Minimization of the Energy of the Nonrelativistic One-Electron Pauli-Fierz Model over Quasifree States

Volker Bach, Sébastien Breteaux, Tim Tzaneteas

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Abstract. In this article the existence of a minimizer for the energy for the nonrelativistic one-electron Pauli-Fierz model within the class of quasifree states is established. To this end it is shown that the minimum of the energy on quasifree states coincides with the minimum of the energy on pure quasifree states, where existence and uniqueness of a minimizer holds. Infrared and ultraviolet cutoffs are assumed, along with sufficiently small coupling constant and momentum of the dressed electron. A perturbative expression of the minimum of the energy on quasifree states for a small momentum of the dressed electron and small coupling constant is given. We also express the Lagrange equation for the minimizer in terms of the generalized one particle density matrix of the pure quasifree state.

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I Introduction and Main Results

We begin by introducing the mathematical model studied in this paper and mention some well-known results before we describe the main results of the paper.

I.1 The Hamiltonian

According to the *Standard Model of Nonrelativistic Quantum Electrodynamics* [4] the unitary time evolution of a free nonrelativistic particle coupled to the quantized radiation field is generated by the Hamiltonian

$$\widetilde{H}_g \;:=\; \frac{1}{2}\big(\tfrac{1}{i}\vec{\nabla}_x - \vec{\mathbb{A}}(\vec{x})\big)^2 + H_f \tag{I.1}$$

acting on the Hilbert space $L^2(\mathbb{R}^3_x; \mathfrak{F})$ of square-integrable functions with values in the photon Fock space

$$\mathfrak{F} \;:=\; \mathfrak{F}_+(\mathfrak{h}) \;:=\; \bigoplus_{n=0}^{\infty} \mathfrak{F}_+^{(n)}(\mathfrak{h}). \tag{I.2}$$

Here $\mathfrak{F}_+^{(0)}(\mathfrak{h}) = \mathbb{C}\cdot\Omega$ is the vacuum sector and the n-photon sector $\mathfrak{F}_+^{(n)}(\mathfrak{h}) = \mathcal{S}_n(\mathfrak{h}^{\otimes n})$ is the subspace of totally symmetric vectors on the n-fold tensor product of the one-photon Hilbert space

$$\mathfrak{h} \;=\; \big\{\vec{f} \in L^2(S_{\sigma,\Lambda}; \mathbb{C}\otimes\mathbb{R}^3) \;\big|\; \forall \vec{k} \in S_{\sigma,\Lambda},\, a.e.: \quad \vec{k}\cdot\vec{f}(\vec{k}) = 0\big\} \tag{I.3}$$

of square-integrable, transversal vector fields which are supported in the momentum shell

$$S_{\sigma,\Lambda} \;:=\; \big\{\vec{k} \in \mathbb{R}^3 \;\big|\; \sigma \le |\vec{k}| \le \Lambda\big\}, \tag{I.4}$$

where $0 \le \sigma < \Lambda < \infty$ are infrared and ultraviolet cutoffs, respectively. The condition $\vec{k}\cdot\vec{f}(\vec{k}) = 0$ reflects our choice of gauge, namely, the Coulomb gauge. It is convenient to fix real polarization vectors $\vec{\varepsilon}_\pm(\vec{k}) \in \mathbb{R}^3$ such that $\{\vec{\varepsilon}_+(\vec{k}), \vec{\varepsilon}_-(\vec{k}), \frac{\vec{k}}{|\vec{k}|}\} \subseteq \mathbb{R}^3$ form a right-handed orthonormal basis (Dreibein) and replace (I.3) by

$$\mathfrak{h} \;=\; L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2), \tag{I.5}$$

with the understanding that $\vec{f}(\vec{k}) = \vec{\varepsilon}_+\, f(\vec{k},+) + \vec{\varepsilon}_-\, f(\vec{k},-)$.
In (I.1) the energy of the photon field is represented by

$$H_f \;=\; \int |k|\, a^*(k)\, a(k)\, dk, \tag{I.6}$$

where $\int f(k)dk \;:=\; \sum_{\tau=\pm}\int_{S_{\sigma,\Lambda}} f(\vec{k},\tau)\, d^3k$ and $\{a(k), a^*(k)\}_{k\in S_{\sigma,\Lambda}\times\mathbb{Z}_2}$ are the usual boson creation and annihilation operators constituting a Fock representation of the CCR on $\mathfrak{F}$, i.e.,

$$[a(k)\,,\, a(k')] \;= [a^*(k)\,,\, a^*(k')] \;=\; 0, \tag{I.7}$$

$$[a(k)\,,\, a^*(k')] \;= \delta(k-k')\,\mathbf{1}, \quad a(k)\Omega \;=\; 0, \tag{I.8}$$

for all $k, k' \in S_{\sigma,\Lambda} \times \mathbb{Z}_2$. The magnetic vector potential $\vec{\mathbb{A}}(\vec{x})$ is given by

$$\vec{\mathbb{A}}(\vec{x}) \;=\; \int \vec{G}(k)\Big(e^{-i\vec{k}\cdot\vec{x}}\, a^*(k) + e^{i\vec{k}\cdot\vec{x}}\, a(k)\Big)\, dk, \tag{I.9}$$

with $k = (\vec{k}, \tau) \in \mathbb{R}^3 \times \mathbb{Z}_2$,

$$\vec{G}(\vec{k}, \tau) \;:=\; g\, \vec{\varepsilon}_\tau(\vec{k})\, |\vec{k}|^{-1/2}, \tag{I.10}$$

and $g \in \mathbb{R}$ being the coupling constant. In our units, the mass of the particle and the speed of light equal one, so the coupling constant is given as $g = \frac{1}{4\pi}\sqrt{\alpha}$, with $\alpha \approx 1/137$ being Sommerfeld's fine structure constant.

The Hamiltonian $\widetilde{H}_g$ preserves (i.e., commutes with) the total momentum operator $\vec{p} = \frac{1}{i}\vec{\nabla}_x + \vec{P}_f$ of the system, where

$$\vec{P}_f \;=\; \int \vec{k}\, a^*(k)\, a(k)\, dk \tag{I.11}$$

is the photon field momentum. This fact allows us to eliminate the particle degree of freedom. More specifically, introducing the unitary operator

$$\mathbb{U} \;: L^2(\mathbb{R}^3_x; \mathfrak{F}) \;\to\; L^2(\mathbb{R}^3_p; \mathfrak{F})\,, \quad \big(\mathbb{U}\Psi\big)(\vec{p}) \;:=\; \int e^{-i\vec{x}\cdot(\vec{p}-\vec{P}_f)}\, \Psi(\vec{x})\, \frac{d^3x}{(2\pi)^{3/2}}, \tag{I.12}$$

one finds that

$$\mathbb{U}\, \widetilde{H}_g\, \mathbb{U}^* \;=\; \int^{\oplus} H_{g,\vec{p}}\, d^3p, \tag{I.13}$$

where

$$H_{g,\vec{p}} \;=\; \frac{1}{2}\big(\vec{P}_f + \vec{\mathbb{A}}(\vec{0}) - \vec{p}\big)^2 \;+\; H_f \tag{I.14}$$

is a self-adjoint operator on $\mathrm{dom}(H_{0,\vec{0}})$, the natural domain of $H_{0,\vec{0}} = \frac{1}{2}\vec{P}_f^{\,2} + H_f$.

I.2 Ground State Energy and Bogolubov-Hartree-Fock Energy

Due to (I.13), all spectral properties of $\widetilde{H}_g$ are obtained from those of $\{H_{g,\vec{p}}\}_{\vec{p}\in\mathbb{R}^3}$. Of particular physical interest is the mass shell for fixed total momentum $\vec{p} \in \mathbb{R}^3$, coupling constant $g \geq 0$, and infrared and ultraviolet cutoffs $0 \leq \sigma < \Lambda < \infty$, i.e., the value of the ground state energy

$$E_{\mathrm{gs}}(g, \vec{p}, \sigma, \Lambda) \;:=\; \inf \sigma[H_{g,\vec{p}}] \;\geq\; 0 \tag{I.15}$$

and the corresponding ground states (or approximate ground states).

We express the ground state energy in terms of density matrices with finite energy expectation value and accordingly introduce

$$\widetilde{\mathfrak{DM}} := \Big\{\rho \in \mathcal{L}^1(\mathfrak{F}) \ \Big| \ \rho \geq 0, \ \mathrm{Tr}_{\mathfrak{F}}[\rho] = 1, \ \rho\, H_{0,\vec{0}}, \ H_{0,\vec{0}}\, \rho \in \mathcal{L}^1(\mathfrak{F})\Big\}, \tag{I.16}$$

so that the Rayleigh-Ritz principle appears in the form

$$E_{\mathrm{gs}}(g,\vec{p}) \ = \ \inf\Big\{\mathrm{Tr}_{\mathfrak{F}}\big[\rho\, H_{g,\vec{p}}\big] \ \Big| \ \rho \in \widetilde{\mathfrak{DM}}\Big\}. \tag{I.17}$$

Note that $\mathrm{Tr}_{\mathfrak{F}}[\rho\, H_{g,\vec{p}}] = \mathrm{Tr}_{\mathfrak{F}}[\rho^{1-\beta}\, H_{g,\vec{p}}\, \rho^{\beta}]$, for all $0 \leq \beta \leq 1$, due to our assumption $\rho H_{0,\vec{0}}, H_{0,\vec{0}}\rho \in \mathcal{L}^1(\mathfrak{F})$.
The determination of $E_{\mathrm{gs}}(g,\vec{p})$ and the corresponding ground state $\rho_{\mathrm{gs}}(g,\vec{p}) \in \widetilde{\mathfrak{DM}}$ (provided the infimum is attained) is a difficult task. In this paper we rather study approximations to $E_{\mathrm{gs}}(g,\vec{p})$ and $\rho_{\mathrm{gs}}(g,\vec{p})$ that we borrow from the quantum mechanics of atoms and molecules, namely, the Bogolubov-Hartree-Fock (BHF) approximation. We define the BHF energy as

$$E_{BHF}(g,\vec{p},\sigma,\Lambda) \ = \ \inf\Big\{\mathrm{Tr}_{\mathfrak{F}}\big[\rho\, H_{g,\vec{p}}(\sigma,\Lambda)\big] \ \Big| \ \rho \in \mathfrak{QF}\Big\}, \tag{I.18}$$

with corresponding BHF ground state(s) $\rho_{BHF}(g,\vec{p},\sigma,\Lambda) \in \mathfrak{QF}$, determined by

$$\mathrm{Tr}_{\mathfrak{F}}\big[\rho_{BHF}(g,\vec{p},\sigma,\Lambda)\ H_{g,\vec{p}}(\sigma,\Lambda)\big] \ = \ E_{BHF}(g,\vec{p},\sigma,\Lambda), \tag{I.19}$$

where

$$\mathfrak{QF} \ := \ \Big\{\rho \in \mathfrak{DM} \ \Big| \ \rho \text{ is quasifree}\Big\} \ \subseteq \ \mathfrak{DM} \tag{I.20}$$

denotes the subset of quasifree density matrices (of finite particle number; see Sect. II.1).

I.3 Results

Our first result in Theorem IV.5 is that the minimal energy expectation value for all quasifree density matrices $\mathfrak{QF}$ is already obtained if the variation is restricted to pure quasifree density matrices $\mathfrak{pQF}$, i.e.,

$$E_{BHF}(g,\vec{p},\sigma,\Lambda) \ := \ \inf_{\rho\in\mathfrak{QF}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho] \ = \ \inf_{\rho\in\mathfrak{pQF}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho]\,, \tag{I.21}$$

see (I.20) and (II.40). The physical relevance of the minimization over (pure) quasifree density matrices is seen by the fact that it includes density matrices of the form

$$\rho_{sq} \ = \ \Big|e^{i[(a^*)^2+a^2]}\,\Omega\Big\rangle\Big\langle e^{i[(a^*)^2+a^2]}\,\Omega\Big|, \tag{I.22}$$

where $a \equiv a(f)$ for some one-photon state f. These are important states in quantum optics known as *squeezed light*.

The restriction to pure quasifree states has the great advantage that the latter have a very convenient parametrization of their reduced one-particle density matrix given in Proposition IV.12. This enables us to prove the existence and uniqueness of a (pure) quasifree minimizer $(f_{g,\vec{p}}, \gamma_{g,\vec{p}}, \tilde{\alpha}_{g,\vec{p}})$ which minimizes the energy $(f, \gamma, \tilde{\alpha}) \mapsto \mathcal{E}_{g,\vec{p}}(f, \gamma, \tilde{\alpha})$ in Theorem VIII.3. The minimizer is characterized in Theorem VIII.8 by the Euler-Lagrange equations corresponding to $\mathcal{E}_{g,\vec{p}}$. We obtain expansions of the minimizer and the corresponding minimal energy for small g and $\vec{p}$ in Theorem VIII.6. Our proof uses a convexity and coercivity argument and the assumption that $|g|, |\vec{p}| \leq C$ are smaller than a certain constant $C \equiv C(\sigma, \Lambda)$ which, however, is not uniformly bounded as $\Lambda \to \infty$ or $\sigma \to 0$.

We also determine the minimizer in the case where the variation over pure quasifree density matrices is further restricted to coherent states introduced in (II.41). More precisely, we minimize the energy functional $L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2) \ni f \mapsto \mathcal{E}_{g,\vec{p}}(f, 0, 0)$ and obtain the existence of a minimizer $f_{g,\vec{p}}$ and its uniqueness in Theorem VI.2 again by a fixed-point argument. Compared to the general case studied in Theorem VIII.3, our assumption for the minimizing coherent state is much milder, namely, that $|\vec{p}| \leq 1/3$ and that g^2 is small compared to $1/\ln[\Lambda + 2]$. As our equations are fairly explicit in the coherent state case, we determine the leading orders in the expansions of the minimizer $f_{g,\vec{p}}$ and of the minimal energy $\mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}, 0, 0)$ in powers of g and $|\vec{p}|$. In particular, the coefficient for the term proportional to $|\vec{p}|^2$, which gives the "renormalized electron mass for coherent states", is computed in Proposition VII.1 and is found to agree with the first order expansion in α of the renormalized mass of the electron, as computed for example in [12]. Our result holds uniformly in $\sigma \to 0$ but not in $\Lambda \to \infty$.

Outline of the article In Section II we discuss density matrices, density matrices of finite particle number, pure density matrices and quasifree density matrices in greater detail. We introduce our notation to describe the second quantization framework in Section III. Section IV introduces two parametrizations of pure quasifree states and contains the proof of Theorem IV.5. The energy functional for a fixed value of the momentum $\vec{p}$ of the dressed electron is computed in Section V, and some positivity properties of the different parts of the energy are established. From Section VI on we tacitly assume that the coupling constant $|g| > 0$ is small. The energy is then minimized in the particular case of coherent states in Section VI, providing a first upper bound to the energy of the ground state and a proof of Theorem VI.2. We then turn in Section VIII to the problem of minimizing the energy over all pure quasifree states. The existence and uniqueness of a minimizer among the class of pure quasifree state is then proven in Section VIII.1 provided $|\vec{p}|$ is small enough. The first terms of a perturbative expansion for small g and $\vec{p}$ of the energy at the minimizer is computed in Section VIII.2. Finally the Lagrange equations associated with the problem of minimization in the generalized one particle density matrix variables are presented in Section VIII.3.

II Density Matrices and Quasifree Density Matrices

We now further discuss density matrices on Fock space and in particular give more details about quasifree density matrices.

II.1 Density Matrices of Finite Particle Number

Recall that the ground state energy is obtained as

$$E_{\mathrm{gs}}(g,\vec{p}) \; = \; \inf\Big\{\mathrm{Tr}_{\mathfrak{F}}\big[\rho\, H_{g,\vec{p}}\big] \;\Big|\; \rho \in \widetilde{\mathfrak{DM}}\Big\}. \tag{II.23}$$

It is not difficult to see that $E_{\mathrm{gs}}(g,\vec{p})$ is already obtained as an infimum over all density matrices

$$\mathfrak{DM} \; := \; \Big\{\rho \in \widetilde{\mathfrak{DM}} \;\Big|\; \rho\, N_f,\; N_f\, \rho \,\in \mathcal{L}^1(\mathfrak{F})\Big\} \tag{II.24}$$

of finite photon number expectation value, where

$$N_f \; = \; \int a^*(k)\, a(k)\, dk \tag{II.25}$$

is the photon number operator. Indeed, if $\sigma > 0$ then

$$H_{g,\vec{p}} \;\geq\; H_f \;\geq\; \sigma\, N_f, \tag{II.26}$$

and $\mathfrak{DM} = \widetilde{\mathfrak{DM}}$ is automatic. Furthermore, if $\sigma = 0$ then it is not hard to see [4] that $E_{\mathrm{gs}}(g,\vec{p},0,\Lambda) = \lim_{\sigma\searrow 0} E_{\mathrm{gs}}(g,\vec{p},\sigma,\Lambda)$, by using the standard relative bound

$$\big\|\vec{\mathbb{A}}_{<\sigma}(\vec{0})\,\psi\big\| \;\leq\; \mathcal{O}(\sigma)\,\big\|(H_{f,<\sigma}+1)^{1/2}\,\psi\big\|, \tag{II.27}$$

where $\vec{\mathbb{A}}_{<\sigma}(\vec{0})$ and $H_{f,<\sigma}$ are the quantized magnetic vector potential and field energy, respectively, for momenta below σ. So, for all $0 \leq \sigma < \Lambda < \infty$, we have that

$$E_{\mathrm{gs}}(g,\vec{p},\sigma,\Lambda) \; = \; \inf\Big\{\mathrm{Tr}_{\mathfrak{F}}\big[\rho\, H_{g,\vec{p}}(\sigma,\Lambda)\big] \;\Big|\; \rho \in \mathfrak{DM}\Big\}. \tag{II.28}$$

Indeed, if the infimum (II.28) is attained at $\rho_{\mathrm{gs}}(g,\vec{p},\sigma,\Lambda) \in \mathfrak{DM}$ then we call $\rho_{\mathrm{gs}}(g,\vec{p},\sigma,\Lambda)$ a ground state of $H_{g,\vec{p}}(\sigma,\Lambda)$.
Since $\mathfrak{DM}$ is convex, we may restrict the density matrices in (II.28) to vary only over pure density matrices,

$$E_{\mathrm{gs}}(g,\vec{p},\sigma,\Lambda) \; = \; \inf\Big\{\mathrm{Tr}_{\mathfrak{F}}\big[\rho\, H_{g,\vec{p}}(\sigma,\Lambda)\big] \;\Big|\; \rho \in \mathfrak{p}\mathfrak{DM}\Big\}, \tag{II.29}$$

where *pure* density matrices are those of rank one,

$$\widetilde{\mathfrak{p}\mathfrak{DM}} \; := \; \Big\{\rho \in \widetilde{\mathfrak{DM}} \;\Big|\; \exists \Psi \in \mathfrak{F},\; \|\Psi\| = 1 : \;\; \rho = |\Psi\rangle\langle\Psi|\Big\}, \tag{II.30}$$

and

$$\mathfrak{pDM} := \mathfrak{DM} \cap \widetilde{\mathfrak{pDM}}. \tag{II.31}$$

Another class of states that play an important role in our work is the set of *centered* density matrices,

$$\mathfrak{cDM} := \Big\{ \rho \in \mathfrak{DM} \;\Big|\; \forall f \in \mathfrak{h} : \;\; \mathrm{Tr}_{\mathfrak{F}}\big[\rho\, a^*(f)\big] = 0 \Big\}. \tag{II.32}$$

II.2 Quasifree Density Matrices

A density matrix $\rho \in \mathfrak{DM}$ is called *quasifree*, if there exist $f_\rho \in \mathfrak{h}$, a symplectomorphism T_ρ (see Definition III.6) and a positive, self-adjoint operator $h_\rho = h_\rho^* \geq 0$ on $\mathfrak{h}$ such that

$$\begin{aligned}\big\langle W(\sqrt{2}f/i)\big\rangle_\rho &:= \mathrm{Tr}_{\mathfrak{F}}\big[\rho\, W(\sqrt{2}f/i)\big] \\ &= \exp\Big[2i\,\mathrm{Im}\langle f_\rho | f\rangle - \frac{1}{2}\big\langle T_\rho f \big| (1+h_\rho) T_\rho f\big\rangle\Big],\end{aligned} \tag{II.33}$$

for all $f \in \mathfrak{h}$, where

$$W(f) := \exp\big[i\Phi(f)\big] := \exp\big[\tfrac{i}{\sqrt{2}}\big(a^*(f) + a(f)\big)\big] \tag{II.34}$$

denotes the Weyl operator corresponding to f and we write expectation values w.r.t. the density matrix ρ as $\langle\cdot\rangle_\rho$.

There are several important facts about quasifree density matrices, which do not hold true for general density matrices in $\mathfrak{DM}$. See, e.g., [5, 13, 7, 8]. The first such fact is that if $\rho \in \mathfrak{QF}$ is a quasifree density matrix then so is $W(g)^*\rho W(g) \in \mathfrak{QF}$, for any $g \in \mathfrak{h}$, as follows from the Weyl commutation relations

$$\forall\, f, g \in \mathfrak{h} : \qquad W(f)\, W(g) = e^{-\frac{i}{2}\mathrm{Im}\langle f|g\rangle}\, W(f+g). \tag{II.35}$$

Choosing $g := -i\sqrt{2}f_\rho$, we find that $\tilde\rho := W(-i\sqrt{2}f_\rho)^*\,\rho\, W(-i\sqrt{2}f_\rho)$ is a centered quasifree density matrix, i.e.,

$$\tilde\rho := W(\sqrt{2}f_\rho/i)^*\,\rho\, W(\sqrt{2}f_\rho/i) \;\in\; \mathfrak{cQF} := \mathfrak{QF} \cap \mathfrak{cDM}. \tag{II.36}$$

A characterization of centered quasifree density matrices is given in Appendix VII. A second important fact is that any quasifree state $\rho \in \mathfrak{QF}$ is completely determined by its one-point function $\langle a(\varphi)\rangle_\rho = \langle \varphi, f_\rho\rangle$ and its two-point function (one-particle reduced density matrix)

$$\Gamma[\gamma_\rho, \tilde\alpha_\rho] := \begin{pmatrix} \gamma_\rho & \tilde\alpha_\rho \\ \tilde\alpha_\rho^* & \mathbf{1} + \mathcal{J}\,\gamma_\rho\,\mathcal{J} \end{pmatrix} \in \mathcal{B}\big(\mathfrak{h} \oplus \mathfrak{h}\big), \tag{II.37}$$

where the operators $\gamma_\rho, \tilde\alpha_\rho \in \mathcal{B}(\mathfrak{h})$ are defined as

$$\langle \varphi,\, \gamma_\rho\, \psi\rangle := \langle a^*(\psi)\, a(\varphi)\rangle_{\tilde\rho} \quad \text{and} \quad \langle \varphi,\, \tilde\alpha_\rho\, \psi\rangle := \langle a(\varphi)\, a(\mathcal{J}\psi)\rangle_{\tilde\rho}, \tag{II.38}$$

and $\mathcal{J} : \mathfrak{h} \to \mathfrak{h}$ is a conjugation. See Definition IV.8 and Remark IV.10. The positivity of the density matrix ρ implies that $\Gamma[\gamma_\rho, \tilde{\alpha}_\rho] \geq 0$ and, in particular, $\gamma_\rho \geq 0$, too. Moreover, the additional finiteness of the particle number expectation value, which distinguishes $\mathfrak{DM}$ from $\widetilde{\mathfrak{DM}}$, ensures that $\gamma_\rho \in \mathcal{L}^1(\mathfrak{h})$ is trace-class, namely,

$$\mathrm{Tr}_{\mathfrak{h}}[\gamma_\rho] \; = \; \langle N_f \rangle_\rho \; < \; \infty, \tag{II.39}$$

and that $\tilde{\alpha}_\rho \in \mathcal{L}^2(\mathfrak{h})$ is Hilbert-Schmidt.
Similar to (II.30)-(II.31), we introduce pure quasifree density matrices,

$$\mathfrak{pQF} \; := \; \mathfrak{QF} \, \cap \, \widetilde{\mathfrak{pDM}}. \tag{II.40}$$

A subset of $\mathfrak{pQF}$ of special interest is given by *coherent states*, i.e., pure quasifree states of the form $|W(-i\sqrt{2}f)\Omega\rangle\langle W(-i\sqrt{2}f)\Omega|$, which we collect in

$$\mathrm{coh} \; := \; \big\{ |W(-i\sqrt{2}f)\Omega\rangle\langle W(-i\sqrt{2}f)\Omega| \; \big| \; f \in \mathfrak{h} \big\}. \tag{II.41}$$

For these, $\gamma_\rho = \tilde{\alpha}_\rho = 0$.
Conversely, if $\gamma \in \mathcal{L}^1_+(\mathfrak{h})$ is a positive trace-class operator and $\tilde{\alpha} \in \mathcal{L}^2(\mathfrak{h})$ is a Hilbert-Schmidt operator such that $\Gamma[\gamma, \tilde{\alpha}] \geq 0$ is positive then there exists a unique centered quasifree density matrix $\rho \in \mathfrak{cQF}$ such that $\gamma = \gamma_\rho$ and $\alpha = \alpha_\rho$ are its one-particle reduced density matrices.
Summarizing these two relations, the set $\mathfrak{QF}$ of quasifree density matrices is in one-to-one correspondence to the convex set

$$1\!-\!\mathrm{pdm} \; := \; \Big\{ (f, \gamma, \tilde{\alpha}) \in \mathfrak{h} \oplus \mathcal{L}^1_+(\mathfrak{h}) \oplus \mathcal{L}^2(\mathfrak{h}) \; \Big| \; \Gamma[\gamma, \tilde{\alpha}] \geq 0 \Big\}. \tag{II.42}$$

Note that coherent states correspond to elements of $1\!-\!\mathrm{pdm}$ of the form $(f, 0, 0)$.
Next, we observe in accordance with (II.42) that, if $\rho \in \mathfrak{QF}$ is quasifree then its energy expectation value $\langle H_{g,\vec{p}} \rangle_\rho$ is a functional of $(f_\rho, \gamma_\rho, \tilde{\alpha}_\rho)$, namely,

$$\big\langle H_{g,\vec{p}} \big\rangle_\rho \; = \; \mathcal{E}_{g,\vec{p}}(f_\rho, \gamma_\rho, \tilde{\alpha}_\rho), \tag{II.43}$$

where, as shown in Section V,

$$\begin{aligned}
\mathcal{E}_{g,\vec{p}}(f, \gamma, \tilde{\alpha}) = \frac{1}{2} \big\{ & (\mathrm{Tr}[\gamma \vec{k}] + \langle f, \vec{k} f \rangle + 2\mathrm{Re}(\langle f, \vec{G} \rangle) - \vec{p})^{\cdot 2} \\
& + \mathrm{Tr}[\gamma \vec{k} \cdot \gamma \vec{k}] + \mathrm{Tr}[\tilde{\alpha}^* \vec{k} \cdot \tilde{\alpha} \vec{k}] + \mathrm{Tr}[|\vec{k}|^2 \gamma] \\
& + 2\mathrm{Re} \langle \overline{\vec{G} + \vec{k} f}, \cdot \tilde{\alpha} (\vec{G} + \vec{k} f) \rangle + \langle \vec{G} + \vec{k} f, \cdot (2\gamma + \mathbf{1})(\vec{G} + \vec{k} f) \rangle \big\} \\
& + \mathrm{Tr}[\gamma |\vec{k}|] + \langle f, |\vec{k}| f \rangle \,,
\end{aligned} \tag{II.44}$$

where $|\vec{a}\rangle \cdot \langle \vec{a}| = \sum_{j=1}^{3} |a_j\rangle\langle a_j|$. Note that in this expression $\vec{k}$ denotes the triple of multiplication operators (k_1, k_3, k_3). We also use the same notation $\vec{k}$ for the momentum variable, the meaning being clear from the context.

III SECOND QUANTIZATION

In this section we describe in detail the second quantization framework we use, and in particular we explain the notation introduced below, which may be unfamiliar to some readers.
In what follows $\mathfrak{h}$ will denote a $\mathbb{C}$-Hilbert space with a scalar product $\mathbb{C}$-linear in the right variable and $\mathbb{C}$-antilinear in the left variable.
Let $\mathcal{B}(X;Y)$ be the space of bounded operators between two Banach spaces X and Y, and $\mathcal{L}^1(\mathfrak{h})$ the space of trace class operators on $\mathfrak{h}$. Given two $\mathbb{C}$-Hilbert spaces $(\mathfrak{h}_j, \langle\cdot,\cdot\rangle_j)$, $j = 1, 2$ and a bounded linear operator $A : \mathfrak{h}_1 \to \mathfrak{h}_2$, set $A^* : \mathfrak{h}_2 \to \mathfrak{h}_1$ to be the operator such that

$$\forall z_1 \in \mathfrak{h}_1,\, z_2 \in \mathfrak{h}_2, \qquad \langle z_2, Az_1\rangle_2 = \overline{\langle z_1, A^* z_2\rangle_1}\,,$$

and $\mathrm{Re}A := \frac{1}{2}(A \oplus A^*)$, $\mathrm{Im}A := \frac{1}{2i}(A \oplus (-A^*)) \in \mathcal{B}(\mathfrak{h}_1, \mathfrak{h}_2) \oplus \mathcal{B}(\mathfrak{h}_2, \mathfrak{h}_1)$.

EXAMPLE III.1. For $z, z' \in \mathfrak{h}$,

$$\langle z, z'\rangle = z^* z'\,.$$

The adjoint of a bounded operator A on $\mathfrak{h}$ is A^*.

REMARK III.2. *This notation applies in particular to one-particle vectors $f \in \mathfrak{h}$ identified with linear applications from $\mathbb{C}$ to $\mathfrak{h}$ or to two-particle vectors $\alpha \in \mathfrak{h}^{\otimes 2}$ identified with linear applications from $\mathbb{C}$ to $\mathfrak{h}^{\otimes 2}$. For this purpose a slight generalization of the Dirac notation with bras and kets would have been sufficient, but we would like to emphasize that in some situations, like in Equation* (IV.58)*, it is natural to apply this operation to more general objects. For vectors and operators in a finite dimensional space $\mathfrak{h}$ this notation is consistent with the usual notation on matrices.*

The symmetrization operator $\mathcal{S}_n$ on $\mathfrak{h}^{\otimes n}$ is the orthogonal projection defined by

$$\mathcal{S}_n(z_1 \otimes \cdots \otimes z_n) = \frac{1}{n!}\sum_{\pi\in\mathfrak{S}_n} z_{\pi_1} \otimes \cdots \otimes z_{\pi_n}$$

and extension by linearity and continuity. The symmetric tensor product for vectors is $z_1 \vee z_2 = \mathcal{S}_{n_1+n_2}(z_1 \otimes z_2)$ and more generally for operators is $A_1 \vee A_2 = \mathcal{S}_{q_1+q_2} \circ (A_1 \otimes A_2) \circ \mathcal{S}_{p_1+p_2}$ for $A_j \in \mathcal{B}(\mathfrak{h}^{\otimes p_j}; \mathfrak{h}^{\otimes q_j})$. We set

$$\mathfrak{h}^{\vee n} := \mathcal{S}_n\mathfrak{h}^{\otimes n}, \qquad \mathcal{B}^{p,q} := \mathcal{B}(\mathfrak{h}^{\otimes p}; \mathfrak{h}^{\otimes q}).$$

DEFINITION III.3. The symmetric Fock space on a Hilbert space $\mathfrak{h}$ is defined to be

$$\mathfrak{F}_+(\mathfrak{h}) := \bigoplus_{n=0}^{\infty} \mathfrak{h}^{\vee n}\,,$$

where $\mathfrak{h}^{\vee 0} := \mathbb{C}\Omega$, Ω being the normalized vacuum vector.

For a linear operator C on $\mathfrak{h}$ such that $\|C\|_{\mathcal{B}(\mathfrak{h})} \leq 1$, let $\Gamma(C)$ defined on each $\mathfrak{h}^{\vee n}$ by $C^{\vee n}$ and extended by continuity to the symmetric Fock space on $\mathfrak{h}$.
For an operator A on $\mathfrak{h}$, the second quantization $d\Gamma(A)$ of A is defined on each $\mathfrak{h}^{\vee n}$ by

$$d\Gamma(A)\Big|_{\mathfrak{h}^{\vee n}} = n\, \mathbf{1}_{\mathfrak{h}}^{\vee n-1} \vee A$$

and extended by linearity to $\bigoplus_{n\geq 0}^{alg} \mathfrak{h}^{\vee n}$. The number operator is $N_f = d\Gamma(\mathbf{1}_{\mathfrak{h}})$. For a vector f in $\mathfrak{h}$, the creation and annihilation operators in f are the linear operators such that $a(f)\Omega = 0$, $a^*(f)\Omega = f$, and

$$a(f)g^{\vee n} = \sqrt{n}(f^* g)\, g^{\vee n-1}\,, \text{ and } a^*(f)g^{\vee n} = \sqrt{n+1} f \vee g^{\vee n}\,, \tag{III.45}$$

for all $g \in \mathfrak{h}$. By the polarization identity

$$\forall g_1, \ldots, g_n, \qquad g_1 \vee \cdots \vee g_n = \frac{1}{2^n n!} \sum_{\varepsilon_i = \pm 1} \varepsilon_1 \cdots \varepsilon_n \Big(\sum_{j=1}^{n} \varepsilon_j g_j \Big)^{\otimes n}$$

Eq. (III.45) extends to $\mathfrak{h}^{\vee n}$ and hence also to $\bigoplus_{n\geq 0}^{alg} \mathfrak{h}^{\vee n}$. They satisfy the canonical commutation relations $[a(f), a^*(g)] = f^* g$, $[a(f), a(g)] = [a^*(f), a^*(g)] = 0$.
The self-adjoint field operator associated to f is $\Phi(f) = \frac{1}{\sqrt{2}}\big(a^*(f) + a(f)\big)$. For more details on the second quantization see the book of Berezin [6].

A dot "$\cdot$" denotes an operation analogous to the scalar product in $\mathbb{R}^3$. For every two objects $\vec{a} = (a_1, a_2, a_3)$ and $\vec{b} = (b_1, b_2, b_3)$ with three components such that the products $a_j b_j$ are well defined

$$\vec{a} \cdot \vec{b} := \sum_{j=1}^{3} a_j b_j\,.$$

Example III.4. With $\vec{p} \in \mathbb{R}^3$, $\vec{G} \in \mathfrak{h}^3$, $\vec{k} \in (\mathcal{B}^{1,1})^3$

$$\begin{aligned}
&\vec{p}^{\,\cdot 2} = \sum_{j=1}^{3} p_j^2 \in \mathbb{R}\,, && \vec{k} \cdot \vec{p} = \sum_{j=1}^{3} p_j k_j \in \mathcal{B}^{1,1}, && \vec{p} \cdot \vec{G} = \sum_{j=1}^{3} p_j G_j \in \mathfrak{h}\,,\\
&\vec{k}^{\,\cdot 2} = \sum_{j=1}^{3} k_j^2 \in \mathcal{B}^{1,1}, && \vec{k} \cdot \vec{G} = \sum_{j=1}^{3} k_j G_j \in \mathfrak{h}\,, && \vec{G}^* \cdot \vec{k} = \sum_{j=1}^{3} G_j^* k_j \in \mathfrak{h}^*,\\
&\vec{G} \cdot \vec{G}^* = \sum_{j=1}^{3} G_j G_j^* \in \mathcal{B}^{1,1}, && \vec{G}^* \cdot \vec{G} = \sum_{j=1}^{3} G_j^* G_j \in \mathbb{C}\,,
\end{aligned}$$

where for an object with three components $\vec{a} = (a_1, a_2, a_3)$ such that a_j^* is well-defined, $\vec{a}^* := (a_1^*, a_2^*, a_3^*)$. We sometimes use the notation $\vec{p}^{\,\cdot 2} = |\vec{p}|^2$, or $\vec{k}^{\,\cdot 2} = |\vec{k}|^2$. And with another product, such as the symmetric tensor product $\vee$,

$$\vec{k}^{\,\cdot \vee 2} = \sum_{j=1}^{3} k_j^{\vee 2} \in \mathcal{B}^{2,2}\,, \qquad \vec{k} \cdot\vee \vec{G} = \sum_{j=1}^{3} k_j \vee G_j \in \mathcal{B}^{2,3}\,.$$

Recall that the Weyl operators are the unitary operators $W(f) = \exp(i\Phi(f))$ satisfying the relations

$$\forall z_1,\, z_2 \in \mathfrak{h} : \qquad W(z_1)W(z_2) = e^{-\frac{i}{2}\mathrm{Im}(z_1^* z_2)} W(z_1 + z_1)\,, \tag{III.46}$$

$$\forall z \in \mathfrak{h} : \qquad W(-i\sqrt{2}z)\Omega = e^{-\frac{|z|^2}{2}} \sum_{n=0}^{\infty} \frac{z^{\vee n}}{\sqrt{n!}}\,. \tag{III.47}$$

We now introduce the usual parametrization of coherent states by vectors in $\mathfrak{h}$ and of Bogolubov transformations by symplectomorphisms.

DEFINITION III.5. The *coherent vectors* are the vectors of the form

$$E_z = W(-i\sqrt{2}z)\Omega$$

for some $z \in \mathfrak{h}$ and the *coherent states* are the states of the form

$$|E_z\rangle\langle E_z|\,.$$

DEFINITION III.6. A *symplectomorphism* T for the symplectic form $\mathrm{Im}\langle\cdot,\cdot\rangle$ on a $\mathbb{C}$-Hilbert space $\mathfrak{h}$ is a continuous $\mathbb{R}$-linear automorphism on $\mathfrak{h}$ which preserves this symplectic form, i.e.,

$$\forall z_1,\, z_2 \in \mathfrak{h} : \qquad \mathrm{Im}\langle Tz_1, Tz_2\rangle = \mathrm{Im}\langle z_1, z_2\rangle\,.$$

A symplectomorphism T is *implementable* if there is a unitary operator $\mathbb{U}_T$ on $\mathfrak{F}_+(\mathfrak{h})$ such that

$$\forall z \in \mathfrak{h}\,, \quad \mathbb{U}_T W(z)\mathbb{U}_T^* = W(Tz)\,.$$

In this case $\mathbb{U}_T$ is a *Bogolubov transformation* corresponding to T.

We recall a well-known parametrization, in the spirit of the polar decomposition, of implementable symplectomorphisms.

PROPOSITION III.7. *The set of implementable symplectomorphisms is the set of operators*

$$T = u\exp[\hat{r}] = u\,\sum_{n=0}^{\infty} \frac{1}{n!}\hat{r}^n\,,$$

where u is an isometry and $\hat{r}$ is an antilinear operator, self-adjoint in the sense that $\forall z, z' \in \mathfrak{h}$, $\langle z, \hat{r}z'\rangle = \langle z', \hat{r}z\rangle$, and Hilbert-Schmidt in the sense that the positive operator $\hat{r}^2$ is trace-class. Equivalently, there exist a Hilbert basis $(\varphi_j)_{j\in\mathbb{N}}$ of $\mathfrak{h}$ and $(\hat{r}_{i,j})_{i,j} \in \ell^2(\mathbb{N}^2;\mathbb{C})$ such that

$$\hat{r} = \sum_{i,j=1}^{\infty} \hat{r}_{i,j}\,\langle\cdot,\varphi_j\rangle\,\varphi_i\,, \quad \forall i,j \in \mathbb{N}^2 : \quad \hat{r}_{i,j} = \hat{r}_{j,i}\,, \quad \textit{and} \quad \sum_{i,j=1}^{\infty} |\hat{r}_{i,j}|^2 < \infty.$$

Proof. On the one hand, every operator of the form $T = u \exp[\hat{r}]$ with u a unitary operator and $\hat{r}$ a self-adjoint antilinear operator is a symplectomorphism. Since a unitary operator is a symplectomorphism, and the set of symplectomorphisms is a group for the composition, it is enough to prove that $\exp[\hat{r}]$ is a symplectomorphism. It is indeed the case since, for all z, z' in $\mathfrak{h}$,

$$\begin{aligned}
\operatorname{Im}\langle e^{\hat{r}} z, e^{\hat{r}} z' \rangle &= \operatorname{Im}\langle e^{\hat{r}} z, \cosh(\hat{r}) z' \rangle + \operatorname{Im}\langle e^{\hat{r}} z, \sinh(\hat{r}) z' \rangle \\
&= \operatorname{Im}\langle \cosh(\hat{r}) e^{\hat{r}} z, z' \rangle + \operatorname{Im}\langle z', \sinh(\hat{r}) e^{\hat{r}} z \rangle \\
&= \operatorname{Im}\langle \cosh(\hat{r}) e^{\hat{r}} z, z' \rangle - \operatorname{Im}\langle \sinh(\hat{r}) e^{\hat{r}} z, z' \rangle \\
&= \operatorname{Im}\langle e^{-\hat{r}} e^{\hat{r}} z, z' \rangle \,.
\end{aligned}$$

The implementability condition is then satisfied if we suppose $\hat{r}$ to be Hilbert-Schmidt. On the other hand, to get exactly this formulation we give the step to go from the result given in Appendix A in [9] to the decomposition in Proposition III.7. In [9] an implementable symplectomorphism is decomposed as

$$T = u e^{c\tilde{r}} \,, \tag{III.48}$$

where u is a unitary operator, c is a conjugation and $\tilde{r}$ is a Hilbert-Schmidt, self-adjoint, non-negative operator commuting with c. It is then enough to set $\hat{r} = c\tilde{r}$ to get the expected decomposition. To check the self-adjointness of $\hat{r}$, observe that, for all z, z' in $\mathfrak{h}$,

$$\langle z', \hat{r} z \rangle = \langle z', \tilde{r} c z \rangle = \langle \tilde{r} z', c z \rangle = \langle z, c \tilde{r} z' \rangle = \langle z, \hat{r} z' \rangle \,.$$

For the convenience of the reader we recall the main steps to obtain the decomposition in Eq. (III.48). First decompose T in its $\mathbb{C}$-linear and antilinear parts, $T = L + A$, then write the polar decomposition $L = u|L|$. It is then enough to prove that $|L| + u^* A$ is of the form $e^{c\tilde{r}}$. >From certain properties of symplectomorphisms (also recalled in [9]) it follows that the antilinear operator $u^* A$ is self-adjoint and $|L|^2 + \mathbf{1}_{\mathfrak{h}} = (u^* A)^2$. A decomposition of the positive trace class operator $(u^* A)^2 = \sum_j \lambda_j^2 e_j e_j^*$ with e_j an orthonormal basis of $\mathfrak{h}$ yields $|L| = \sum_j (1 + \lambda_j^2)^{1/2} e_j e_j^*$. Using that $\lambda_j \to 0$ one can study the operator $|L|$ and $u^* A$ on the finite dimensional subspaces $\ker(|L| - \mu \mathbf{1}_{\mathfrak{h}})$ which are invariant under $u^* A$. It is then enough to prove that for a $\mathbb{C}$-antilinear self-adjoint operator f such that $f f^* = \lambda^2$ on a finite dimensional space, there is an orthonormal basis $\{\varphi_k\}_k$ such that $f(\varphi_k) = \lambda \varphi_k$. The conjugation is then defined such that $c(\sum \beta_k \varphi_k) = \sum \bar{\beta}_k \varphi_k$ and $\tilde{r} = \sinh^{-1}(\lambda_j) \mathbf{1}$ on that subspace. □

IV Pure Quasifree States

In this section we give a characterization of quasifree states and use this to show that the infimum of the energy over quasifree states is equal to the infimum of the energy over pure quasifree states. This result has been generalized to a wider class of Hamiltonians and also to the case of fermion Fock space in [2].

IV.1 From Quasifree States to Pure Quasifree States

Let $\mathfrak{h}$ be the $\mathbb{C}$-Hilbert space $L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$. We make use of the following characterization of quasifree density matrices.

Lemma IV.1. *The set of quasifree density matrices and pure quasifree density matrices, respectively, of finite photon number expectation value can be characterized by*

$$\mathfrak{QF} = \mathfrak{DM} \bigcap \Big\{ W(-i\sqrt{2}f)\mathbb{U}^* \frac{\Gamma(C)}{\mathrm{Tr}[\Gamma(C)]} \mathbb{U} W(-i\sqrt{2}f)^* \\ \Big| \, f \in \mathfrak{h},\ \mathbb{U} \text{ a Bogolubov transformation}, \\ C \in \mathcal{L}^1(\mathfrak{h}),\ C \geq 0,\ \|C\|_{\mathcal{B}(\mathfrak{h})} < 1 \Big\}$$

$$\mathfrak{pQF} = \mathfrak{DM} \bigcap \Big\{ W(-i\sqrt{2}f)\mathbb{U}^* |\Omega\rangle\langle\Omega| \mathbb{U} W(-i\sqrt{2}f)^* \\ \Big| \, f \in \mathfrak{h},\ \mathbb{U} \text{ a Bogolubov transformation} \Big\}$$

Proof. We only sketch the argument, details can be found in [6, 13]. It is not difficult to see that any density matrix of the form $W(-i\sqrt{2}f)\mathbb{U}^* \frac{\Gamma(C)}{\mathrm{Tr}[\Gamma(C)]} \mathbb{U} W(-i\sqrt{2}f)^*$ is indeed quasifree. Conversely, if $\rho \in \mathfrak{QF}$ is a quasifree density matrix then it is fully characterized by its one-point function $f_\rho \in \mathfrak{h}$ and two-point functions $(\gamma_\rho, \tilde{\alpha}_\rho)$. Moreover, $W(-i\sqrt{2}f_\rho)^* \, \rho \, W(-i\sqrt{2}f_\rho) \in \mathfrak{cQF}$ is a centered quasifree density matrix with the same one-particle density matrix, that is, the density matrix $W(-i\sqrt{2}f_\rho)^* \, \rho \, W(-i\sqrt{2}f_\rho)$ corresponds to $(0, \gamma_\rho - f_\rho f_\rho^*, \tilde{\alpha}_\rho - f_\rho \bar{f}_\rho^*)$. Obviously, $\gamma_\rho - f_\rho f_\rho^*$ is again trace-class and $\tilde{\alpha}_\rho - f_\rho \bar{f}_\rho^*$ is Hilbert-Schmidt. Now, we use that there exists a Bogolubov transformation $\mathbb{U}$ which eliminates $\tilde{\alpha}_\rho$, i.e., $\mathbb{U}^* W(\sqrt{2}f_\rho/i)^* \, \rho \, W(\sqrt{2}f_\rho/i)\mathbb{U}$ corresponds to $(0, \tilde{\gamma}_\rho, 0)$. While this is the only nontrivial step of the proof, we note that if $\mathbb{U}$ is characterized by u and v as in Lemma IV.2 then there is an involved, but explicit formula that determines u and v. Again $\tilde{\gamma}_\rho$ is trace-class because the photon number operator N_f transforms under $\mathbb{U}^*$ to itself plus lower order corrections, $\mathbb{U}^* \, N_f \, \mathbb{U} = N_f + \mathcal{O}(N_f^{1/2} + 1)$. Finally, it is easy to see that $(0, \tilde{\gamma}_\rho, 0)$ corresponds to the quasifree density matrix $\Gamma(C_\rho)/\mathrm{Tr}[\Gamma(C_\rho)]$ with $C_\rho := \tilde{\gamma}_\rho(1 + \tilde{\gamma}_\rho)^{-1}$. Following these steps we finally obtain

$$\rho = W(f_\rho)\mathbb{U} \frac{\Gamma(C_\rho)}{\mathrm{Tr}[\Gamma(C_\rho)]} \mathbb{U}^* W(f_\rho)^* ,$$

as asserted. The additional characterization of pure quasifree density matrices is obvious. □

Lemma IV.2. *Let* $\mathbb{U} \in \mathcal{B}(\mathfrak{F})$ *be a unitary operator. The following statements are* *equivalent:*

$$\mathbb{U} \in \mathcal{B}(\mathfrak{F}) \text{ is a Bogolubov transformation;} \tag{IV.49}$$

$$\Leftrightarrow \exists T \text{ implementable symplectomorphism,} \tag{IV.50}$$
$$\mathbb{U} = \tilde{U}_T\,, \quad \tilde{U}_T W(f) \tilde{U}^* = W(Tf).$$

$$\Leftrightarrow \exists u \in \mathcal{B}(\mathfrak{h}),\ v \in \mathcal{L}^2(\mathfrak{h})\ \forall f \in \mathfrak{h}: \tag{IV.51}$$
$$\mathbb{U} a^*(f) \mathbb{U}^* = a^*(uf) + a(\mathcal{J} v \mathcal{J} f);$$

$$\Leftrightarrow \mathbb{U} = \exp(iH), \text{ where } H = H^* \text{ is a semibounded operator,} \tag{IV.52}$$
$$\text{quadratic in } a^* \text{ and } a \text{ and without linear term.}$$

Proof. Again, we only sketch the argument. First note that (IV.49)⇔(IV.50) is the definition of a Bogolubov transformation. Secondly, $\tilde{U}_T W(f) \tilde{U}_T^* = W(Tf)$ is equivalent to $\tilde{U}_T \Phi(f) \tilde{U}_T^* = \Phi(Tf)$. Hence, using that $a^*(f) = \frac{1}{\sqrt{2}}[\Phi(f) - i\Phi(if)]$ and $a(f) = \frac{1}{\sqrt{2}}[\Phi(f) + i\Phi(if)]$ we obtain the equivalence (IV.50)⇔(IV.51). Thirdly, setting $U_\lambda = \exp(i\lambda H)$ and $a^*_\lambda(f) := U_\lambda a^*(f) U^*_\lambda$, we observe that $\partial_\lambda a^*_\lambda(f) = i[H, a^*_\lambda(f)]$. Furthermore, $[H, a^*_\lambda(f)]$ is linear in a^* and a if, and only if, H is quadratic in a^* and a. Solving this linear differential equation, we finally obtain (IV.51)⇔(IV.52). ☐

As a consequence, the class of quasifree states (resp. centered quasifree states) is invariant under conjugation by Weyl transformations and Bogolubov transformations (resp. Bogolubov transformations):

Lemma IV.3. *For all Bogolubov transformations $\mathbb{U}$ and all $g \in \mathfrak{h}$:*

$$W(g)\mathbb{U}\, \mathfrak{Q}\mathfrak{F}\, \mathbb{U}^* W(g)^* = \mathfrak{Q}\mathfrak{F}, \tag{IV.53}$$
$$\mathbb{U}\, \mathfrak{c}\mathfrak{Q}\mathfrak{F}\, \mathbb{U}^* = \mathfrak{c}\mathfrak{Q}\mathfrak{F}. \tag{IV.54}$$

Remark IV.4. A pure quasifree state is a particular case of quasifree state with $C = 0$, that is $\Gamma(C) = |\Omega\rangle\langle\Omega|$.

We come to the main result of this section.

Theorem IV.5. *Let $0 \leq \sigma < \Lambda < \infty$, $g \in \mathbb{R}$ and $\vec{p} \in \mathbb{R}^3$. Minimizing the energy over quasifree states is the same as minimizing the energy over pure quasifree states, i.e.,*

$$E_{BHF}(g, \vec{p}, \sigma, \Lambda) := \inf_{\rho \in \mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho] = \inf_{\rho \in \mathfrak{p}\mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho]\,.$$

For the proof of Theorem IV.5 we derive a couple of preparatory lemmata.

Proposition IV.6. *Let C be a non-negative operator on $\mathfrak{h}$, then*

$$\Big\{ \mathrm{Tr}[\Gamma(C)] < \infty \Big\} \qquad \Leftrightarrow \qquad \Big\{ C \in \mathcal{L}^1(\mathfrak{h}) \quad \text{and} \quad \|C\|_{\mathcal{B}(\mathfrak{h})} < 1 \Big\}\,.$$

In this case $\mathrm{Tr}[\Gamma(C)] = \det(1 - C)^{-1}$. (We refrain from defining the determinant.) For the direction ⇐ the non-negativity assumption is not necessary.

Proof. Let us decompose $\mathfrak{h} = \bigoplus_{j\geq 0} \mathbb{C}e_j$ where $C = \sum c_j e_j e_j^*$ with $(e_j)_{j\geq 0}$ an orthonormal basis of $\mathfrak{h}$. Then $\mathfrak{F}_+(\mathfrak{h}) = \bigotimes_{j\geq 0} \mathfrak{F}_+(\mathbb{C}e_j)$ and

$$\mathrm{Tr}[\Gamma(C)] = \mathrm{Tr}[\bigotimes_{j\geq 0} \Gamma(c_j)] = \prod_{j\geq 0} \mathrm{Tr}[\Gamma(c_j)] = \prod_{j\geq 0} \frac{1}{1-c_j}$$

and the infinite product converges exactly when $C \in \mathcal{L}^1(\mathfrak{h})$ and $\|C\|_{\mathcal{B}(\mathfrak{h})} < 1$. □

Lemma IV.7. *Suppose $\mathfrak{h}_d$ is of dimension $d < \infty$. Then, for any non-negative operator $C_d \neq 0$ such that $C_d \in \mathcal{L}^1(\mathfrak{h}_d)$ and $\|C_d\|_{\mathcal{B}(\mathfrak{h}_d)} < 1$, there exist a non-negative measure μ_d (depending on C) of mass one on $\mathfrak{h}_d$ and a family $\{\rho_d(z_d)\}_{z_d\in\mathfrak{h}_d}$ of pure quasifree states such that*

$$\frac{\Gamma(C)}{\mathrm{Tr}[\Gamma(C)]} = \int_{\mathfrak{h}_d} \rho_d(z_d)\, d\mu_d(z_d)\,.$$

Proof. In finite dimension d we can use a resolution of the identity with coherent states (see, e.g., [6])

$$\mathbf{1}_{\Gamma(\mathfrak{h}_d)} = \int_{\mathfrak{h}_d} |E_{z_d}\rangle\langle E_{z_d}|\, \frac{dz_d}{\pi^d},$$

where $\mathfrak{h}_d$ is identified with $\mathbb{C}^d$ and $dz_d = dx_d\, dy_d$, $z_d = x_d + iy_d$. Using Equation (III.47) we get

$$\begin{aligned}\Gamma(C) &= \int_{\mathfrak{h}_d} \Gamma(C^{1/2})|E_{z_d}\rangle\langle E_{z_d}|\Gamma(C^{1/2})\, \frac{dz_d}{\pi^d} \\ &= \int_{\mathfrak{h}_d} |E_{C^{1/2}z_d}\rangle\langle E_{C^{1/2}z_d}|\, \frac{\exp(|C^{1/2}z_d|^2 - |z_d|^2)dz_d}{\pi^d}\,.\end{aligned}$$

The measure $d\mu_d(z_d) = \pi^{-d}\exp(|C^{1/2}z_d|^2 - |z_d|^2)dz_d/\mathrm{Tr}[\Gamma(C)]$ has mass one. Indeed

$$\begin{aligned}\int_{\mathfrak{h}_d} \exp(-z_d^*(\mathbf{1}_{\mathfrak{h}_d} - C)z_d)\frac{dz_d}{\pi^d} &= \prod_{j=1}^d \int_{\mathbb{R}^2} \exp(-(1-c_j)(x^2+y^2))\frac{dx\,dy}{\pi} \\ &= \prod_{j=1}^d \frac{1}{1-c_j} = \mathrm{Tr}[\Gamma(C)],\end{aligned}$$

where $C = \sum_{j=1}^d c_j e_j e_j^*$ with $(e_j)_{j=1}^d$ an orthonormal basis of $\mathfrak{h}_d$. □

Proof of Theorem IV.5. The inclusion $\mathfrak{pQF} \subset \mathfrak{QF}$ implies that

$$\inf_{\rho\in\mathfrak{QF}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho] \;\leq\; \inf_{\rho\in\mathfrak{pQF}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho]\,,$$

and it is hence enough to prove for any quasifree state

$$\rho_{qf} \;=\; W(-i\sqrt{2}f)\,\mathbb{U}_T^*\,\frac{\Gamma(C)}{\mathrm{Tr}[\Gamma(C)]}\,\mathbb{U}_T\,W(-i\sqrt{2}f)^*\,,$$

that the inequality

$$\mathrm{Tr}[H_{g,\vec{p}}\,\rho_{qf}] \;\geq\; \inf_{\rho\in\mathfrak{p}\mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho]$$

holds true. The operator C is decomposed as $C = \sum_{j\geq 0} c_j e_j e_j^*$ where (e_j) is an orthonormal basis of the Hilbert space $\mathfrak{h}$ and $c_j \geq 0$. Let $C_d = \sum_{j\leq d} c_j e_j e_j^*$. Let

$$\rho_{qf,d} = W(-i\sqrt{2}f)\,\mathbb{U}_T^*\,\frac{\Gamma(C_d)}{\mathrm{Tr}[\Gamma(C_d)]}\,\mathbb{U}_T\,W(-i\sqrt{2}f)^*\,,$$

then using Lemma IV.7 with $\mathfrak{h}_d = \bigoplus_{j\leq d}\mathbb{C}e_j$, $\mathfrak{F}_+\mathfrak{h} = \mathfrak{F}_+(\mathfrak{h}_d\oplus\mathfrak{h}_d^\perp) \cong \mathfrak{F}_+\mathfrak{h}_d\otimes\mathfrak{F}_+\mathfrak{h}_d^\perp$ and the extension of the operator $\Gamma(C_d)$ on $\mathfrak{F}_+\mathfrak{h}_d$ to $\mathfrak{F}_+\mathfrak{h}_d\otimes\mathfrak{F}_+\mathfrak{h}_d^\perp$ by $\Gamma(C_d)\otimes(|\Omega_{\mathfrak{h}_d^\perp}\rangle\langle\Omega_{\mathfrak{h}_d^\perp}|)$ (which we still denote by $\Gamma(C_d)$), we obtain

$$\rho_{qf,d} \;=\; \int_{\mathfrak{h}_d} \rho_d(z_d)\,d\mu_d(z_d)\,,$$

where $\rho_d(z_d)$ are pure quasifree states and the μ_d are non-negative measures with mass one. Note that

$$\nu_d \;:=\; \frac{\mathrm{Tr}[\Gamma(C_d)]}{\mathrm{Tr}[\Gamma(C)]} = \prod_{j>d}(1-c_j) \;\nearrow\; 1\,,$$

as $d\to\infty$. Further note that $\rho_{qf} \geq \nu_d\,\rho_{qf,d}$, for any $d\in\mathbb{N}$, since $\Gamma(C)\geq\Gamma(C_d)$. Thus

$$\begin{aligned}
\mathrm{Tr}[H_{g,\vec{p}}\,\rho_{qf}] \;&\geq\; \mathrm{Tr}[H_{g,\vec{p}}\,\nu_d\rho_{qf,d}] \\
&=\; \nu_d \int_{\mathfrak{h}_d} \mathrm{Tr}[H_{g,\vec{p}}\,\rho_d(z_d)]\,d\mu_d(z_d) \\
&\geq\; \nu_d \inf_{z_d\in\mathfrak{h}_d} \mathrm{Tr}[H_{g,\vec{p}}\,\rho_d(z_d)] \\
&\geq\; \nu_d \inf_{\rho\in\mathfrak{p}\mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho]\,,
\end{aligned}$$

for all $d\in\mathbb{N}$, and in the limit $d\to\infty$, we obtain

$$\mathrm{Tr}[H_{g,\vec{p}}\,\rho_{qf}] \;\geq\; \lim_{d\to\infty}\{\nu_d\} \inf_{\rho\in\mathfrak{p}\mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho] \;=\; \inf_{\rho\in\mathfrak{p}\mathfrak{Q}\mathfrak{F}} \mathrm{Tr}[H_{g,\vec{p}}\,\rho]\,. \qquad \square$$

IV.2 Pure Quasifree States and their One-Particle Density Matrices

We now define reduced density matrices $\rho^{p,q}$ resulting as marginals from a given density matrix ρ on Fock space and derive a convenient parametrization for them in case ρ is pure and quasifree. We also recall a characterization of the admissible one-particle density matrices for pure quasifree states.
Let $\mathfrak{h}$ be a $\mathbb{C}$-Hilbert space.

DEFINITION IV.8. Let $\rho \in \mathfrak{DM}$ be a density matrix on the bosonic Fock space $\mathfrak{F}_+(\mathfrak{h})$ over $\mathfrak{h}$. If $\mathrm{Tr}[\rho N_f^{\frac{p+q}{2}}] < \infty$, we define $\rho^{p,q} \in \mathcal{B}^{p,q}(\mathfrak{h})$ through

$$\forall \varphi, \psi \in \mathfrak{h}\,, \qquad \psi^{*\vee p} \rho^{p,q} \varphi^{\vee q} = \mathrm{Tr}[a^*(\varphi)^q a(\psi)^p \rho]\,.$$

We single out

$$f = \rho^{0,1} \in \mathcal{B}^{0,1} \cong \mathfrak{h}\,,$$

i.e., $f_\rho \in \mathfrak{h}$ is the unique vector such that $\mathrm{Tr}[a(\psi)\,\rho] = \psi^* f_\rho$, for all $\psi \in \mathfrak{h}$. Furthermore, with $\tilde{\rho} = W(\sqrt{2} f_\rho/i)^* \rho W(\sqrt{2} f_\rho/i)$, the matrix elements of the (generalized) one-particle density matrix are defined by

$$\gamma_\rho = \tilde{\rho}^{1,1} \in \mathcal{B}^{1,1} \qquad \text{and} \qquad \alpha_\rho = \tilde{\rho}^{0,2} \in \mathcal{B}^{0,2} \cong \mathfrak{h}^{\vee 2}\,,$$

in other words

$$\begin{aligned} \forall \varphi, \psi \in \mathfrak{h}\ : \qquad \langle \psi\,, \gamma_\rho\, \varphi \rangle &= \mathrm{Tr}[\tilde{\rho}\, a^*(\varphi) a(\psi)]\,, \\ \langle \psi \otimes \varphi\,, \alpha_\rho \rangle &= \mathrm{Tr}[\tilde{\rho}\, a(\psi) a(\varphi)]\,. \end{aligned}$$

Note that f_ρ, γ_ρ, and α_ρ exist for any $\rho \in \mathfrak{DM}$ since $N_f \rho, \rho N_f \in \mathcal{L}^1(\mathfrak{F}_+)$.

REMARK IV.9. For a centered pure quasifree state $\tilde{\rho}$, $\tilde{\rho}^{p,q}$ vanishes when $p+q$ is odd.

REMARK IV.10. Another definition of the one-particle density matrix γ_ρ would be through the relation $\langle \psi, \gamma_\rho \varphi \rangle = \mathrm{Tr}[a^*(\varphi) a(\psi) \rho]$. We prefer here a definition with a "centered" version $\tilde{\rho}$ of the state ρ, because this centered quasifree state $\tilde{\rho}$ then satisfies the usual Wick theorem. The same considerations hold for α_ρ.
Hence, any quasifree density matrix is characterized by $(f_\rho, \gamma_\rho, \alpha_\rho)$, since $\rho^{p,q}$ can be expressed in terms of $(f_\rho, \gamma_\rho, \alpha_\rho)$.
When $f_\rho = 0$, the definition of γ_ρ is consistent with the usual one, for z_1, $z_2 \in \mathfrak{h}$, $\langle z_1, \gamma_\rho z_2 \rangle = \mathrm{Tr}[a^*(z_2) a(z_1) \rho]$. The definition of α_ρ is related with the definition of the operator $\hat{\alpha}_\rho$ (here denoted with a hat for clarity) used in the article of Bach, Lieb and Solovej [5], through the relation $\langle z_1 \otimes z_2, \alpha_\rho \rangle_{\mathfrak{h}^{\otimes 2}} = \langle z_1, \tilde{\alpha}_\rho c z_2 \rangle_{\mathfrak{h}}$ with c a conjugation on $\mathfrak{h}$.

EXAMPLE IV.11. A centered pure quasifree state satisfies the relation,

$$\tilde{\rho}^{2,2} = \gamma \otimes \gamma + \gamma \otimes \gamma\ \mathrm{Ex} + \alpha \alpha^* \in \mathcal{B}^{2,2}\,, \tag{IV.55}$$

where the exchange operator is the linear operator on $\mathfrak{h}^{\otimes 2}$ such that

$$\forall z_1,\, z_2 \in \mathfrak{h}, \qquad \mathrm{Ex}(z_1 \otimes z_2) = z_2 \otimes z_1$$

and where for any $b \in \mathfrak{h}^{\otimes 2}$, $\alpha \alpha^* b = \langle \alpha, b \rangle_{\mathfrak{h}^{\otimes 2}}\, \alpha$.

We now turn to another parametrization of quasifree states, by vectors in a real Hilbert space. This parametrization enables us to use convexity arguments.

Proposition IV.12. *Let $T = ue^{\hat{r}}$ be an implementable symplectomorphism and ρ a quasifree state of the form $\rho = \mathbb{U}_T^*|\Omega\rangle\langle\Omega|\mathbb{U}_T$. Then*

$$\gamma_\rho = \tfrac{1}{2}(\cosh(2\hat{r}) - \mathbf{1}), \tag{IV.56}$$

$$\forall z_1, z_2 \in \mathfrak{h} : \quad \langle z_1 \otimes z_2, \alpha_\rho\rangle_{\mathfrak{h}^{\otimes 2}} = \langle z_1, \tfrac{1}{2}\sinh(2\hat{r}) z_2\rangle . \tag{IV.57}$$

Proof of Proposition IV.12. We have $Ti = ue^{\hat{r}}i = uie^{-\hat{r}} = iue^{-\hat{r}}$ and for all $z \in \mathfrak{h}$

$$\begin{aligned}
\mathrm{Tr}[\rho W(-i\sqrt{2}z)] &= \mathrm{Tr}\big[\mathbb{U}_T^*|\Omega\rangle\langle\Omega|\mathbb{U}_T W(-i\sqrt{2}z)\big] \\
&= \langle\Omega|W(ue^{\hat{r}}(-i\sqrt{2}z))|\Omega\rangle \\
&= \langle\Omega|W(-i\sqrt{2}ue^{-\hat{r}}z)|\Omega\rangle \\
&= \exp\big(-\tfrac{1}{2}|ue^{-\hat{r}}z|^2\big) \\
&= \exp\big(-\tfrac{1}{2}|e^{-\hat{r}}z|^2\big).
\end{aligned}$$

>From this formula we can easily compute the function

$$h(t,s) := \mathrm{Tr}\big[\rho W(-ti\sqrt{2}z)W(-si\sqrt{2}z)\big] = \exp\big(-\tfrac{1}{2}|e^{-\hat{r}}(t+s)z|^2\big),$$

whose derivative $\partial_t\partial_s$ at $(t,s) = (0,0)$ involves α and γ:

$$\begin{aligned}
\partial_t\partial_s h(0,0) &= \mathrm{Tr}\big[\rho(a^*(z) - a(z))^2\big] \\
&= -2z^*\gamma z + 2\mathrm{Re}(\alpha^* z^{\vee 2}) - z^* z .
\end{aligned}$$

But we also have

$$\begin{aligned}
&\partial_t\partial_s \exp(-\frac{1}{2}|e^{-\hat{r}}(t+s)z|^2)\Big|_{t=s=0} \\
&\quad = -(e^{-\hat{r}}z)^*(e^{-\hat{r}}z) \\
&\quad = -(\cosh(\hat{r})z - \sinh(\hat{r})z)^*(\cosh(\hat{r})z - \sinh(\hat{r})z) \\
&\quad = -(\cosh(\hat{r})z)^*(\cosh(\hat{r})z) \\
&\qquad\quad + 2\mathrm{Re}(\sinh(\hat{r})z)^*(\cosh(\hat{r})z) - (\sinh(\hat{r})z)^*(\sinh(\hat{r})z) \\
&\quad = -z^*(\cosh^2\hat{r} + \sinh^2\hat{r})z + 2\mathrm{Re}(z^*(\sinh\hat{r}\cosh\hat{r})z) \\
&\quad = -z^*\cosh(2\hat{r})z + 2\mathrm{Re}(z^*\frac{1}{2}\sinh(2\hat{r})z)
\end{aligned}$$

and hence, using the polarization identity

$$4z \vee z' = (z+z')^{\otimes 2} - (z-z')^{\otimes 2}$$

to recover every vector from $\mathfrak{h}^{\vee 2}$ from linear combinations of vectors of the form $z^{\vee 2}$, we arrive at (IV.56)-(IV.57). ☐

Proposition IV.13. *The admissible γ, α for a pure quasifree state are exactly those satisfying the relation*

$$\gamma + \gamma^2 = (\alpha \otimes \mathbf{1})^*(\mathbf{1} \otimes \alpha), \tag{IV.58}$$

with $\gamma \geq 0$.

This is the constraint when we minimize the energy as a function of (f, γ, α) with the method of Lagrange multipliers in Section VIII.3.

Proof. If γ, α are associated with a quasifree state, then there is an $\hat{r}$ such that γ, α and $\hat{r}$ satisfy Equations (IV.56) and (IV.57), then

$$\begin{aligned}
\langle z_1, (\alpha^* \otimes \mathbf{1})(\mathbf{1} \otimes \alpha) z_2 \rangle &= (\alpha^* \otimes z_1^*)(z_2 \otimes \alpha) \\
&= ([\alpha^*(z_2 \otimes \mathbf{1})] \otimes z_1^*)\alpha \\
&= \left\langle \alpha^*(z_2 \otimes \mathbf{1}), \tfrac{1}{2}\sinh(2\hat{r}) z_1 \right\rangle_{\mathfrak{h}} \\
&= \left\langle \alpha^*, z_2 \otimes \tfrac{1}{2}\sinh(2\hat{r}) z_1 \right\rangle_{\mathfrak{h}^{\otimes 2}} \\
&= \left\langle \tfrac{1}{4}\sinh^2(2\hat{r}) z_1, z_2 \right\rangle_{\mathfrak{h}} \\
&= \left\langle (\tfrac{1}{2}(\cosh(2\hat{r}) - \mathbf{1}) + \tfrac{1}{4}(\cosh(2\hat{r}) - \mathbf{1})^2) z_1, z_2 \right\rangle_{\mathfrak{h}} .
\end{aligned}$$

Conversely, if γ and α satisfy Eq. (IV.58) then we define the $\mathbb{C}$-antilinear operator $\hat{\alpha}$ such that $\langle z_1, \hat{\alpha} z_2 \rangle = (z_1 \otimes z_2)^* \alpha$, and set $\hat{r} = \frac{1}{2}\sinh^{-1}(2\hat{\alpha})$, then

$$\forall z_1, z_2 \in \mathfrak{h}: \quad \langle z_1 \otimes z_2, \alpha_\rho \rangle_{\mathfrak{h}^2} \;=\; \langle z_1, \hat{\alpha} z_2 \rangle \;=\; \left\langle z_1, \tfrac{1}{2}\sinh(2\hat{r}) z_2 \right\rangle ,$$

which, in turn, implies that $(\alpha^* \otimes \mathbf{1})(\mathbf{1} \otimes \alpha) = \frac{1}{4}\sinh^2(2\hat{r})$. Hence, we have

$$\gamma + \gamma^2 = \frac{1}{4}\sinh^2(2\hat{r})$$

and as $\gamma \geq 0$, it follows that $\gamma = \frac{1}{2}(\cosh(2\hat{r}) - \mathbf{1})$. Then γ, α is associated with the centered pure quasifree state whose symplectic transformation is $\exp[\hat{r}]$.

□

V Energy Functional

In this section we calculate the energy of a quasifree state in terms of its characterizing parameters, i.e., in terms of (f, γ, α) and (f, r).

Notation: We first recall that, as before, we denote by $\vec{k}$, and $|\vec{k}|$ the multiplication operators $\vec{k} \otimes \mathbf{1}_{\mathbb{C}^2}$ and $|\vec{k}| \otimes \mathbf{1}_{\mathbb{C}^2}$ on $\mathfrak{h} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$, with three components in the case of $\vec{k}$.

We now work at fixed values of total momentum $\vec{p} \in \mathbb{R}^3$. The operator $H_{g,\vec{p}}$ is given by

$$H_{g,\vec{p}} = \frac{1}{2}(d\Gamma(\vec{k}) + 2\mathrm{Re}\, a^*(\vec{G}) - \vec{p})^{\cdot 2} + d\Gamma(|\vec{k}|) ,$$

where $\vec{G}(k) = \vec{G}(\vec{k}, \pm) := g|\vec{k}|^{-1/2}\vec{\varepsilon}_\pm(\vec{k})$. The energy of a quasifree state ρ associated with $f \in \mathfrak{h}$, $\gamma \in \mathcal{L}^1(\mathfrak{h})$, $\alpha \in \mathfrak{h}^{\vee 2}$ is

$$\mathcal{E}_{g,\vec{p}}(f, \gamma, \alpha) \;:=\; \mathrm{Tr}[H_{g,\vec{p}}\, \rho] , \tag{V.59}$$

where $\mathfrak{h}$ is the $\mathbb{C}$-Hilbert space $\mathfrak{h} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$ and $\mathcal{L}^1(\mathfrak{h})$ is the space of trace class operators on $\mathfrak{h}$.

Proposition V.1. *The energy functional* (V.59) *is*

$$\begin{aligned}\mathcal{E}_{g,\vec{p}}(f,\gamma,\alpha) = \frac{1}{2}\Big\{&(\mathrm{Tr}[\gamma\vec{k}] + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p})^{\cdot 2}\\ &+ \mathrm{Tr}[\gamma\vec{k}\cdot\gamma\vec{k}] + \alpha^*(\vec{k}\cdot\otimes\vec{k})\alpha + \mathrm{Tr}[|\vec{k}|^2\gamma]\\ &+ 2\mathrm{Re}\{\alpha^*[(\vec{G}+\vec{k}f)^{\cdot\vee 2}]\} + \mathrm{Tr}[(2\gamma+\mathbf{1})(\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*]\Big\}\\ &+ \mathrm{Tr}[\gamma|\vec{k}|] + f^*|\vec{k}|f\,. \end{aligned} \tag{V.60}$$

where the following positivity properties hold

$$\begin{aligned}(\mathrm{Tr}[\gamma\vec{k}] + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p})^{\cdot 2} \geq 0\,,\\ \mathrm{Tr}[\gamma\vec{k}\cdot\gamma\vec{k}] + \mathrm{Tr}[\gamma\vec{k}]^{\cdot 2} + \alpha^*(\vec{k}\cdot\otimes\vec{k})\alpha + \mathrm{Tr}[|\vec{k}|^2\gamma] \geq 0\,,\\ (\mathrm{Tr}[\gamma\vec{k}] + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p})^{\cdot 2}\\ +\mathrm{Tr}[\gamma\vec{k}\cdot\gamma\vec{k}] + \alpha^*(\vec{k}\cdot\otimes\vec{k})\alpha + \mathrm{Tr}[|\vec{k}|^2\gamma] \geq 0\,,\\ 2\mathrm{Re}(\alpha^*((\vec{G}+\vec{k}f)^{\cdot\vee 2})) + \mathrm{Tr}[(2\gamma+\mathbf{1})(\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*] \geq 0\,.\end{aligned}$$

The energy of a pure quasifree state in the variables f and $\hat{r}$ is

$$\begin{aligned}\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r}) = \tfrac{1}{2}\big\{&(\mathrm{Tr}[\tfrac{1}{2}(\cosh(2\hat{r})-1)\vec{k}] + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p})^{\cdot 2}\\ &+ \mathrm{Tr}[\tfrac{1}{2}(\cosh(2\hat{r})-1)\vec{k}\cdot\tfrac{1}{2}(\cosh(2\hat{r})-1)\vec{k}]\\ &+ \mathrm{Tr}[\tfrac{1}{2}\sinh(2\hat{r})\vec{k}\cdot\tfrac{1}{2}\sinh(2r)\vec{k}] + \mathrm{Tr}[|\vec{k}|^2\tfrac{1}{2}(\cosh(2\hat{r})-1)]\\ &+ 2\mathrm{Re}\langle\tfrac{1}{2}\sinh(2\hat{r})(\vec{G}+\vec{k}f);(\vec{G}+\vec{k}f)\rangle\\ &+ \mathrm{Tr}[(2\tfrac{1}{2}(\cosh(2\hat{r})-1)+\mathbf{1})(\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*]\big\}\\ &+ \mathrm{Tr}[\tfrac{1}{2}(\cosh(2\hat{r})-1)|\vec{k}|] + f^*|\vec{k}|f\,. \end{aligned} \tag{V.61}$$

Proof. Using the Weyl operators,

$$\mathcal{E}_{g,\vec{p}}(f,\gamma,\alpha) := \mathrm{Tr}[H_{g,\vec{p}}\rho] = \mathrm{Tr}[H_{g,\vec{p}}(f)\tilde{\rho}]$$

where $H_{g,\vec{p}}(f) = W(\sqrt{2}f/i)^* H_{g,\vec{p}} W(\sqrt{2}f/i)$ and $\tilde{\rho} = W(\sqrt{2}f/i)^*\rho W(\sqrt{2}f/i)$, so that $\tilde{\rho}$ is centered. Modulo terms of odd order, which vanish when we take the trace against a centered quasifree state, $H_{g,\vec{p}}(f)$ equals

$$\begin{aligned}H_{g,\vec{p}}(f) &= \frac{1}{2}\big(d\Gamma(\vec{k}) + f^*\vec{k}f + 2\mathrm{Re}\big(a^*(\vec{k}f+\vec{G})\big) + 2\mathrm{Re}(f^*\vec{G}) - \vec{p}\big)^{\cdot 2}\\ &\qquad + d\Gamma(|\vec{k}|) + f^*|\vec{k}|f + \mathrm{odd}\\ &= \frac{1}{2}\big(d\Gamma(\vec{k}) + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p}\big)^{\cdot 2}\\ &\qquad + \frac{1}{2}\big(2\mathrm{Re}\big(a^*(\vec{k}f+\vec{G})\big)\big)^{\cdot 2} + d\Gamma(|\vec{k}|) + f^*|\vec{k}|f + \mathrm{odd}\,.\end{aligned}$$

To compute $\mathcal{E}(f,\gamma,\alpha)$ we are thus lead to compute, for $\vec{\varphi} \in \mathfrak{h}^3$ and $\vec{u} \in \mathbb{R}^3$,

$$\mathrm{Tr}\big[\tilde{\rho}\,(d\Gamma(\vec{k}) + \vec{u})^{\cdot 2}\big] \qquad \text{and} \qquad \mathrm{Tr}\big[\tilde{\rho}\,(2\mathrm{Re}\{a(\vec{\varphi})\})^{\cdot 2}\big]\,.$$

The expression of the energy as a function of (f,γ,α) then follows from Propositions V.2 and V.4. The expression of the energy as a function of (f,r) follows from Proposition IV.12. □

PROPOSITION V.2. *Let $\vec{u} \in \mathbb{R}^3$, then*

$$\begin{aligned} 0 \leq \mathrm{Tr}[\tilde{\rho}(d\Gamma(\vec{k}) + \vec{u})^{\cdot 2}] &= (\mathrm{Tr}[\gamma\vec{k}] + \vec{u})^{\cdot 2} - \mathrm{Tr}[\gamma\vec{k}]^{\cdot 2} \\ &\quad + \mathrm{Tr}[\gamma\vec{k}\cdot\gamma\vec{k}] + \mathrm{Tr}[\gamma\vec{k}]^{\cdot 2} + \alpha^*(\vec{k}\cdot\otimes\vec{k})\alpha + \mathrm{Tr}[|\vec{k}|^2\gamma]\,. \end{aligned}$$

This condition is used with $\vec{u} = \vec{p} - f^*\vec{k}f - 2\mathrm{Re}(f^*\vec{G})$.

Proof. Indeed,

$$(d\Gamma(\vec{k}) + \vec{u})^{\cdot 2} \;=\; d\Gamma(\vec{k})^{\cdot 2} + 2d\Gamma(\vec{k})\cdot\vec{u} + \vec{u}^{\,\cdot 2}\,.$$

Then we use that $\mathrm{Tr}[\tilde{\rho}\,d\Gamma(\vec{k})] = \mathrm{Tr}[\gamma\vec{k}]$, add and substract $\mathrm{Tr}[\gamma\vec{k}]^{\cdot 2}$ to complete the square and compute $\mathrm{Tr}[\tilde{\rho}\,d\Gamma(\vec{k})^{\cdot 2}]$ using Lemma V.3. □

LEMMA V.3. *Let $X \in \mathcal{B}^{1,1}$, then*

$$\begin{aligned} 0 \;\leq\; \mathrm{Tr}\big[\tilde{\rho}d\Gamma(X)d\Gamma(X)^*\big] \;=& \\ = \mathrm{Tr}[\gamma X\gamma X^*] + |\mathrm{Tr}[\gamma X]|^2 &+ \alpha^*(X\otimes X^*)\alpha + \mathrm{Tr}[XX^*\gamma]\,. \end{aligned}$$

Proof. Indeed, using Equation (IV.55),

$$\begin{aligned} &\mathrm{Tr}[\tilde{\rho}d\Gamma(X)d\Gamma(X)^*] \\ &= \mathrm{Tr}[\tilde{\rho}(\int X(k_1,k_1')X(k_2,k_2')a^*(k_1)a^*(k_2)a(k_2')a(k_1')dk_1dk_2dk_1'dk_2' + d\Gamma(XX^*)] \\ &= \mathrm{Tr}[(\gamma\otimes\gamma + \gamma\otimes\gamma\,Ex + \alpha\alpha^*)(X\otimes X^*)] + \mathrm{Tr}[\gamma\,XX^*] \\ &= \mathrm{Tr}[\gamma X]\mathrm{Tr}[\gamma X^*] + \mathrm{Tr}[\gamma X\gamma X^*] + \alpha^*(X\otimes X^*)\alpha + \mathrm{Tr}[\gamma\,XX^*]\,. \end{aligned}$$ □

PROPOSITION V.4. *Let $\varphi \in \mathfrak{h}$, then*

$$0 \leq \mathrm{Tr}[\tilde{\rho}(a^*(\varphi) + a(\varphi))^2] = 2\mathrm{Re}(\alpha^*(\varphi^{\vee 2})) + \mathrm{Tr}[(2\gamma + \mathbf{1})\varphi\varphi^*] \tag{V.62}$$

and $|2\mathrm{Re}(\alpha^*(\varphi^{\cdot\vee 2}))| \leq \mathrm{Tr}[(2\gamma + \mathbf{1})\varphi\varphi^*]$.

This condition is used with the three components of $\vec{\varphi} = \vec{G} + \vec{k}f$.

Proof. A computation using the canonical commutation relations yields

$$\begin{aligned} &Tr[\tilde{\rho}\,(a^*(\varphi) + a(\varphi))^2] \\ &\quad = \mathrm{Tr}[\tilde{\rho}\,(a^*(\varphi))^2 + \tilde{\rho}\,(a(\varphi))^2 + \tilde{\rho}\,(a^*(\varphi)a(\varphi) + a(\varphi)a^*(\varphi))] \\ &\quad = \alpha^*\varphi^{\vee 2} + \varphi^{\vee 2*}\alpha + \mathrm{Tr}[\gamma\,\varphi\varphi^* + (\gamma + \mathbf{1})\psi\psi^*]. \end{aligned}$$

□

VI Minimization over Coherent States

In this section we consider the problem of minimizing the energy over coherent states and show that there is a unique minimizer. We also calculate the lower orders of the energy at the minimizer seen as a function of the total momentum $\vec{p}$.
For this section we can take $\sigma = 0$ if we consider the parameter f in the energy to be in $\widetilde{\mathfrak{h}} := L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)dk)$. Recall that $S_{\sigma,\Lambda} = \{\vec{k} \in \mathbb{R}^3 \,|\, \sigma \leq |\vec{k}| \leq \Lambda\}$.
We also recall that for z and z' in some Hilbert space, $z^* z' = \langle z, z' \rangle$ (see Section III).

Remark VI.1. For a coherent state (see Definition III.5) the energy reduces to

$$\mathcal{E}_{g,\vec{p}}(f) = \frac{1}{2}\|\vec{G}\|^2 + \frac{1}{2}(f^* \vec{k} f + 2\mathrm{Re}(f^* \vec{G}) - \vec{p})^{\cdot 2} + f^*(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|)f\,. \tag{VI.63}$$

Note that, for $\sigma > 0$, $\mathfrak{h} = L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2, dk) = \widetilde{\mathfrak{h}}$, while for $\sigma = 0$, $\mathfrak{h} \subset \widetilde{\mathfrak{h}}$, and $\mathcal{E}_{g,\vec{p}}(f)$ extends to $\widetilde{\mathfrak{h}}$ by using Equation (VI.63).

Theorem VI.2. *There exists a universal constant $C < \infty$ such that, for $0 \leq \sigma < \Lambda < \infty$, $g^2 \ln(\Lambda + 2) \leq C$ and $|\vec{p}| \leq 1/3$, there exists a unique $f_{\vec{p}}$ which minimizes $\mathcal{E}_{g,\vec{p}}$ in $\widetilde{\mathfrak{h}}$. The minimizer $f_{\vec{p}}$ solves the system of equations*

$$f_{\vec{p}} = \frac{\vec{u}_{\vec{p}} \cdot \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k} \cdot \vec{u}_{\vec{p}}}\,, \tag{VI.64}$$

$$\vec{u}_{\vec{p}} = \vec{p} - 2\mathrm{Re}(f_{\vec{p}}^* \vec{G}) - f_{\vec{p}}^* \vec{k} f_{\vec{p}}\,, \tag{VI.65}$$

with $|\vec{u}_{\vec{p}}| \leq |\vec{p}|$.

Remark VI.3. Our hypotheses are similar those of Chen, Fröhlich, and Pizzo [10], where their vector $\vec{\nabla} E^{\sigma}_{\vec{p}}$ is analogous to $\vec{u}_{\vec{p}}$ in our notations.
The construction of $\vec{u}_{\vec{p}}$ as the solution of a fixed point problem and the dependency in the parameter $\vec{p}$ imply that the map $\vec{p} \mapsto \vec{u}_{\vec{p}}$ is of class $\mathcal{C}^\infty$.

Remark VI.4. We note that we also expect to have $\vec{u}_{\vec{p}}$ in the neighborhood of $\vec{p}$.

Remark VI.5. The minimizer is constructed as the solution of a fixed point problem. As a result the application

$$(\sigma, \Lambda, g, \vec{p}) \mapsto \inf_{\rho \in \mathrm{coh}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho]$$

is continuous on the domain defined by Theorem VI.2, and at σ, Λ fixed,

$$(g, \vec{p}) \mapsto \inf_{\rho \in \mathrm{coh}} \mathrm{Tr}[H_{g,\vec{p}}\, \rho]$$

is analytic for $g^2 < C/\ln(\Lambda + 2)$ and $|\vec{p}| < 1/3$.

REMARK VI.6. The assumption on $|\vec{p}| \leq 1/3$ is much weaker than in the quasifree state case where we need to have $\vec{p}$ smaller than a constant C which may be small. In fact the $1/3$ is arbitrary and one may suppose only $|\vec{p}| \leq R$ for some constant $R < 1$, but since this would result in a heavier exposition without providing additional relevant information, we restrict to $|\vec{p}| \leq 1/3$.

To prove Theorem VI.2 we first show that the Equations (VI.64) and (VI.65) are necessarily verified by a minimizer. We then show the existence and uniqueness of a solution to these equations by a fixed point argument.

Proof of Theorem VI.2. Assume there is a point $f_{\vec{p}}$ where the minimum is attained. The partial derivative of the energy at the point $f_{\vec{p}}$

$$\begin{aligned}&\partial_{f^*}\mathcal{E}(f_{\vec{p}})\\ &= ((f_{\vec{p}}^*\vec{k}f_{\vec{p}} - \vec{p} + 2\mathrm{Re}(f_{\vec{p}}^*\vec{G}))\cdot\vec{k} + \frac{1}{2}|\vec{k}|^2 + |\vec{k}|)f_{\vec{p}} - (\vec{p} - f_{\vec{p}}^*\vec{k}f_{\vec{p}} - 2\mathrm{Re}(f_{\vec{p}}^*\vec{G}))\cdot\vec{G}\end{aligned}$$

then vanishes, where the derivative $\partial_{f^*}\mathcal{E}(f)$ at a point f is the unique vector in $\widetilde{\mathfrak{h}}^* \cong L^2(S_{\sigma,\Lambda}, (\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)^{-1}dk)$ defined by

$$\mathcal{E}(f + \delta f) - \mathcal{E}(f) = 2\mathrm{Re}(\delta f^*\,\partial_{f^*}\mathcal{E}(f)) + o(\|\delta f\|_{\widetilde{\mathfrak{h}}})$$

with $f,\, \delta f \in \widetilde{\mathfrak{h}}$. Observe that

$$\begin{aligned}0 &\leq \mathcal{E}_{g,\vec{p}}(0) - \mathcal{E}_{g,\vec{p}}(f_{\vec{p}})\\ &= \frac{1}{2}|\vec{p}|^{\cdot 2} - \frac{1}{2}(f_{\vec{p}}^*\vec{k}f_{\vec{p}} + 2\mathrm{Re}(f_{\vec{p}}^*\vec{G}) - \vec{p})^{\cdot 2} - f_{\vec{p}}^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)f_{\vec{p}}\end{aligned}$$

and hence $|\vec{p}| \geq |\vec{u}_{\vec{p}}|$ with $\vec{u}_{\vec{p}} := \vec{p} - f_{\vec{p}}^*\vec{k}f_{\vec{p}} - 2\mathrm{Re}(f_{\vec{p}}^*\vec{G})$. Since $|\vec{u}_{\vec{p}}| \leq |\vec{p}| < 1$, it makes sense to write

$$f_{\vec{p}} = \frac{\vec{u}_{\vec{p}}\cdot\vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{u}_{\vec{p}}\cdot\vec{k}}\,.$$

Hence the minimum point $f_{\vec{p}}$ satisfies Equations (VI.64) and (VI.65). It is in particular sufficient to prove that there exist a unique $\vec{u}_{\vec{p}}$ in a ball $\bar{B}(0,r)$ with $r \geq |\vec{p}|$ such that the function in Equation (VI.64) satisfies also Equation (VI.65) to prove the existence and uniqueness of a minimizer.

Proof of the existence and uniqueness of a solution. Let $\frac{1}{3} < r < 1$, $\vec{u} \in \mathbb{R}^3$, $|\vec{u}| \leq r < 1$ and

$$\Phi_{\vec{u}}(\vec{k}) = \frac{\vec{u}\cdot\vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{u}}\,.$$

Observe that $\Phi_{\vec{u}} \in \tilde{\mathcal{Z}}$, indeed, if $|\vec{u}| < 1$ then $\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{u} \geq (1-r)(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)$, and with $\vec{\varepsilon}(\vec{k}) = \vec{\varepsilon}(\vec{k},+) + \vec{\varepsilon}(\vec{k},-)$,

$$\begin{aligned}\int_{|\vec{k}|\in[\sigma,\Lambda]} (\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|)|\Phi_{\vec{u}}(\vec{k})|^2 dk &\leq g^2 \int_{|\vec{k}|\in[\sigma,\Lambda]} \frac{1}{|\vec{k}|}\frac{1}{(1-r)^2}\frac{|\vec{u}\cdot\vec{\varepsilon}(\vec{k})|^2}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|} dk < +\infty\,. \\ &\leq C_0 g^2 \ln(\Lambda+2)\frac{|\vec{u}|^2}{(1-r)^2}\end{aligned}$$

for some universal constant $C_0 > 0$. Observe then that

$$\int_{|\vec{k}|\in[\sigma,\Lambda]} \frac{|\vec{G}(k)|^2}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|} dk \leq C_0 g^2 \ln(\Lambda+2)$$

for some universal constant $C_0 > 0$. It follows that $\Phi_{\vec{u}}^* \vec{G} \in L^1(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$. Note that if $\sigma = 0$ then $\Phi_{\vec{u}} \notin L^2(S_{\sigma,\Lambda} \times \mathbb{Z}_2)$ (for $\vec{u} \neq 0$).
We can thus define the application

$$\bar{B}(0,r) \ni \vec{u} \mapsto \vec{\Psi}(\vec{u}) := \vec{p} - \Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}} - 2\mathrm{Re}(\Phi_{\vec{u}}^* \vec{G}) \in \mathbb{R}^3\,.$$

We check that the hypotheses of the Banach-Picard fixed point theorem are verified on the ball $\bar{B}(0,r)$, which will prove the result.
Stability: If $g^2 \ln(\Lambda+2)$ is sufficiently small, we get from

$$|\vec{\Psi}(\vec{u})| \leq |\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}}| + |2\mathrm{Re}(\Phi_{\vec{u}}^* \vec{G})| + |\vec{p}|$$

and the estimates above that the sum of the two first terms is smaller than $r - 1/3$ and since $|\vec{p}| \leq 1/3$ the map $\vec{\Psi}$ sends $\bar{B}(0,r)$ into itself,

$$\vec{\Psi}(\bar{B}(0,r)) \subseteq \bar{B}(0,r)\,.$$

Contraction: For $\vec{u}$ and $\vec{v}$ in $\bar{B}(0,r)$, we have that

$$\begin{aligned}&|\Phi_{\vec{u}}(\vec{k}) - \Phi_{\vec{v}}(\vec{k})|(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\ &\quad = \Big|\frac{\vec{u}.\vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}\cdot\vec{u}} - \frac{\vec{v}.\vec{G}(\vec{k})}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}.\vec{v}}\Big|(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\ &\quad \leq \Big(\frac{|\vec{u}-\vec{v}||\vec{G}(\vec{k})|}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}\cdot\vec{u}} \\ &\qquad + |\vec{v}||\vec{G}(\vec{k})|\,\Big|\frac{1}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}\cdot\vec{v}} - \frac{1}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}\cdot\vec{u}}\Big|\Big)(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|) \\ &\quad \leq |\vec{u}-\vec{v}||\vec{G}(\vec{k})|\frac{1}{(1-r)}(1 + \frac{r|\vec{k}|}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|(1-r)}) \\ &\quad \leq |\vec{u}-\vec{v}||\vec{G}(\vec{k})|\frac{1}{(1-r)^2}\,.\end{aligned}$$

For the term $2\mathrm{Re}(\Phi_{\vec{u}}^* \vec{G})$, we observe that

$$\begin{aligned}
&|2\mathrm{Re}(\Phi_{\vec{u}}^* \vec{G}) - 2\mathrm{Re}(\Phi_{\vec{v}}^* \vec{G})| \\
&\qquad \le g^2 2|\vec{u} - \vec{v}| \frac{1}{(1-r)^2} \int_{|\vec{k}| \in [\sigma,\Lambda]} \frac{1}{|\vec{k}|} \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} d^3k \\
&\qquad \le C_1 g^2 \ln(2+\Lambda) 2|\vec{u} - \vec{v}| \frac{1}{(1-r)^2} .
\end{aligned}$$

Note that, for $g^2 \ln(2+\Lambda) < (1-r)^2/(3C_1)$,

$$|2\mathrm{Re}(\Phi_{\vec{u}}^* \vec{G}) - 2\mathrm{Re}(\Phi_{\vec{v}}^* \vec{G})| < \frac{1}{3} |\vec{u} - \vec{v}| .$$

Finally, for the term $\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}}$, we obtain the estimate

$$\begin{aligned}
&|\Phi_{\vec{u}}^* \vec{k} \Phi_{\vec{u}} - \Phi_{\vec{v}}^* \vec{k} \Phi_{\vec{v}}| \\
&\quad \le \int_{|\vec{k}| \in [\sigma,\Lambda]} (\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|) |\Phi_{\vec{u}}(\vec{k}) - \Phi_{\vec{v}}(\vec{k})| (|\Phi_{\vec{u}}(\vec{k})| + |\Phi_{\vec{v}}(\vec{k})|) d^3k \\
&\quad \le \frac{|\vec{u} - \vec{v}|}{(1-r)^2} \int_{|\vec{k}| \in [\sigma,\Lambda]} |\vec{G}(\vec{k})| (|\Phi_{\vec{u}}(\vec{k})| + |\Phi_{\vec{v}}(\vec{k})|) d\vec{k} \\
&\quad \le \frac{|\vec{u} - \vec{v}|}{(1-r)^2} \|(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|)^{-1/2} G\| (\| \sqrt{\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Phi_{\vec{u}}\| + \| \sqrt{\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Phi_{\vec{v}}\|) \\
&\quad \le C_2 |\vec{u} - \vec{v}| \, (|\vec{u}| + |\vec{v}|) g^2 \ln(\Lambda + 2) ,
\end{aligned}$$

and thus this term can be controlled for $|g \ln(\Lambda + 2)|^2$ sufficiently small by $\frac{1}{3}|\vec{u} - \vec{v}|$. We thus get a contraction

$$|\vec{\Psi}(\vec{u}) - \vec{\Psi}(\vec{u}')| \le \frac{2}{3} |\vec{u} - \vec{u}'|$$

and with $f_{\vec{p}} = \Phi_{\vec{u}_{\vec{p}}}$ Equation (VI.64) is solved. □

We then obtain several explicit results from the expression of this minimizer.

COROLLARY VI.7. *With the same hypotheses as in Theorem VI.2:*

1. *For* $0 \le \sigma < \Lambda < \infty$,

$$\inf_{f \in \mathfrak{h}} \mathcal{E}_{g,\vec{p}}(f) \;=\; \inf_{f \in \widetilde{\mathfrak{h}}} \mathcal{E}_{g,\vec{p}}(f) \;=\; \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) ,$$

and for $0 < \sigma < \Lambda < \infty$, *we have that* $f_{\vec{p}} \in \mathfrak{h}$.

2. *For fixed* g, σ, Λ, *as a function of* $\vec{p}$,

$$\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) = \mathcal{E}_{g,\vec{p}}(0) - \vec{p} \cdot \vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G} \cdot \vec{G}^*} \vec{G} \cdot \vec{p} + \mathcal{O}(|\vec{p}|^3) .$$

3. For all f in $\widetilde{\mathfrak{h}}$,

$$\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}+f) = \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) + f^*(\tfrac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{u}_{\vec{p}}\cdot\vec{k})f \\ + \tfrac{1}{2}\big(f^*\vec{k}f + 2\mathrm{Re}(f_{\vec{p}}^*\vec{k}f) + 2\mathrm{Re}(f^*\vec{G})\big)^{\cdot 2}. \quad \text{(VI.66)}$$

4. The energy $\mathcal{E}_{g,\vec{p}}(f_{\vec{p}})$ of the minimizer compared to the energy of the vacuum state $\mathcal{E}_{g,\vec{p}}(0)$ is

$$\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) \;=\; \mathcal{E}_{g,\vec{p}}(0) - \tfrac{1}{2}2\mathrm{Re}(f_{\vec{p}}^*\vec{u}_{\vec{p}}\cdot\vec{G}) - \tfrac{1}{2}|\vec{u}_{\vec{p}}-\vec{p}|^2\,.$$

Note that the term $2\mathrm{Re}(f_{\vec{p}}^*\vec{u}_{\vec{p}}\cdot\vec{G})$ is non-negative.

Proof of 1. is straightforward for $\sigma > 0$. For $\sigma = 0$ one can approximate the minimizer in $\tilde{\mathfrak{h}}$ by functions in $\mathfrak{h}$.

Proof of 2. The expression of the energy $\mathcal{E}_{g,\vec{p}}(f)$ given in Equation (VI.63) implies that $\mathcal{E}_{g,\vec{p}}(f) \ge \frac{1}{2}\|\vec{G}\|^2$, and for $\vec{p}=\vec{0}$ this minimum is only attained at the point $f_{\vec{0}}=0$. It follows that $f_{\vec{p}} = \partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p} + \mathcal{O}(|\vec{p}|^2)$. >From Equation (VI.65) we deduce

$$\vec{u}_{\vec{p}} = \vec{p} - 2\mathrm{Re}((\partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p})^*\vec{G}) + \mathcal{O}(|\vec{p}|^2)$$

and thus

$$\begin{aligned} f_{\vec{p}} &= \frac{(\vec{p}-2\mathrm{Re}((\partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p})^*\vec{G})).\vec{G}}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|-\vec{k}\cdot\vec{u}_{\vec{p}}} + \mathcal{O}(|\vec{p}|^2) \\ &= (\frac{1}{2}|\vec{k}|^2+|\vec{k}|)^{-1}(\vec{p}-2\mathrm{Re}((\partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p})^*\vec{G}))\cdot\vec{G} + \mathcal{O}(|\vec{p}|^2)\,. \end{aligned}$$

Expanding the left hand side of this equality in $\vec{0}$ brings

$$\partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p} = (\frac{1}{2}|\vec{k}|^2+|\vec{k}|)^{-1}(\vec{p}-2\mathrm{Re}((\partial_{\vec{p}}f_{\vec{0}}\cdot\vec{p})^*\vec{G}))\cdot\vec{G}$$

and hence $\partial_{\vec{p}}f_{\vec{0}} = (\frac{1}{2}|\vec{k}|^2+|\vec{k}|+2\vec{G}\cdot\vec{G}^*)^{-1}\vec{G}$. The expansion of $f_{\vec{p}}$ to the second order is then

$$f_{\vec{p}} = (\frac{1}{2}|\vec{k}|^2+|\vec{k}|+2\vec{G}\cdot\vec{G}^*)^{-1}\vec{G}\cdot\vec{p} + \mathcal{O}(|\vec{p}|^2)\,.$$

We can compute the energy modulo error terms in $\mathcal{O}(|\vec{p}|^3)$. To have less heavy computations we set $A = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G}\cdot\vec{G}^*$ and get

$$
\begin{aligned}
&\mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) - \frac{1}{2}\|\vec{G}\|^2 - \frac{1}{2}|\vec{p}|^2 \\
&\quad \equiv -\frac{1}{2}|\vec{p}|^2 + \frac{1}{2}(2\mathrm{Re}(\vec{p}\cdot\partial_{\vec{p}} f^*_{\vec{0}}\vec{G}) - \vec{p})^{\cdot 2} + \vec{p}\cdot\partial_{\vec{p}} f^*_{\vec{0}}(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)\partial_{\vec{p}} f^*_{\vec{0}}\cdot\vec{p} \\
&\quad \equiv \frac{1}{2}(2\mathrm{Re}(\vec{p}\cdot\vec{G}^* A^{-1}\vec{G}))^{\cdot 2} - 2\vec{p}\cdot\vec{G}^* A^{-1}\vec{G}\cdot\vec{p} \\
&\qquad\quad + \vec{p}\cdot\vec{G}^* A^{-1}(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)A^{-1}\vec{G}\cdot\vec{p} \\
&\quad \equiv 2(\vec{p}\cdot\vec{G}^* A^{-1}\vec{G})^{\cdot 2} + \vec{p}\cdot\vec{G}^* A^{-1}((\frac{1}{2}|\vec{k}|^2 + |\vec{k}|) - 2A)A^{-1}\vec{G}\cdot\vec{p} \\
&\quad \equiv \vec{p}\cdot\vec{G}^* A^{-1} 2\vec{G}\cdot\vec{G}^* A^{-1}\vec{G}\cdot\vec{p} - \vec{p}\cdot\vec{G}^* A^{-1}(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 4\vec{G}\cdot\vec{G}^*))A^{-1}\vec{G}\cdot\vec{p} \\
&\quad \equiv -\vec{p}\cdot\vec{G}^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G}\cdot\vec{G}^*)^{-1}\vec{G}\cdot\vec{p}
\end{aligned}
$$

which yields the result.

Proof of 3. The Taylor expansion of the energy around $f_{\vec{p}}$ is

$$
\begin{aligned}
\mathcal{E}_{g,\vec{p}}(f_{\vec{p}} + f) = {}& \mathcal{E}_{g,\vec{p}}(f_{\vec{p}}) + f^*\,\partial_{f^*}\mathcal{E}(f_{\vec{p}}) + \partial_f\mathcal{E}(f_{\vec{p}})\,f \\
& + \frac{1}{2}\Big\{(f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) + 2\mathrm{Re}(f^*_{\vec{p}}\vec{k}f))^{\cdot 2} \\
& \qquad + 2(f^*_{\vec{p}}\vec{k}f_{\vec{p}} + 2\mathrm{Re}(f^*_{\vec{p}}\vec{G}) - \vec{p})\cdot f^*\vec{k}f + f^*|\vec{k}|^2 f\Big\} + f^*|\vec{k}|f\,.
\end{aligned}
$$

Since $\partial_{f^*}\mathcal{E}(f_{\vec{p}})$ vanishes this gives Equation (VI.66).

Proof of 4. It is sufficient to replace f by $-f_{\vec{p}}$ in Equation (VI.66). The observation

$$
f^*_{\vec{p}}\vec{u}_{\vec{p}}\cdot\vec{G} = \int \frac{(\vec{u}_{\vec{p}}\cdot\vec{G}(\vec{k}))^2 dk}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{u}_{\vec{p}}}
$$

shows that $2\mathrm{Re}(f^*_{\vec{p}}\vec{u}_{\vec{p}}\cdot\vec{G})$ is non-negative since $|\vec{u}_{\vec{p}}| < 1$. □

VII Renormalized Electron Mass for Coherent states

In this section we use the coherent state minimizer found in Section VI in order to determine the renormalized electron mass.

Proposition VII.1. *The renormalized electron mass for coherent states $m_{coh}(g,\Lambda)$ defined by*

$$
\mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{0}}(f_{g,\vec{0}}) = \frac{1}{2m_{coh}(g,\Lambda)}|\vec{p}|^2 + \mathcal{O}(|\vec{p}|^3)\,.
$$

is

$$
m_{coh}(g,\Lambda) = 1 + \frac{32\pi}{3}g^2\ln(1 + \frac{\Lambda}{2})\,.
$$

Remark VII.2. This result agrees with m_{eff}/m obtained in [12] to second order in g, taking into account that g in [12] equals $\frac{\sqrt{\alpha}}{2\pi}$ in the present paper, that $\omega(\vec{k}) = |\vec{k}|$, and that the mass m of the electron is one in our units. See also (among others) [11] or [3].

Proof. From

$$\mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{p}}(0) = \frac{1}{2}|\vec{p}|^2 - \vec{p}\cdot\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G}\cdot\vec{G}^*} \vec{G}\cdot\vec{p} + \mathcal{O}(|\vec{p}|^3)$$

and the fact that for $\vec{p} = \vec{0}$ the minimizer is $f_{g,\vec{0}} = 0$, it follows that

$$\begin{aligned}\mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{0}}(f_{g,\vec{0}}) &= \mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{0}}(0) \\ &= \mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{p}}(0) + \frac{1}{2}|\vec{p}|^2 \\ &= \frac{1}{2}|\vec{p}|^2 - \vec{p}\cdot\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G}\cdot\vec{G}^*} \vec{G}\cdot\vec{p} + \mathcal{O}(|\vec{p}|^3)\end{aligned}$$

where we used point 2 of Theorem VI.2 for the last equality. The power expansion of $(1-t)^{-1}$ yields

$$\frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}| + 2\vec{G}\cdot\vec{G}^*} = \sum_{j=0}^{\infty} \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Big(- 2\vec{G}\cdot\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \Big)^j$$

and hence

$$\begin{aligned}\mathcal{E}_{g,\vec{p}}(f_{g,\vec{p}}) - \mathcal{E}_{g,\vec{0}}(f_{g,\vec{0}}) &= \frac{1}{2}|\vec{p}|^2 - \frac{1}{2}\sum_{j=1}^{\infty} \vec{p}\cdot\Big(- 2\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \vec{G}\Big)^j \cdot\vec{p} + \mathcal{O}(|\vec{p}|^3) \\ &= \frac{1}{2}\vec{p}\cdot \Big(Id_{\mathbb{R}^3} + 2\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \vec{G}\Big)^{-1} \cdot\vec{p} + \mathcal{O}(|\vec{p}|^3)\,.\end{aligned}$$

The coherent renormalized mass is thus

$$m_{coh} = Id_{\mathbb{R}^3} + 2\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \vec{G}\,.$$

The proof is achieved by the computation of an integral that we give in a separate lemma since it will be useful again later. ☐

Lemma VII.3. *With* $\sigma = 0$,

$$2\vec{G}^* \frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \vec{G} = g^2\, 8\pi\, \frac{4}{3}\, \ln(1 + \frac{\Lambda}{2})\, Id_{\mathbb{R}^3}\,.$$

Proof. Using spherical coordinates

$$\begin{aligned}
2\vec{p}\cdot\vec{G}^*\frac{1}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|}\vec{G}\cdot\vec{p} &= 2g^2\int_{|\vec{k}|\leq\Lambda}\frac{|\vec{p}\cdot\vec{\varepsilon}_+(\vec{k})|^2+|\vec{p}\cdot\vec{\varepsilon}_-(\vec{k})|^2}{\frac{1}{2}|\vec{k}|^3+|\vec{k}|^2}d\vec{k}\\
&= 2g^2|\vec{p}|^2\int_{|\vec{k}|\leq\Lambda}\frac{1-|\frac{\vec{p}}{|\vec{p}|}\cdot\frac{\vec{k}}{|\vec{k}|}|^2}{\frac{1}{2}|\vec{k}|^3+|\vec{k}|^2}d\vec{k}\\
&= 2g^2|\vec{p}|^2\int_0^\Lambda\int_0^{2\pi}\int_0^\pi\frac{1-\cos^2\varphi}{\frac{1}{2}\rho^3+\rho^2}\sin\varphi\,d\varphi\,d\theta\,\rho^2d\rho\\
&= g^2|\vec{p}|^2\,8\pi\,\frac{4}{3}\,\ln(1+\frac{\Lambda}{2})\,,
\end{aligned}$$

which yields the result. □

VIII Minimization over Quasifree States

In this section we minimize the energy functional over the set of pure quasifree states. We first obtain the existence and uniqueness of a pure quasifree state in Theorem VIII.3. As shown in Section IV this proves the existence (but not the uniqueness) of a minimizer in the class of quasifree states. We then compute asymptotics for small coupling g and momentum p of the parameters $f_{g,\vec{p}}$ and $r_{g,\vec{p}}$ describing the pure quasifree state minimizing the energy in Theorem VIII.6. From these asymptotics we deduce an expansion of the energy at the minimizer. Finally we give in Theorem VIII.8 the Lagrange equations in terms of the parameters f, α and γ.

Remark VIII.1. We believe that the assumption $\sigma > 0$ is unnecessary, but we have no proof for this assertion and do not follow it here, because the infrared singular limit $\sigma \to 0$ is not our concern in this paper.

VIII.1 Existence and Uniqueness of a Minimizer of the Energy over Pure Quasifree States

In this section we minimize the energy over all pure quasifree states and show that there is a unique minimizer.

Definition VIII.2. Let $\mathfrak{h}$ be a $\mathbb{C}$-Hilbert space. Let Y be the $\mathbb{R}$-Hilbert space of antilinear operators $\hat{r}$ on $\mathfrak{h}$, self-adjoint in the sense that $\forall z, z' \in \mathfrak{h}$, $\langle z, \hat{r}z'\rangle = \langle z', \hat{r}z\rangle$, and Hilbert-Schmidt in the sense that the positive operator $\hat{r}^2$ is trace class. The space $X = \mathfrak{h}\times Y$ with the scalar product

$$\langle (f,\hat{r}),(f',\hat{r}')\rangle_X = f^*f' + \mathrm{Tr}[\hat{r}\hat{r}']$$

is an $\mathbb{R}$-Hilbert space.
Keeping $\sigma > 0$, we only need to use $\mathfrak{h} = L^2(S_{\sigma,\Lambda}\times\mathbb{Z}_2)$ in this section.

Theorem VIII.3. *Let $0 < \sigma < \Lambda < \infty$. There exists $C > 0$ such that for $g, |\vec{p}| \le C$ there exists a unique minimizer for $\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$.*

Proof. This result follows from convexity and coercivity arguments. By Proposition VIII.4, $\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$ is strictly θ-convex (i.e., uniformly strictly convex) on $\bar{B}_X(0,R)$ for some $R > 0$ and $\theta > 0$. Since $\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$ is strongly continuous on the closed and convex set $\bar{B}_X(0,R)$ of the Hilbert space X we get the existence and uniqueness of a minimizer in $\bar{B}_X(0,R)$. (See for example [1]. The uniform strict convexity allows to prove directly that a minimizing sequence is a Cauchy sequence.) Proposition VIII.5 then proves that it is the only minimum of $\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$ on the whole space.
Note that to use Propositions VIII.4 and VIII.5 we need to restrict to values of g and $|\vec{p}|$ smaller than some constant $C > 0$. ☐

Proposition VIII.4 (Convexity). *There exist $0 < C, R < \infty$ such that for $g \le C$ and $|\vec{p}| \le \frac{1}{2}$, the Hessian of the energy satisfies $\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r}) \ge \frac{\sigma}{4}\mathbf{1}_X$ on the ball $B_X(0,R)$.*

Proof. We use that strict positivity of the Hessian implies strict convexity and thus first compute the Hessian in $(0,0)$. The Hessian $\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r}) \in \mathcal{B}(X)$ is defined using the Fréchet derivative

$$\begin{aligned}&\hat{\mathcal{E}}_{g,\vec{p}}(f+\delta f,\hat{r}+\delta\hat{r}) - \hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})\\ &= D\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})(\delta f,\delta\hat{r}) + \frac{1}{2}\big\langle(\delta f,\delta\hat{r})\,,\,\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})\,(\delta f,\hat{r})\big\rangle_X + o(\|(\delta f,\delta\hat{r})\|_X^2)\end{aligned}$$

with $D\hat{\mathcal{E}}_{g,\vec{p}}(0,0) \in \mathcal{B}(X,\mathbb{R})$. (Note that differentiability is granted in this case because $|\vec{k}| \le \Lambda < \infty$.) For any $\mu > 0$, $\forall(f,\hat{r}) \in X$,

$$\begin{aligned}&\langle(f,\hat{r})\,,\,\frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0,0)\,(f,\hat{r})\rangle_X\\
&\quad= 2\mathrm{Re}\langle\hat{r}\vec{k}f;\vec{G}\rangle + \frac{1}{2}(2\mathrm{Re}(f^*\vec{G}))^{\cdot 2} + \mathrm{Tr}[\hat{r}^2\vec{G}\cdot\vec{G}^*]\\
&\qquad+ \frac{1}{2}\big\{\mathrm{Tr}[\hat{r}\vec{k}\cdot\hat{r}\vec{k}] + \mathrm{Tr}[|\vec{k}|^2\hat{r}^2]\big\}\\
&\qquad+ \mathrm{Tr}[\hat{r}^2(|\vec{k}| - \vec{k}\cdot\vec{p})] + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{p})f\\
&\quad\ge \mathrm{Tr}[\hat{r}^2\vec{G}\cdot\vec{G}^*] - \mu\|\hat{r}\vec{G}\|^2 - \frac{1}{\mu}\|\vec{k}f\|^2\\
&\qquad+ \frac{1}{2}\big\{(2\mathrm{Re}(\delta f^*\vec{G}))^{\cdot 2} + \mathrm{Tr}[\hat{r}\vec{k}\cdot\hat{r}\vec{k}] + \mathrm{Tr}[|\vec{k}|^2\hat{r}^2]\big\}\\
&\qquad+ \mathrm{Tr}[\hat{r}^2(|\vec{k}| - \vec{k}\cdot\vec{p})] + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{p})f\\
&\quad\ge \mathrm{Tr}[\hat{r}^2(|\vec{k}| - \vec{k}\cdot\vec{p} + (1-\mu)\vec{G}\cdot\vec{G}^*)] + f^*((\frac{1}{2} - \frac{1}{\mu})|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{p})f\,,\end{aligned}$$

since

$$|2\mathrm{Re}\langle\hat{r}\vec{k}f;\vec{G}\rangle| \le 2\|\hat{r}\vec{G}\|\|\vec{k}f\| = 2\sqrt{\mu}\|\hat{r}\vec{G}\|\frac{1}{\sqrt{\mu}}\|\vec{k}f\| \le \mu\|\hat{r}\vec{G}\|^2 + \frac{1}{\mu}\|\vec{k}f\|^2\,.$$

With $\mu = 2$ we obtain (with $|\vec{p}| \leq \frac{1}{2}$)

$$\begin{aligned}\frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0,0)(f,\hat{r}) &\geq \mathrm{Tr}[\hat{r}^2(|\vec{k}| - \vec{k}\cdot\vec{p} - \vec{G}\cdot\vec{G}^*)] + f^*(|\vec{k}| - \vec{k}\cdot\vec{p})f \\ &\geq \mathrm{Tr}[\hat{r}^2(|\vec{k}|(1 - \||\vec{k}|^{-1/2}\vec{G}\|^2) - \vec{k}\cdot\vec{p})] + f^*(|\vec{k}| - \vec{k}\cdot\vec{p})f \\ &\geq \mathrm{Tr}[\hat{r}^2\sigma(\frac{1}{2} - \||\vec{k}|^{-1/2}\vec{G}\|^2)] + f^*\frac{\sigma}{2}f\end{aligned}$$

and for g small enough

$$\frac{1}{2}\mathcal{H}\hat{\mathcal{E}}_{g,\vec{p}}(0,0) \geq \frac{\sigma}{4}\,.$$

We then compare it with the Hessian in points near zero. Observing that the Hessian is continuous with respect to $(f,\hat{r},\vec{p},g)$, we deduce that there exist $R < \infty$ and $C > 0$, as asserted. □

PROPOSITION VIII.5 (Coercivity). *Suppose $\vec{p}$ and $C > 0$ are fixed such that $\frac{1}{2}|\vec{p}|^2 + \frac{1}{2}\|\vec{G}\|^2 < \sigma R^2$, with the value of R given by Proposition VIII.4, for any $0 < g < C$. For every $(f,\hat{r}) \in X$,*

$$\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r}) \;\geq\; \mathrm{Tr}[\hat{r}^2|\vec{k}|] + f^*|\vec{k}|f \;\geq\; \sigma\left\|(f,\hat{r})\right\|_X^2.$$

Since $\hat{\mathcal{E}}_{g,\vec{p}}(0,0) = \frac{1}{2}|\vec{p}|^2 + \frac{1}{2}\|\vec{G}\|^2 < \sigma R^2$, any minimizing sequence can be assumed to take its values in $B_X(0,R)$.

VIII.2 ASYMPTOTICS FOR SMALL COUPLING AND MOMENTUM

In this section we calculate the ground state energy for small orders of the coupling constant g and total momentum $\vec{p}$.
We use below an identification between self-adjoint $\mathbb{C}$-antilinear Hilbert-Schmidt operator $\hat{r}$ and symmetric two vector r given by the relation $\langle\varphi,\hat{r}\psi\rangle_{\mathfrak{h}} = \langle\varphi\otimes\psi, r\rangle_{\mathfrak{h}^{\otimes 2}}$. Note that the self-adjointness condition for $\hat{r}$ is equivalent to the symmetry condition $r \in \mathfrak{h}^{\vee 2}$.

THEOREM VIII.6. *Let $0 < \sigma < \Lambda < \infty$. There exists $C > 0$ such that for $|g|, |\vec{p}| < C$, there exist two functions $f_{g,\vec{p}}$ and $\hat{r}_{g,\vec{p}}$ which are smooth in $(g,\vec{p})$ such that the minimum of the energy $\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$ is attained at $(f_{g,\vec{p}},\hat{r}_{g,\vec{p}})$. These functions satisfy*

$$\begin{aligned}f_{g,\vec{p}} &= \frac{\vec{p}\cdot\vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} + \mathcal{O}(\|(g,\vec{p})\|^3) \\ r_{g,\vec{p}} &= -S^{-1}\vec{G}^{\cdot\vee 2} + \mathcal{O}(\|(g,\vec{p})\|^3)\,,\end{aligned}$$

with $S = \vec{k}\cdot\otimes\vec{k} + 2(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)\vee\mathbf{1}_{\mathfrak{h}}$ and where $\vec{G}^{\cdot\vee 2} = \sum_{j=1}^3 \vec{G}_j \vee \vec{G}_j \in \mathfrak{h}\vee\mathfrak{h}$ (recall that $\vee$ denotes the symmetric tensor product). As a consequence

$$\begin{aligned}&E_{BHF}(g,\vec{p},\sigma,\Lambda) \\ &\quad= \hat{\mathcal{E}}_{g,\vec{p}}(0_X) - \vec{p}\cdot\vec{G}^*\frac{1}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|}\vec{G}\cdot\vec{p} - \frac{1}{2}\vec{G}^{\cdot\vee 2*}S^{-1}\vec{G}^{\cdot\vee 2} + \mathcal{O}(\|(g,\vec{p})\|^5)\,.\end{aligned}$$

Recall that for z and z' in a Hilbert space, $z^* z' = \langle z, z' \rangle$.

Remark VIII.7. The energy in 0_X is the energy of the vacuum state and is $\hat{\mathcal{E}}_{g,\vec{p}}(0_X) = \frac{1}{2}\vec{p}^{\,2} + \frac{1}{2}\|\vec{G}\|^2$. Further note that by Lemma VII.3

$$2(\vec{p}\cdot\vec{G}^*)\frac{1}{\frac{1}{2}|\vec{k}|^2+|\vec{k}|}(\vec{G}\cdot\vec{p}) \ = \ g^2|\vec{p}|^2\frac{32\pi}{3}\ \ln\left(\frac{\Lambda+2}{\sigma+2}\right)$$

and in particular does not depend on the choice of the polarization vectors $\vec{\varepsilon}$.
The quantity $\vec{G}^{\cdot\vee 2*}S^{-1}\vec{G}^{\cdot\vee 2}$ does not depend on the choice of the vectors $\vec{\varepsilon}$ either since

$$\vec{G}^{\cdot\vee 2*}S^{-1}\vec{G}^{\cdot\vee 2} = \sum_{\mu,\nu=\pm}\int\frac{|\vec{\varepsilon}(\vec{k}_1,\mu)\cdot\vec{\varepsilon}(\vec{k}_2,\nu)|^2}{\sqrt{|\vec{k}_1||\vec{k}_2|}S(\vec{k}_1,\vec{k}_2)}d^3k_1d^3k_2$$

and with $P_{\vec{u}}$ is the orthogonal projection on $\vec{u}$ in $\mathbb{R}^3$,

$$\begin{aligned}\sum_{\mu,\nu=\pm}|\vec{\varepsilon}(\vec{k}_1,\mu)\cdot\vec{\varepsilon}(\vec{k}_2,\nu)|^2 &= \sum_{\mu,\nu=\pm}\mathrm{Tr}_{\mathbb{R}^3}[P_{\vec{\varepsilon}(\vec{k}_1,\mu)}P_{\vec{\varepsilon}(\vec{k}_2,\nu)}] \\ &= 1+\mathrm{Tr}_{\mathbb{R}^3}[P^{\perp}_{\vec{k}_1}P^{\perp}_{\vec{k}_2}] \\ &= 1+\left(\frac{\vec{k}_1}{|\vec{k}_1|}\cdot\frac{\vec{k}_2}{|\vec{k}_2|}\right)^2 .\end{aligned}$$

Proof of Theorem VIII.6. Let

$$F:(g,\vec{p},f,\hat{r})\mapsto\partial_{f,\hat{r}}\hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r})$$

and $\left(\begin{smallmatrix}f\\ \hat{r}\end{smallmatrix}\right)(g,\vec{p}) := \left(\begin{smallmatrix}f(g,\vec{p})\\ \hat{r}(g,\vec{p})\end{smallmatrix}\right)$ such that

$$F(g,\vec{p},\left(\begin{smallmatrix}f\\ \hat{r}\end{smallmatrix}\right)(g,\vec{p}))=0\,, \qquad \text{(VIII.67)}$$

then a derivation of Equation (VIII.67) with respect to $(f,\hat{r})$ brings

$$\partial_{g,\vec{p}}\left(\begin{smallmatrix}f\\ \hat{r}\end{smallmatrix}\right)(0_{g,\vec{p}}) = -\left[\partial_{f,\hat{r}}F(0_{g,\vec{p}},0_{f,\hat{r}})\right]^{-1}\partial_{g,\vec{p}}F(0_{g,\vec{p}},0_{f,\hat{r}})\,.$$

The term which is independent of $(g,\vec{p})$ and quadratic in $\left(\begin{smallmatrix}f\\ \hat{r}\end{smallmatrix}\right)$ in the energy is

$$\frac{1}{2}\{\mathrm{Tr}[\hat{r}S\hat{r}]+f^*(|\vec{k}|^2+2|\vec{k}|)f\}$$

thus, in $(0_{g,\vec{p}},0_{f,\hat{r}})$,

$$\partial_{f,\hat{r}}F = \begin{pmatrix} |\vec{k}|^2+2|\vec{k}| & 0\\ 0 & S\end{pmatrix}.$$

To compute $\partial_{g,\vec{p}}F$ in 0, observe that no part in the energy is linear in $(g,\vec{p})$ and linear in $(f,\hat{r})$. Thus $\partial_{g,\vec{p}}F(0_{g,\vec{p}},0_{f,\hat{r}})=0$ and we get

$$\partial_{g,\vec{p}}f(0_{g,\vec{p}})=0\,.$$

Differentiating a second time Equation (VIII.67) brings

$$0 = \partial^2_{g,\vec{p}} F + 2\partial_{f,\hat{r}}\partial_{g,\vec{p}} F \circ \partial_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right) + \partial_{f,\hat{r}} F \circ \partial^2_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right) + \partial^2_{f,\hat{r}} F(\partial_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right), \partial_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right)) .$$

Since $\partial_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right)(0_{g,\vec{p}}) = 0$, it follows that

$$\partial^2_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right)(0_{g,\vec{p}}) = -[\partial_{f,\hat{r}} F(0_{g,\vec{p}}, 0_{f,\hat{r}})]^{-1} \partial^2_{g,\vec{p}} F(0_{g,\vec{p}}, 0_{f,\hat{r}}) .$$

The part of the energy which is quadratic in $(g,\vec{p})$ and linear in $(f,\hat{r})$ is $-2\mathrm{Re}(f^*\vec{G}) \cdot \vec{p} + \mathrm{Re}\langle \hat{r}\vec{G}; \vec{G}\rangle$, it follows that, in $(0_{g,\vec{p}}, 0_{f,\hat{r}})$,

$$\partial^2_{g,\vec{p}} F = 2 \begin{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \vee \begin{pmatrix} 0 & -2\partial_g \vec{G} \end{pmatrix} \\ \begin{pmatrix} \partial_g \vec{G} & 0 \end{pmatrix} \cdot \vee \begin{pmatrix} \partial_g \vec{G} & 0 \end{pmatrix} \end{pmatrix} ,$$

which gives in $0_{g,\vec{p}}$

$$\partial^2_{g,\vec{p}} \left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right) = 2 \begin{pmatrix} \begin{pmatrix} 1 & 0 \end{pmatrix} \vee \begin{pmatrix} 0 & \frac{\partial_g \vec{G}}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} \end{pmatrix} \\ -S^{-1} \begin{pmatrix} \partial_g \vec{G} & 0 \end{pmatrix} \cdot \vee \begin{pmatrix} \partial_g \vec{G} & 0 \end{pmatrix} \end{pmatrix} .$$

Hence the expansion of $\left(\begin{smallmatrix} f \\ \hat{r} \end{smallmatrix}\right)$ up to order 2.
We can thus express the energy around $0_{g,\vec{p}}$ modulo error terms in $\mathcal{O}(\|(g,\vec{p})\|^5)$

$$\begin{aligned}
&\min_{f,\hat{r}} \hat{\mathcal{E}}_{g,\vec{p}}(f,\hat{r}) - \hat{\mathcal{E}}_{g,\vec{p}}(0,0) \\
&\quad \equiv \tfrac{1}{2}\big\{ (\mathrm{Tr}[\hat{r}^2\vec{k}] + f^*\vec{k}f + 2\mathrm{Re}(f^*\vec{G}) - \vec{p})^{\cdot 2} + \mathrm{Tr}[\hat{r}\vec{k} \cdot \hat{r}\vec{k}] + \mathrm{Tr}[|\vec{k}|^2\hat{r}^2] \\
&\qquad + 2\mathrm{Re}\langle \hat{r}(\vec{G} + \vec{k}f); (\vec{G} + \vec{k}f)\rangle + \|\vec{G}\|^2 + f^*|\vec{k}|^2 f \big\} \\
&\qquad + \mathrm{Tr}[\hat{r}^2|\vec{k}|] + f^*|\vec{k}|f - \hat{\mathcal{E}}_{g,\vec{p}}(0,0) \\
&\quad \equiv -2\mathrm{Re}(f^*\vec{G}) \cdot \vec{p} + \tfrac{1}{2}\mathrm{Tr}[\hat{r}S\hat{r}] + \mathrm{Re}\langle \hat{r}\vec{G}; \vec{G}\rangle + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)f \\
&\quad \equiv -2\mathrm{Re}(f^*\vec{p} \cdot \vec{G}) + \tfrac{1}{2}\mathrm{Tr}[\hat{r}S\hat{r}] + \mathrm{Re}\langle \hat{r}\vec{G}; \vec{G}\rangle + f^*(\frac{1}{2}|\vec{k}|^2 + |\vec{k}|)f \\
&\quad \equiv -2\frac{(\vec{p} \cdot \vec{G})^*(\vec{p} \cdot \vec{G})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|} + \frac{1}{2}\vec{G}^{\cdot\vee 2*}S^{-1}\vec{G}^{\cdot\vee 2} - \vec{G}^{\cdot\vee 2*}S^{-1}\vec{G}^{\cdot\vee 2} + \frac{(\vec{p} \cdot \vec{G})^*(\vec{p} \cdot \vec{G})}{\frac{1}{2}|\vec{k}|^2 + |\vec{k}|}
\end{aligned}$$

which completes the proof. □

VIII.3 Lagrange Equations

In this section we derive a system of equations that determine critical points of the energy functional. We formulate the results of Section VIII.1 in terms of γ and α subject to the constraints $\gamma + \gamma^2 = (\alpha^* \otimes \mathbf{1}_{\mathfrak{h}})(\mathbf{1}_{\mathfrak{h}} \otimes \alpha)$, without reference to the parametrization of γ and α in terms of $\hat{r}$.
Suppose $f \in \mathfrak{h}$, $\alpha \in \mathfrak{h}^{\vee 2}$, $\gamma \in \mathcal{L}^1(\mathfrak{h})$, $\lambda \in \mathcal{B}(\mathfrak{h}) = \mathcal{B}$ and $\vec{u} \in \mathbb{R}^3$. Let $\mathcal{A}(\lambda) = \frac{1}{2}\vec{k} \cdot\vee \vec{k} + \lambda \vee \mathbf{1}$ and $\mathcal{G}(\gamma) = \gamma + \gamma^2$.

Theorem VIII.8. *Suppose (f,γ,α) is a minimizer of the energy functional $\mathcal{E}$ such that $\|\gamma\|_{\mathcal{B}(\mathfrak{h})} < \frac{1}{2}$. Then there is a unique $(\lambda,\vec{u})$ such that $(f,\gamma,\alpha,\lambda,\vec{u})$ satisfies the following equations, equivalent to Lagrange equations*

$$M(\gamma,\vec{u})f = -(\vec{k}\gamma-\vec{u})\cdot\vec{G} - \vec{k}\cdot\vee(\vec{G}+\vec{k}f)^*\alpha \tag{VIII.68}$$

$$\mathcal{A}(\lambda)\alpha = -\frac{1}{2}(\vec{G}+\vec{k}f)^{\cdot\vee 2} \tag{VIII.69}$$

$$\gamma = \mathcal{G}^{-1}((\alpha^*\otimes\mathbf{1}_{\mathfrak{h}})(\mathbf{1}_{\mathfrak{h}}\otimes\alpha)) \tag{VIII.70}$$

$$\lambda = \int_0^\infty e^{-t(\frac{1}{2}+\gamma)}(M(\gamma,\vec{u}) + (\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*)e^{-t(\frac{1}{2}+\gamma)}dt \tag{VIII.71}$$

$$\vec{u} = \vec{p} - \mathrm{Tr}[\gamma\vec{k}] - f^*\vec{k}f - 2\mathrm{Re}(f^*\vec{G}) \tag{VIII.72}$$

with $M(\gamma,\vec{u}) = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{u} + \vec{k}\cdot\gamma\vec{k}$.
Assuming $|\vec{p}| < \frac{1}{2}$, sufficient conditions such that $M(\gamma,\vec{u})$ and $\mathcal{A}(\lambda)$ are invertible operators are $|\vec{u}| < 1/2$, $\gamma \geq 0$ and $\|\lambda - (|\vec{k}|^2/2 + |\vec{k}| - \vec{p}\cdot\vec{k})\|_{\mathcal{B}} < \sigma/2$. Equations (VIII.68) to (VIII.72) then form a system of coupled explicit equations.

Remark VIII.9. To prove that Equations (VIII.68) to (VIII.72) admit a solution we use here the result of existence of a minimizer proved in Section VIII.1. It can also be proved directly by a fixed point argument by defining the applications

$$\begin{aligned}
\Psi_f(f,\alpha,\gamma,\vec{u}) &= -M(\gamma,\vec{u})^{-1}(\vec{k}\gamma-\vec{u})\cdot\vec{G} - \vec{k}\cdot\vee(\vec{G}+\vec{k}f)^*\alpha \\
\Psi_\alpha(f,\lambda) &= -\mathcal{A}(\lambda)^{-1}\frac{1}{2}(\vec{G}+\vec{k}f)^{\cdot\vee 2} \\
\Psi_\gamma(\alpha) &= \mathcal{G}^{-1}((\alpha^*\otimes\mathbf{1}_{\mathfrak{h}})(\mathbf{1}_{\mathfrak{h}}\otimes\alpha)) \\
\Psi_\lambda(f,\gamma,\vec{u}) &= \int_0^\infty e^{-t(\frac{1}{2}+\gamma)}(M(\gamma,\vec{u}) + (\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*)e^{-t(\frac{1}{2}+\gamma)}dt \\
\Psi_{\vec{u}}(f,\gamma) &= \vec{p} - \mathrm{Tr}[\gamma\vec{k}] - f^*\vec{k}f - 2\mathrm{Re}(f^*\vec{G})
\end{aligned}$$

defined on balls of centers 0, 0, 0, $\frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{p}$ and $\vec{p}$ and proving that the application

$$\begin{aligned}
\Psi_{(f,\lambda)}(f,\lambda) = (\Psi_f&[f,\Psi_\alpha\{f,\lambda\},\Psi_\gamma\{\Psi_\alpha(f,\lambda)\},\Psi_{\vec{u}}\{f,\Psi_\gamma(\Psi_\alpha[f,\lambda])\}], \\
&\Psi_\lambda[f,\Psi_\gamma\{\Psi_\alpha(f,\lambda)\},\Psi_{\vec{u}}\{f,\Psi_\gamma(\Psi_\alpha[f,\lambda])\}])
\end{aligned}$$

is a contraction for a convenient choice of the radiuses and a sufficiently small coupling constant g. Note that it is then convenient to consider the norm of $L^2(S_{\sigma,\Lambda}\times\mathbb{Z}_2,|\vec{k}|^2)$ for f.

Proof of Theorem VIII.8. Indeed, set $\vec{u} = \vec{p} - \mathrm{Tr}[\gamma\vec{k}] - f^*\vec{k}f - 2\mathrm{Re}(f^*\vec{G})$ and define the partial derivatives as $\partial_{f^*}\mathcal{E}(f,\gamma,\alpha) \in \mathfrak{h}$, $\partial_{\alpha^*}\mathcal{E}(f,\gamma,\alpha) \in \mathfrak{h}^{\vee 2}$ and $\partial_\gamma\mathcal{E}(f,\gamma,\alpha) \in$

$\mathcal{B}(\mathfrak{h}) \cong \mathcal{L}^1(\mathfrak{h})'$ such that

$$\begin{aligned}&\mathcal{E}(f+\delta f,\gamma+\delta\gamma,\alpha+\delta\alpha)-\mathcal{E}(f,\gamma,\alpha)\\&\quad=2\mathrm{Re}(\delta f^*\,\partial_{f^*}\mathcal{E}(f,\gamma,\alpha))+2\mathrm{Re}(\delta\alpha^*\,\partial_{\alpha^*}\mathcal{E}(f,\gamma,\alpha))\\&\qquad+\mathrm{Tr}[\delta\gamma\,\partial_\gamma\mathcal{E}(f,\gamma,\alpha)]+o(\|(\delta f,\delta\gamma,\delta\alpha)\|_{\mathfrak{h}\times\mathcal{L}^1(\mathfrak{h})\times\mathfrak{h}^{\vee 2}})\,.\end{aligned}$$

Recall the energy functional is given by Equation (V.60) and this yields

$$\begin{aligned}\partial_{f^*}\mathcal{E}(f,\gamma,\alpha)&=\frac{1}{2}\big\{2(\vec{k}f+\vec{G})\cdot(\mathrm{Tr}[\gamma\vec{k}]+f^*\vec{k}f+2\mathrm{Re}(f^*\vec{G})-\vec{p})\\&\qquad+2\vec{k}\cdot\vee(\vec{G}+\vec{k}f)^*\alpha+\vec{k}\cdot(2\gamma+\mathbf{1})(\vec{G}+\vec{k}f)\big\}+|\vec{k}|f\\&=-(\vec{k}f+\vec{G})\cdot\vec{u}+\vec{k}\cdot\vee(\vec{G}+\vec{k}f)^*\alpha+\vec{k}\cdot\gamma(\vec{G}+\vec{k}f)+|\vec{k}|f\\&=M(\gamma,\vec{u})f+(\vec{k}\gamma-\vec{u})\cdot\vec{G}+\vec{k}\cdot\vee(\vec{G}+\vec{k}f)^*\alpha\,,\\\partial_{\alpha^*}\mathcal{E}(f,\gamma,\alpha)&=\frac{1}{2}(\vec{k}\cdot\otimes\vec{k})\alpha+\frac{1}{2}(\vec{G}+\vec{k}f)^{\cdot\vee 2}\,,\\\partial_\gamma\mathcal{E}(f,\gamma,\alpha)&=\frac{1}{2}\big\{2\vec{k}\cdot(\mathrm{Tr}[\gamma\vec{k}]+f^*\vec{k}f+2\mathrm{Re}(f^*\vec{G})-\vec{p})\\&\qquad+2\vec{k}\cdot\gamma\vec{k}+|\vec{k}|^2+2(\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*\big\}+|\vec{k}|\\&=M(\gamma,\vec{u})+(\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^*\,.\end{aligned}$$

The constraint given by Equation (IV.58) can be expressed as

$$\mathcal{C}(f,\gamma,\alpha)=0 \tag{VIII.73}$$

with

$$\begin{aligned}&\mathcal{C}:\mathfrak{h}\times\mathcal{L}^1(\mathfrak{h})\times\mathfrak{h}^{\vee 2}\to\mathcal{L}^1(\mathfrak{h})\\&\qquad\qquad(f,\gamma,\alpha)\mapsto\gamma+\gamma^2-(\alpha^*\otimes\mathbf{1}_\mathfrak{h})(\mathbf{1}_\mathfrak{h}\otimes\alpha)\,.\end{aligned}$$

Equation (VIII.73) is equivalent to Equation (VIII.70). The application $\mathcal{C}$ has a differential $D\mathcal{C}(f,\gamma,\alpha):\mathfrak{h}\times\mathcal{L}^1(\mathfrak{h})\times\mathfrak{h}^{\vee 2}\to\mathcal{L}^1(\mathfrak{h})$ such that

$$\begin{aligned}&D\mathcal{C}(f,\gamma,\alpha)(\delta f,\delta\gamma,\delta\alpha)\\&\quad=\delta\gamma+\delta\gamma\,\gamma+\gamma\,\delta\gamma-(\delta\alpha^*\otimes\mathbf{1}_\mathfrak{h})(\mathbf{1}_\mathfrak{h}\otimes\alpha)-(\alpha^*\otimes\mathbf{1}_\mathfrak{h})(\mathbf{1}_\mathfrak{h}\otimes\delta\alpha)\,.\end{aligned}$$

For $\|\gamma\|_{\mathcal{B}(\mathfrak{h})}<\frac{1}{2}$ the application $D\mathcal{C}(f,\gamma,\alpha)$ is surjective. Indeed it is already surjective on $\{0\}\times\mathcal{L}^1(\mathfrak{h})\times\{0\}$, since, for every $\gamma'\in\mathcal{L}^1(\mathfrak{h})$ the equation $\delta\gamma+\delta\gamma\,\gamma+\gamma\,\delta\gamma=\gamma'$ with unknown $\delta\gamma$ has at least one solution, see Proposition VIII.10. We can then apply the Lagrange multiplier rule (see for example the book of Zeidler [14]) which tells us that there exists a $\lambda\in\mathcal{B}(\mathfrak{h})$ such that

$$\forall(\delta f,\delta\alpha,\delta\gamma)\,,\quad D\mathcal{E}(f,\alpha,\gamma)(\delta f,\delta\alpha,\delta\gamma)+\mathrm{Tr}[D\mathcal{C}(f,\alpha,\gamma)(\delta f,\delta\alpha,\delta\gamma)\,\lambda]=0\,,$$

that is to say

$$\begin{aligned}&2\mathrm{Re}(\delta f^*\partial_{f^*}\mathcal{E}(f,\gamma,\alpha)+\delta\alpha^*\partial_{\alpha^*}\mathcal{E}(f,\gamma,\alpha))+\mathrm{Tr}[\partial_\gamma\mathcal{E}(f,\gamma,\alpha)\delta\gamma]\\&+\mathrm{Tr}[(\delta\gamma+\delta\gamma\,\gamma+\gamma\,\delta\gamma-(\delta\alpha^*\otimes\mathbf{1}_\mathfrak{h})(\mathbf{1}_\mathfrak{h}\otimes\alpha)-(\alpha^*\otimes\mathbf{1}_\mathfrak{h})(\mathbf{1}_\mathfrak{h}\otimes\delta\alpha))\lambda]=0\,.\end{aligned}$$

This is equivalent to Equations (VIII.68), (VIII.69) and

$$\lambda(\frac{1}{2}+\gamma)+(\frac{1}{2}+\gamma)\lambda = M(\gamma,\vec{u}) + (\vec{G}+\vec{k}f)\cdot(\vec{G}+\vec{k}f)^* \tag{VIII.74}$$

Using again Proposition VIII.10 we get that Equation (VIII.74) is equivalent to Equation (VIII.71).
For the invertibility of $\mathcal{A}(\lambda)$ note that

$$\begin{aligned}\mathcal{A}(\lambda) &= \frac{1}{4}(\vec{k}\otimes\mathbf{1}+\mathbf{1}\otimes\vec{k})^{\cdot 2} + (|\vec{k}| - \vec{k}.\vec{p} + \lambda - \frac{1}{2}|\vec{k}|^2 - |\vec{k}| + \vec{k}\cdot\vec{p})\vee\mathbf{1}\\ &\geq (\frac{\sigma}{2} - \lambda - \|(|\vec{k}|^2/2 + |\vec{k}| - \vec{p}\cdot\vec{k})\|_{\mathcal{B}})\,\mathbf{1}\vee\mathbf{1}\,.\end{aligned}$$

For $M(\gamma,\vec{u})$, $M(\gamma,\vec{u}) = \frac{1}{2}|\vec{k}|^2 + |\vec{k}| - \vec{k}\cdot\vec{u} + \vec{k}\cdot\gamma\vec{k} \geq \sigma/2$ if $\gamma\geq 0$ and $|\vec{u}|<1/2$. □

Let us recall a well known expression for the solution of the Sylvester or Lyapunov equation.

Proposition VIII.10. *Let A and B be bounded self-adjoint operators on a Hilbert space. Suppose $A\geq a\,\mathbf{1}$ with $a>0$. Then the equation*

$$AX + XA = B$$

for X a bounded operator has a unique solution $\chi_A(B) = \int_0^\infty e^{-tA}Be^{-tA}dt$. If B a trace class operator then the solution X is also trace class.

Proof. Indeed, $\chi_A(B)$ is a solution because

$$\begin{aligned}A\chi_A(B)+\chi_A(B)A &= \int_0^\infty e^{-tA}(AB+BA)e^{-tA}dt\\ &= -\int_0^\infty \frac{d}{dt}(e^{-tA}Be^{-tA})dt = B\,.\end{aligned}$$

Conversely, suppose that $AX+XA=B$, then

$$\begin{aligned}\chi_A(B) &= \int_0^\infty e^{-tA}(AX+XA)e^{-tA}dt\\ &= -\int_0^\infty \frac{d}{dt}(e^{-tA}Xe^{-tA})dt = X\,,\end{aligned}$$

and thus any solution X is equal to $\chi_A(B)$. Hence the solution is unique. □

A Equivalent Characterizations of Centered Quasifree Density Matrices

In this appendix we give various equivalent characterizations of quasifree states. In particular we remark that (ii) in Lemma A.1 below corresponds to the definition of quasifree states in terms of Wick's Theorem.

LEMMA A.1. *Let $\rho \in \mathfrak{cDM}$ be a centered density matrix and denote $\langle A \rangle_\rho := \mathrm{Tr}_{\mathfrak{F}}\{\rho A\}$. Then $(i) \Leftrightarrow (ii) \Leftrightarrow (iii)$, where*

(i) $\rho \in \mathfrak{cQF}$ *is centered and quasifree;*

(ii) All odd correlation functions and all even truncated correlation functions of ρ vanish, i.e., for all $N \in \mathbb{N}$ and $\varphi_1, \ldots, \varphi_{2N} \in \mathfrak{h}$, let either $b_n := a^*(\varphi_n)$ or $b_n := a(\varphi_n)$, for all $1 \leq n \leq 2N$. Then $\langle b_1 \cdots b_{2N-1} \rangle_\rho = 0$ and

$$\left\langle b_1 \, b_2 \cdots b_{2N} \right\rangle_\rho \; = \sum_{\pi \in \mathfrak{P}_{2N}} \left\langle b_{\pi(1)} \, b_{\pi(2)} \right\rangle_\rho \cdots \left\langle b_{\pi(2N-1)} \, b_{\pi(2N)} \right\rangle_\rho, \quad \text{(A.75)}$$

where $\mathfrak{P}_{2N}$ denotes the set of pairings, i.e., the set of all permutations $\pi \in \mathfrak{S}_{2N}$ of $2N$ elements such that $\pi(2n-1) < \pi(2n+1)$ and $\pi(2n-1) < \pi(2n)$, for all $1 \leq n \leq N-1$ and $1 \leq n \leq N$, respectively.

(iii) There exist two commuting quadratic, semibounded Hamiltonians

$$H \; = \sum_{i,j} \Big\{ B_{i,j} \, a^*(\psi_i) \, a(\psi_j) \; + \; C_{i,j} a^*(\psi_i) \, a^*(\psi_j) \; + \; \overline{C_{i,j}} a(\psi_i) \, a(\psi_j) \Big\} \quad \text{(A.76)}$$

$$H' \; = \sum_{i,j} \Big\{ B'_{i,j} \, a^*(\psi_i) \, a(\psi_j) \; + \; C'_{i,j} a^*(\psi_i) \, a^*(\psi_j) \; + \; \overline{C'_{i,j}} a(\psi_i) \, a(\psi_j) \Big\} \quad \text{(A.77)}$$

with $B = B^* \geq 0$, $C = C^T \in \mathcal{L}^2(\mathfrak{h})$, where $\{\psi_i\}_{i \in \mathbb{N}} \subseteq \mathfrak{h}$ is an orthonormal basis, such that $\exp(-H - \beta H')$ is trace class, for all $\beta < \infty$, and

$$\langle A \rangle_\rho \; = \; \lim_{\beta \to \infty} \left\{ \frac{\mathrm{Tr}_{\mathfrak{F}}[A \, \exp(-H - \beta H')]}{\mathrm{Tr}_{\mathfrak{F}}[\exp(-H - \beta H')]} \right\}, \quad \text{(A.78)}$$

for all $A \in \mathcal{B}(\mathfrak{F})$.

Eq. (II.36) and the vanishing (ii) of the truncated correlation functions of a centered quasifree state imply that any quasifree state $\rho \in \mathfrak{QF}$ is completely determined by its one-point function $\langle a(\varphi) \rangle_\rho$ and its two-point function (one-particle reduced density matrix).

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Volker Bach
Technische Universität Braunschweig
Institut für Analysis und Algebra
Rebenring 31, A 14
38106 Braunschweig
Germany
v.bach@tu-bs.de

Sébastien Breteaux
Technische Universität Braunschweig
Institut für Analysis und Algebra
Rebenring 31, A 14
38106 Braunschweig
Germany
sebastien.breteaux@ens-cachan.org

Tim Tzaneteas
Technische Universität Braunschweig
Institut für Analysis und Algebra
Rebenring 31, A 14
38106 Braunschweig
Germany
timmy.tzaneteas@uni-tuebingen.de