},q} = \sum_{\mu,\sigma} K_{\mu,\sigma} \boldsymbol{\Gamma} K^\dagger_{\mu,\sigma}, \qquad \boldsymbol{\Gamma}_{\mathbf{v},q}(\mathbf{x}, \mathbf{x}') = \sum_{\mu,\sigma} K_{\mu,\sigma}(\mathbf{x})\, \boldsymbol{\Gamma}(\mathbf{x}, \mathbf{x}')\, \overline{K_{\mu,\sigma}(\mathbf{x}')}$$

These multipliers are bounded with bounded weak derivatives and hence act boundedly on $\mathcal{Q}_{\mathrm{PF}}$. In particular, $\mathbf{\Gamma}_{\mathbf{v},q}$ has finite form energy. Directly from their definition,

$$\sum_{\mu,\sigma} |K_{\mu,\sigma}(\mathbf{x})|^2 = \frac{1}{6}\sum_{\mu,\sigma}\left(1+\frac{3\sigma v^\mu(\mathbf{x})}{q}\right) = 1,$$

$$\sum_{\mu,\sigma} \overline{K_{\mu,\sigma}(\mathbf{x})}\boldsymbol{\nabla} K_{\mu,\sigma}(\mathbf{x}) = \frac{1}{2}\boldsymbol{\nabla}\sum_{\mu,\sigma}|K_{\mu,\sigma}(\mathbf{x})|^2 + \mathrm{i}q\sum_{\mu,\sigma}\sigma|K_{\mu,\sigma}(\mathbf{x})|^2\mathbf{e}_\mu = \mathrm{i}\mathbf{v}(\mathbf{x}),$$

where $\mathbf{e}_\mu$ is the μth coordinate unit vector. The above scalar relation means that $\sum_{\mu,\sigma} K_{\mu,\sigma}^\dagger K_{\mu,\sigma} = \mathbb{1}$ as an operator. Each summand defining $\mathbf{\Gamma}_{\mathbf{v},q}$ is positive and trace class, and cyclicity of the trace gives

$$\operatorname{Tr}\mathbf{\Gamma}_{\mathbf{v},q} = \operatorname{Tr}\left(\mathbf{\Gamma}\sum_{\mu,\sigma}K_{\mu,\sigma}^\dagger K_{\mu,\sigma}\right) = \operatorname{Tr}\mathbf{\Gamma} = 1.$$

Consequently, $\mathbf{\Gamma}_{\mathbf{v},q} \in \mathcal{D}$.

For the density, write a spectral decomposition $\mathbf{\Gamma} = \sum_r p_r|\Psi_r\rangle\langle\Psi_r|$ with $p_r > 0$. We use the density and current formulas also for unnormalized vectors, with their usual quadratic scaling. Since $N = 1$ and each multiplier is scalar in the photon variables, $\rho_{K_{\mu,\sigma}\Psi_r} = |K_{\mu,\sigma}|^2\rho_{\Psi_r}$. Hence, almost everywhere,

$$\rho_{\mathbf{\Gamma}_{\mathbf{v},q}} = \sum_r p_r\sum_{\mu,\sigma}|K_{\mu,\sigma}|^2\rho_{\Psi_r} = \sum_r p_r\rho_{\Psi_r} = \rho_{\mathbf{\Gamma}}.$$

To check the photon reduced state, let $B \in \mathcal{B}(\mathcal{F}_{\mathrm{ph}})$. Each $K_{\mu,\sigma}$ acts only on the electronic factor and therefore commutes with $\mathbb{1}_{\mathrm{el}}\otimes B$. By the definition (2) of the partial trace and cyclicity of the trace,

$$\begin{aligned}\operatorname{Tr}((\operatorname{Tr}_{\mathrm{el}}\mathbf{\Gamma}_{\mathbf{v},q})B) &= \sum_{\mu,\sigma}\operatorname{Tr}\big(\mathbf{\Gamma}K_{\mu,\sigma}^\dagger(\mathbb{1}_{\mathrm{el}}\otimes B)K_{\mu,\sigma}\big)\\ &= \operatorname{Tr}\left(\mathbf{\Gamma}(\mathbb{1}_{\mathrm{el}}\otimes B)\sum_{\mu,\sigma}K_{\mu,\sigma}^\dagger K_{\mu,\sigma}\right)\\ &= \operatorname{Tr}((\operatorname{Tr}_{\mathrm{el}}\mathbf{\Gamma})B)\,.\end{aligned}$$

Since this holds for every bounded B, it proves $\operatorname{Tr}_{\mathrm{el}}\mathbf{\Gamma}_{\mathbf{v},q} = \operatorname{Tr}_{\mathrm{el}}\mathbf{\Gamma}$.

For the current density, fix one multiplier $K = K_{\mu,\sigma}$. The field operator commutes with electronic scalar multiplication, so the weak product rule gives

$$\mathbf{D}_1(K\Psi) = K\mathbf{D}_1\Psi - \mathrm{i}(\boldsymbol{\nabla}K)\Psi.$$

Using $\mathbf{j}^{\mathrm{c}}_\Psi = \operatorname{Re}\langle\Psi,\mathbf{D}_1\Psi\rangle_{\mathbf{x}}$ for $N = 1$, we obtain

$$\mathbf{j}^{\mathrm{c}}_{K\Psi} = \operatorname{Re}\langle K\Psi, K\mathbf{D}_1\Psi - \mathrm{i}(\boldsymbol{\nabla}K)\Psi\rangle_{\mathbf{x}} = |K|^2\mathbf{j}^{\mathrm{c}}_\Psi + \operatorname{Im}(\overline{K}\boldsymbol{\nabla}K)\rho_\Psi.$$

Summing over the six multipliers therefore yields

$$\sum_{\mu,\sigma}\mathbf{j}^{\mathrm{c}}_{K_{\mu,\sigma}\Psi} = \mathbf{j}^{\mathrm{c}}_\Psi + \rho_\Psi\operatorname{Im}\left(\sum_{\mu,\sigma}\overline{K}_{\mu,\sigma}\boldsymbol{\nabla}K_{\mu,\sigma}\right) = \mathbf{j}^{\mathrm{c}}_\Psi + \rho_\Psi\mathbf{v}.$$

Since the multipliers commute with $\mathfrak{A}(\mathbf{x})$, the field-induced current density is unchanged and the shift is entirely paramagnetic. Apply this to each Ψ_r and sum

with weights p_r to conclude

$$\mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}_{\mathbf{v},q}} = \sum_r p_r \big(\mathbf{j}^{\mathrm{c}}_{\Psi_r} + \rho_{\Psi_r}\mathbf{v}\big) = \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} + \rho_{\mathbf{\Gamma}}\mathbf{v}.$$

The density series converges in L^1 by positivity and normalization, and the current series by Cauchy–Schwarz and the finite mean form energy. Thus the identities hold also for an infinite-rank $\mathbf{\Gamma}$.

Expanding the squared norm in the same product rule gives

$$\begin{aligned}\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_{\mathbf{v},q}\big) - \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) = \int_{\mathbb{R}^3} \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} \cdot \mathbf{v} + \frac{q^2}{2} \\ + \frac{3}{8q^2} \sum_{\mu=1}^{3} \int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} \frac{|\boldsymbol{\nabla} v^\mu|^2}{1 - 9(v^\mu)^2/q^2}. \end{aligned} \tag{240}$$

The radiation energy is unchanged. These identities extend by form approximation, or termwise in a spectral decomposition of $\mathbf{\Gamma}$. Choose

$$q^2 = \max\left\{36\|\mathbf{v}\|_\infty^2, \left(\int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} |\boldsymbol{\nabla}\mathbf{v}|^2\right)^{1/2}\right\},$$

so that $q \geq 6\|\mathbf{v}\|_\infty > 3\|\mathbf{v}\|_\infty$ since $\mathbf{v} \neq 0$. The denominators in (240) are at least $3/4$, and the last two terms are at most

$$\frac{q^2}{2} + \frac{1}{2q^2}\int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} |\boldsymbol{\nabla}\mathbf{v}|^2 \leq q^2 \leq 36\|\mathbf{v}\|_\infty^2 + \left(\int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} |\boldsymbol{\nabla}\mathbf{v}|^2\right)^{1/2}.$$

Set $\mathbf{\Gamma}_{\mathbf{v}} = \mathbf{\Gamma}_{\mathbf{v},q}$ with this choice of q. Photon localization acts only on the photon factor, so equality of photon marginals also preserves the localized photon-number distributions. □

To lift this construction to the antisymmetric N-electron space, we replace tensor products of the one-electron multipliers by symmetric multipliers with the same connection. These are constructed in Appendix B, and only Lemma B.2 is used below. The lift applies to any unit-vector field with connection $\mathrm{i}\mathbf{v}$, not only to the six multipliers above. Part (ii) of the next lemma uses this to remove the boundedness assumptions on $\mathbf{v}$.

Lemma C.2 (Exact current shift for arbitrary particle number)**.** *Let $N \in \mathbb{N}$ and $\mathbf{\Gamma} \in \mathcal{D}$.*

(i) If $\mathbf{v} \in W^{1,\infty}(\mathbb{R}^3, \mathbb{R}^3)$ and $\mathbf{v} \neq 0$, there is a finite electronic multiplication mixture $\mathbf{\Gamma}_{\mathbf{v}} \in \mathcal{D}$ satisfying (239) and

$$\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_{\mathbf{v}}\big) \leq \mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \int_{\mathbb{R}^3} \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} \cdot \mathbf{v} + C_N\big(\|\mathbf{v}\|_\infty^2 + \|\boldsymbol{\nabla}\mathbf{v}\|_\infty\big). \tag{241}$$

(ii) Let $\mathcal{V}$ be a separable complex Hilbert space, let $t \in H^1_{\mathrm{loc}}(\mathbb{R}^3; \mathcal{V})$ satisfy $\|t\| = 1$ and $\int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} \|\boldsymbol{\nabla} t\|^2 < \infty$, and put $\mathbf{v} = \mathrm{Im}\langle t, \boldsymbol{\nabla} t\rangle$. Then there is a countable electronic multiplication mixture $\mathbf{\Gamma}_{\mathbf{v}} \in \mathcal{D}$ satisfying (239) and

$$\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}_{\mathbf{v}}\big) \leq (1 + C_N)\,\mathrm{Tr}\big(H^{0,0}\mathbf{\Gamma}\big) + \int_{\mathbb{R}^3} \mathbf{j}^{\mathrm{c}}_{\mathbf{\Gamma}} \cdot \mathbf{v} + \frac{1}{2}\int_{\mathbb{R}^3} \rho_{\mathbf{\Gamma}} \|\boldsymbol{\nabla} t\|^2. \tag{242}$$

Here C_N depends only on N. In both cases, $\mathbf{\Gamma}_{\mathbf{v}}$ and $\mathbf{\Gamma}$ have the same Coulomb energy.

Proof. *(i)* Let $K_{\mu,\sigma}$ be the six multipliers from the proof of Lemma C.1, with $q^2 = \max\{36\|\mathbf{v}\|_\infty^2, \|\boldsymbol{\nabla}\mathbf{v}\|_\infty\}$, and collect them in the unit vector $t(\mathbf{x}) = (K_{\mu,\sigma}(\mathbf{x}))_{\mu,\sigma} \in \mathbb{C}^6$. By the identities established there, $\langle t, \boldsymbol{\nabla} t\rangle = \mathrm{i}\mathbf{v}$ and

$$|\boldsymbol{\nabla} t|^2 = q^2 + \frac{3}{4q^2}\sum_{\mu=1}^{3}\frac{|\boldsymbol{\nabla} v^\mu|^2}{1-9(v^\mu)^2/q^2} \le q^2 + \frac{\|\boldsymbol{\nabla}\mathbf{v}\|_\infty^2}{q^2} \le 36\|\mathbf{v}\|_\infty^2 + 2\|\boldsymbol{\nabla}\mathbf{v}\|_\infty.$$

Apply Lemma B.2 with $\mathcal{V} = \mathbb{C}^6$ to t, fix an orthonormal basis $(e_\alpha)_{\alpha=1}^{\dim \mathcal{K}_N}$ of $\mathcal{K}_N$, and let $K_\alpha = \langle e_\alpha, K\rangle$. These are finitely many permutation-invariant scalar multipliers with

$$\sum_\alpha |K_\alpha|^2 = 1, \qquad \sum_\alpha \overline{K}_\alpha \boldsymbol{\nabla}_{\mathbf{x}_i} K_\alpha = \mathrm{i}\mathbf{v}(\mathbf{x}_i),$$
$$\sum_{i,\alpha} |\boldsymbol{\nabla}_{\mathbf{x}_i} K_\alpha|^2 \le C_N\big(\|\mathbf{v}\|_\infty^2 + \|\boldsymbol{\nabla}\mathbf{v}\|_\infty\big).$$

Define $\boldsymbol{\Gamma}_{\mathbf{v}} = \sum_\alpha K_\alpha \boldsymbol{\Gamma} K_\alpha^\dagger$. Symmetry and bounded weak derivatives preserve the fermionic form domain. Since the K_α act by multiplication in $\mathbf{X}$ and $\sum_\alpha |K_\alpha|^2 = 1$, the first identity preserves the density, the Coulomb energy, and the photon marginal. The second identity gives the current shift, and the third bounds the kinetic remainder after expanding each covariant derivative. The radiation energy is unchanged.

(ii) Apply Lemma B.2 to t, fix an orthonormal basis (e_α) of $\mathcal{K}_N$, and let $K_\alpha = \langle e_\alpha, K\rangle$. These are countably many permutation-invariant scalar multipliers with

$$\sum_\alpha |K_\alpha|^2 = 1, \qquad \sum_\alpha \overline{K}_\alpha \boldsymbol{\nabla}_{\mathbf{x}_i} K_\alpha = \mathrm{i}\mathbf{v}(\mathbf{x}_i),$$
$$\sum_{i,\alpha} |\boldsymbol{\nabla}_{\mathbf{x}_i} K_\alpha|^2 \le \sum_i \|\boldsymbol{\nabla} t(\mathbf{x}_i)\|^2 + b_N \sum_{i<j}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^2}.$$

Since $\sum_\alpha \mathrm{Tr}\big(K_\alpha \boldsymbol{\Gamma} K_\alpha^\dagger\big) = 1$, the series $\boldsymbol{\Gamma}_{\mathbf{v}} = \sum_\alpha K_\alpha \boldsymbol{\Gamma} K_\alpha^\dagger$ converges in trace norm. The multipliers need not have bounded derivatives. Still, for every eigenvector Ψ of $\boldsymbol{\Gamma}$ with positive eigenvalue, the last bound keeps $\sum_\alpha \|\boldsymbol{\nabla}_{\mathbf{x}_n}(K_\alpha\Psi)\|^2$ finite. Its first part contributes $\int \rho_\Psi \|\boldsymbol{\nabla} t\|^2$, which is finite because $\int \rho_{\boldsymbol{\Gamma}}\|\boldsymbol{\nabla} t\|^2 < \infty$, and its second part is controlled by the Hardy bound below. Hence each $K_\alpha\Psi$ lies in the form domain, and the density, the Coulomb energy, the photon marginal, and the current shift follow as in (i). Expanding each covariant derivative gives exactly

$$\mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}_{\mathbf{v}}\big) = \mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}\big) + \int_{\mathbb{R}^3} \mathbf{j}^{\mathrm{c}}_{\boldsymbol{\Gamma}} \cdot \mathbf{v} + \frac{1}{2}\,\mathrm{Tr}\left(\boldsymbol{\Gamma}\sum_{i,\alpha}|\boldsymbol{\nabla}_{\mathbf{x}_i} K_\alpha|^2\right),$$

where the middle integral converges absolutely by (38) and the Cauchy–Schwarz inequality, since $|\mathbf{v}| \le \|\boldsymbol{\nabla} t\|$. The first part of the multiplier bound contributes $\frac{1}{2}\int \rho_{\boldsymbol{\Gamma}}\|\boldsymbol{\nabla} t\|^2$. For the second, we use the diamagnetic inequality $|\boldsymbol{\nabla}_{\mathbf{x}_n}\|\Psi(\mathbf{X})\|| \le \|(\mathbf{D}_n\Psi)(\mathbf{X})\|$ and Hardy's inequality in the relative coordinate $\mathbf{x}_i - \mathbf{x}_j$. They give

$$\int \frac{\|\Psi(\mathbf{X})\|^2}{|\mathbf{x}_i - \mathbf{x}_j|^2}\,\mathrm{d}\mathbf{X} \le 2\big(\|\mathbf{D}_i\Psi\|^2 + \|\mathbf{D}_j\Psi\|^2\big),$$

and hence

$$\mathrm{Tr}\left(\boldsymbol{\Gamma}\sum_{i<j}\frac{1}{|\mathbf{x}_i - \mathbf{x}_j|^2}\right) \le 2(N-1)\sum_{n=1}^{N}\mathrm{Tr}\big(\mathbf{D}_n^2\boldsymbol{\Gamma}\big) \le 4(N-1)\,\mathrm{Tr}\big(H^{0,0}\boldsymbol{\Gamma}\big).$$

This proves (242) with $C_N^{(\mathrm{ii})} = 2(N-1)b_N$. Taking the maximum of this constant and the constant obtained in part (i) gives a common C_N for both estimates. □

Part (ii) needs a unit-vector field with prescribed connection. For connections of the form $\boldsymbol{\nabla} S + \mathbf{w}$ with $\mathbf{w}$ in a weighted Sobolev space, coherent states provide one.

Lemma C.3 (Coherent-state tags)**.** *Let $\mathcal{V} = \mathcal{F}_s(\mathbb{C}^3)$, with vacuum $\Omega_{\mathcal{V}}$ and Weyl operators $W(z)$, $z \in \mathbb{C}^3$, as in (200). Let $S \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R})$, $\mathbf{w} \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{R}^3)$ and $\lambda > 0$, and put*

$$h(\mathbf{x}) = \frac{1}{\sqrt{2}} \sum_{k=1}^{3} \Big(\lambda w_k(\mathbf{x}) + \frac{\mathrm{i} x_k}{\lambda} \Big) \mathbf{e}_k, \qquad t(\mathbf{x}) = e^{\mathrm{i}(S(\mathbf{x}) + \frac{1}{2}\mathbf{x}\cdot\mathbf{w}(\mathbf{x}))}\, W(h(\mathbf{x}))\Omega_{\mathcal{V}},$$

where $(\mathbf{e}_k)$ is the standard basis of $\mathbb{C}^3$. Then $t \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathcal{V})$, $\|t\| = 1$, and almost everywhere

$$\mathrm{Im}\langle t, \boldsymbol{\nabla} t\rangle = \boldsymbol{\nabla} S + \mathbf{w}, \qquad \|\boldsymbol{\nabla} t\|^2 = |\boldsymbol{\nabla} S + \mathbf{w}|^2 + \frac{1}{2}\big(\lambda^2 |\boldsymbol{\nabla}\mathbf{w}|^2 + 3\lambda^{-2}\big). \tag{243}$$

Proof. The phase $S + \frac{1}{2}\mathbf{x}\cdot\mathbf{w}$ lies in H^1_{loc}, and $h \in H^1_{\mathrm{loc}}(\mathbb{R}^3;\mathbb{C}^3)$. Since $\sum_k x_k \partial_j w_k = \partial_j(\mathbf{x}\cdot\mathbf{w}) - w_j$,

$$\mathrm{Im}\langle h, \partial_j h\rangle = \frac{1}{2}\sum_k \big(w_k \delta_{jk} - x_k \partial_j w_k \big) = w_j - \frac{1}{2}\partial_j(\mathbf{x}\cdot\mathbf{w}),$$

$$\sum_j |\partial_j h|^2 = \frac{1}{2}\big(\lambda^2 |\boldsymbol{\nabla}\mathbf{w}|^2 + 3\lambda^{-2}\big).$$

Hence $\partial_j(S + \frac{1}{2}\mathbf{x}\cdot\mathbf{w}) + \mathrm{Im}\langle h, \partial_j h\rangle = \partial_j S + w_j$, and Proposition A.9(iii) gives (243). Unitarity of $W(h)$ gives $\|t\| = 1$. The right-hand side of the second identity in (243) is locally integrable, so $t \in H^1_{\mathrm{loc}}$ by the same proposition. □

With this tag, the last term in (242) is $\frac{1}{2}\int \rho_{\boldsymbol{\Gamma}} \|\boldsymbol{\nabla} t\|^2$, which involves only the weighted norms $\int \rho_{\boldsymbol{\Gamma}}(|\boldsymbol{\nabla} S + \mathbf{w}|^2 + |\boldsymbol{\nabla}\mathbf{w}|^2)$ and N. For instance, the rigid rotation $\mathbf{w} = \boldsymbol{\omega} \times \mathbf{x}$ is allowed for every $\boldsymbol{\Gamma}$ with $\int \rho_{\boldsymbol{\Gamma}} |\mathbf{x}|^2 < \infty$.

Appendix D. Gaussian representation of the field

In this appendix we represent the field in a subspace of the photon modes by multiplication operators and condition states on its values.

In the solenoidal representation, recall the conjugation $(J\mathbf{f})(\mathbf{k}) = \overline{\mathbf{f}(-\mathbf{k})}$. The symmetry $\widehat{\chi}(\mathbf{k}) = \overline{\widehat{\chi}(-\mathbf{k})}$ in (9) gives $J\mathbf{G}^\mu_{\mathbf{x}} = \mathbf{G}^\mu_{\mathbf{x}}$. Fix an infinite-dimensional closed subspace $\mathfrak{h} \subset \mathfrak{H}_{\mathrm{ph}}$ with $J\mathfrak{h} \subset \mathfrak{h}$, and let $P_{\mathfrak{h}}$ be the orthogonal projection onto it. Since J is an antiunitary involution, also $J\mathfrak{h}^\perp \subset \mathfrak{h}^\perp$, so $P_{\mathfrak{h}}$ commutes with J and every $P_{\mathfrak{h}} G^\mu_{\mathbf{x}}$ is J-real. The exponential law for Fock spaces gives $\mathcal{F}_{\mathrm{ph}} \simeq \mathcal{F}_s(\mathfrak{h}^\perp) \otimes \mathcal{F}_s(\mathfrak{h})$. Put $\mathcal{K} = \mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_s(\mathfrak{h}^\perp)$, so that $\mathcal{H}_N \simeq \mathcal{K} \otimes \mathcal{F}_s(\mathfrak{h})$, and let $\mathfrak{A}_{\mathfrak{h}}(\mathbf{x})$ have components $\mathfrak{A}^\mu_{\mathfrak{h}}(\mathbf{x}) = \Phi(P_{\mathfrak{h}} G^\mu_{\mathbf{x}})$. We use two cases. For the whole field, $\mathfrak{h} = \mathfrak{H}_{\mathrm{ph}}$ and $\mathcal{K} = \mathfrak{H}^N_{\mathrm{el}}$. For the soft field, fix $\kappa > 0$ and use the notation introduced before Lemma 5.8: then $\mathfrak{h} = \mathfrak{H}_{<\kappa}$, $P_{\mathfrak{h}} = \mathbb{1}_{\{\omega<\kappa\}}$, and $\mathcal{K} = \mathfrak{H}^N_{\mathrm{el}} \otimes \mathcal{F}_{\geq\kappa}$. This subspace is J-invariant because $\omega(-\mathbf{k}) = \omega(\mathbf{k})$.

Scalar products of J-real vectors are real, so all components of $\mathfrak{A}_\mathfrak{h}$ commute strongly by Proposition A.6(iii). Let $(\xi_n)_{n\geq 1}$ be a J-real orthonormal basis of $\mathfrak{h}$, equip $\mathcal{Q} = \mathbb{R}^\mathbb{N}$ with its product σ-algebra and the product measure

$$\mu = \bigotimes_{n\geq 1} \gamma, \qquad \mathrm{d}\gamma(t) = (2\pi)^{-1/2} e^{-t^2/2} \mathrm{d}t,$$

and write $u = (u_n)_{n\geq 1} \in \mathcal{Q}$. Mapping the occupation basis associated with (ξ_n) to products of normalized Hermite polynomials in the variables u_n gives a unitary $\mathcal{G} : \mathcal{F}_s(\mathfrak{h}) \to L^2(\mathcal{Q}, \mu)$, the Wiener–Itô–Segal isomorphism [51, 52, 23]. For its use with the Pauli–Fierz model, see [37]. Under $\mathcal{G}$, the field $\Phi(g)$ with $g \in \mathfrak{h}$ and $Jg = g$ becomes multiplication by the real Gaussian variable $\sum_n \langle \xi_n, g\rangle u_n$ of variance $\|g\|^2$. In particular, $\Phi(\xi_n)$ becomes multiplication by u_n. Hence $\mathfrak{A}_\mathfrak{h}(\mathbf{x})$ becomes multiplication by the real random field $\mathbf{a}_u(\mathbf{x})$ with components

$$a^\mu_u(\mathbf{x}) = \sum_{n\geq 1} \langle \xi_n, P_\mathfrak{h} G^\mu_\mathbf{x}\rangle \, u_n,$$

the series converging in $L^2(\mathcal{Q}, \mu)$.

Now let $\mathbf{\Gamma}$ be a positive trace-class operator on $\mathcal{H}_N$. We write $\mathcal{G}$ also for $\mathbb{1} \otimes \mathcal{G}$, which maps $\mathcal{H}_N$ unitarily onto $L^2(\mathcal{Q}, \mu; \mathcal{K})$. If $(\Psi_j)_{j\geq 1}$ is any orthonormal basis of $\mathcal{H}_N$, put

$$\Theta(u) = \sum_{j\geq 1} |(\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u)\rangle\langle(\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u)|.$$

Lemma D.1 (Disintegration over the field)**.** *Let $\mathbf{\Gamma}$ and Θ be as above.*

(i) For μ-almost every u, the series defining $\Theta(u)$ converges in trace norm to a positive trace-class operator on $\mathcal{K}$.

(ii) The family $(\Theta(u))_{u\in\mathcal{Q}}$ disintegrates $\mathbf{\Gamma}$ over the values of $\mathfrak{A}_\mathfrak{h}$: for every bounded operator B on $\mathcal{K}$ and every bounded measurable function f on $\mathcal{Q}$,

$$\mathrm{Tr}\left(\mathbf{\Gamma}\,(B \otimes \mathcal{G}^{-1} M_f \mathcal{G})\right) = \int_\mathcal{Q} f(u)\,\mathrm{Tr}\left(B\Theta(u)\right)\mathrm{d}\mu(u), \tag{244}$$

where M_f is multiplication by f on $L^2(\mathcal{Q}, \mu)$. In particular, $\int_\mathcal{Q} \Theta(u)\mathrm{d}\mu(u)$ is the partial trace of $\mathbf{\Gamma}$ over $\mathcal{F}_s(\mathfrak{h})$.

(iii) Every family of trace-class operators on $\mathcal{K}$ satisfying (244) for all such B and f agrees with $\Theta(u)$ for μ-almost every u. In particular, Θ does not depend on the choice of the basis $(\Psi_j)_{j\geq 1}$, up to a μ-null set.

Proof. (i) Each term of the series is positive and of rank one, and its trace is the squared norm of its vector. By Tonelli's theorem and unitarity of $\mathcal{G}$,

$$\int_\mathcal{Q} \sum_j \|(\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u)\|^2 \mathrm{d}\mu(u) = \sum_j \|\sqrt{\mathbf{\Gamma}}\Psi_j\|^2 = \mathrm{Tr}\,\mathbf{\Gamma} < \infty.$$

Hence the traces are summable for μ-almost every u.

(ii) Expanding the trace in the basis (Ψ_j), the left-hand side of (244) equals

$$\sum_j \langle \sqrt{\mathbf{\Gamma}}\Psi_j, (B \otimes \mathcal{G}^{-1} M_f \mathcal{G})\sqrt{\mathbf{\Gamma}}\Psi_j\rangle$$
$$= \sum_j \int_\mathcal{Q} f(u) \langle (\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u), B(\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u)\rangle \mathrm{d}\mu(u).$$

The integrands are bounded by $\|B\|\|f\|_\infty\|(\mathcal{G}\sqrt{\mathbf{\Gamma}}\Psi_j)(u)\|^2$, so the bound in (i) allows the sum and the integral to be exchanged, which gives (244). For $f = 1$, the definition (2) of the partial trace yields the last identity, the integral converging in trace norm by the same bound.

(iii) Let $(\Theta'(u))_{u\in\mathcal{Q}}$ be another family of trace-class operators satisfying (244). Its left-hand side does not involve the family, so for every bounded B,

$$\int_{\mathcal{Q}} f(u)\,\mathrm{Tr}\left(B(\Theta(u)-\Theta'(u))\right)\mathrm{d}\mu(u) = 0$$

for all bounded measurable f. Hence $\mathrm{Tr}(B(\Theta(u)-\Theta'(u))) = 0$ outside a μ-null set depending on B. Since $\mathcal{K}$ is separable, there is a countable family of finite-rank operators that is norm dense in the compact operators on $\mathcal{K}$. Outside the union of the corresponding null sets, $\mathrm{Tr}(B(\Theta(u)-\Theta'(u))) = 0$ for every compact B, and since the trace class is the dual of the compact operators, $\Theta(u) = \Theta'(u)$. □

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