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Michele Correggi, Marco Falconi and Marco Olivieri

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GROUND STATE PROPERTIES IN THE QUASICLASSICAL REGIME

MICHELE CORREGGI, MARCO FALCONI AND MARCO OLIVIERI

We study the ground state energy and ground states of systems coupling nonrelativistic quantum particles and force-carrying Bose fields, such as radiation, in the quasiclassical approximation. The latter is very useful whenever the force-carrying field has a very large number of excitations and thus behaves in a semiclassical way, while the nonrelativistic particles, on the other hand, retain their microscopic features. We prove that the ground state energy of the fully microscopic model converges to that of a nonlinear quasiclassical functional depending on both the particles' wave function and the classical configuration of the field. Equivalently, this energy can be interpreted as the lowest energy of a Pekar-like functional with an effective nonlinear interaction for the particles only. If the particles are confined, the ground state of the microscopic system converges as well, to a probability measure concentrated on the set of minimizers of the quasiclassical energy.

1. Introduction and main results

The description and rigorous derivation of effective models for complex quantum systems is a flourishing line of research in modern mathematical physics. Typically, in suitable regimes, the fundamental quantum description can be approximated in terms of some simpler model retaining the salient physical features, but also allowing a more manageable computational or numerical treatment. The questions addressed in this work naturally belong to such a wide class of problems.

We consider indeed a quantum system composed of N nonrelativistic particles interacting with a quantized bosonic field in the *quasiclassical regime*. We refer to [Carlone et al. 2021; Correggi and Falconi 2018; Correggi et al. 2019; 2023] for a detailed discussion of such a regime: in extreme synthesis, we plan to study field configurations with a suitable semiclassical behavior. We require indeed that there is a large number of field excitations, although each one of the latter is carrying a very small amount of energy, in such a way that the field's degrees of freedom are almost classical. More precisely, we assume that the average number of force carriers $\langle \mathcal{N} \rangle$ is of order $1/\varepsilon$, for some $0 < \varepsilon \ll 1$, and thus much larger than the commutator between $a^\dagger$ and a, which is of order 1 (we use units in which $\hbar = 1$). Concretely, this can be realized by rescaling the canonical variables $a^\dagger$ and a by $\sqrt{\varepsilon}$, i.e., setting $a_\varepsilon^\sharp := \sqrt{\varepsilon} a^\sharp$, which leads to

$$[a_\varepsilon(\boldsymbol{k}), a_\varepsilon^\dagger(\boldsymbol{k}')] = \varepsilon \delta(\boldsymbol{k} - \boldsymbol{k}'), \quad \varepsilon \ll 1. \tag{1-1}$$

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On the other hand, the degrees of freedom associated with the particles are not affected by the scaling limit $\varepsilon \to 0$ and the particles remain quantum. Our goal is precisely to set up and rigorously derive an effective quantum model for the lowest energy state of the system in the quasiclassical regime $\varepsilon \to 0$, when the field becomes classical.

Let us now describe in more detail the type of microscopic models we plan to address. The space of states of the full system is[1]

$$\mathscr{H}_\varepsilon := L^2(\mathbb{R}^{dN}) \otimes \mathcal{G}_\varepsilon(\mathfrak{h}), \tag{1-2}$$

where $d \in \{1, 2, 3\}$, the single one-excitation space of the field is $\mathfrak{h}$ and $\mathcal{G}_\varepsilon$ stands for the second quantization map, so that $\mathcal{G}_\varepsilon(\mathfrak{h})$ is the bosonic Fock space constructed over $\mathfrak{h}$ with canonical commutation relations

$$[a_\varepsilon(\xi), a_\varepsilon^\dagger(\eta)] = \varepsilon \langle \xi | \eta \rangle_{\mathfrak{h}}, \tag{1-3}$$

for any $\xi, \eta \in \mathfrak{h}$.

The energy of the microscopic system and thus its Hamiltonian is given by the nonrelativistic energy of the particles, the field energy and the interaction between the particles and the field, in such a way that

- the particle and field energies are a priori of the same order $\mathcal{O}(1)$;
- the interaction is weak, i.e., a priori subleading with respect to the unperturbed energies.

This is concretely realized by considering Hamiltonians of the form

$$H_\varepsilon = \mathcal{K}_0 \otimes 1 + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega) + H_I, \tag{1-4}$$

where:

- $\mathcal{K}_0$ is the (ε-independent) free particle Hamiltonian
$$\mathcal{K}_0 = \sum_{j=1}^{N} (-\Delta_j) + \mathcal{W}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) \tag{1-5}$$
which is assumed to be self-adjoint and bounded from below;
- $\mathrm{d}\mathcal{G}_\varepsilon(\omega)$ is the free field energy and is the second quantization of the positive operator ω on $\mathfrak{h}$, admitting a possibly unbounded inverse ω^{-1};
- the interaction H_I is the only nonfactorized term of the Hamiltonian, it depends on ε only through the creation and annihilation operators $a_\varepsilon^\sharp$ and it is a polynomial of such operators of order between one and two.

Such requests meet the scaling conditions mentioned above. Indeed, assuming that the average number $\langle \mathcal{N} \rangle$ of bare excitations of the field is $\mathcal{O}(\varepsilon^{-1})$, the field energy is of order $\varepsilon \langle \mathcal{N} \rangle = \mathcal{O}(1)$, due to the rescaling of $a_\varepsilon^\dagger$ and a_ε. For the same reason and since the interaction is at least of order 1 in the creation and annihilation operators, we have that H_I is of order $\mathcal{O}(\sqrt{\varepsilon})$, i.e., a priori subleading with respect to the rest of H_ε.

[1]We do not take into account the spin degrees of freedom nor the symmetry constraints induced by the presence of identical particles, but such features can be included in the discussion without any effort and the results trivially apply to the corresponding models. In fact, we may even allow for a coupling term between the radiation field and the particle spins [Correggi et al. 2019], as the one often included in the Pauli–Fierz model.

The specific models we consider in the following are:

(a) the *Nelson model* [Nelson 1964]: the coupling in H_I is simply linear, i.e.,

$$H_I = \sum_{j=1}^{N} A_\varepsilon(\boldsymbol{x}_j), \tag{1-6}$$

where

$$A_\varepsilon(\boldsymbol{x}) := a_\varepsilon^\dagger(\boldsymbol{\lambda}(\boldsymbol{x})) + a_\varepsilon(\boldsymbol{\lambda}(\boldsymbol{x})) \tag{1-7}$$

is the field operator and

$$\lambda,\ \omega^{-1/2}\lambda \in L^\infty(\mathbb{R}^3; \mathfrak{h}) \tag{1-8}$$

(a typical choice is $\mathfrak{h} = L^2(\mathbb{R}^d)$, ω a multiplication operator such that $\omega(\boldsymbol{k}) \geq 0$ and also $\lambda(\boldsymbol{x}; \boldsymbol{k}) = \lambda_0(\boldsymbol{k})e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}$, with $\lambda_0, \omega^{-1/2}\lambda_0 \in \mathfrak{h}$);

(b) the *Fröhlich polaron* [Fröhlich 1937]: a variant of the Nelson model where $\mathfrak{h} = L^2(\mathbb{R}^d)$, $\omega = 1$ and

$$\lambda(\boldsymbol{x}; \boldsymbol{k}) = \sqrt{\alpha}\,\frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}}{|\boldsymbol{k}|^{(d-1)/2}}, \tag{1-9}$$

for some $\alpha > 0$;

(c) the *Pauli–Fierz model* [Pauli and Fierz 1938]: the most elaborate model and we consider only its three-dimensional realization, namely $d = 3$; the interaction is provided by the minimal coupling

$$H_\varepsilon = \sum_{j=1}^{N} \frac{1}{2m_j}(-i\nabla_j + e\boldsymbol{A}_{\varepsilon,j}(\boldsymbol{x}_j))^2 + \mathcal{W}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega), \tag{1-10}$$

where $\omega \geq 0$, $m_j > 0$, $j = 1, \ldots, N$, and e are the particles' masses and charge, respectively, and the field operators $\boldsymbol{A}_{\varepsilon,j}$, $j = 1, \ldots, N$, have here the same formal expression as in (1-7) but $\boldsymbol{\lambda}_j = (\lambda_{j,1}, \lambda_{j,2}, \lambda_{j,3})$, with

$$\lambda_{j,\ell},\ \omega^{\pm 1/2}\lambda_{j,\ell} \in L^\infty(\mathbb{R}^3; \mathfrak{h}), \tag{1-11}$$

is a vector function to account for the electromagnetic polarizations and the charge distributions of the particles (the standard choice is, indeed, $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C}^2)$) and we fix for convenience the gauge to be Coulomb's gauge, i.e., $\nabla_j \cdot \boldsymbol{\lambda}_j = 0$.

The physical meaning of the three models above is quite different and we refer, e.g., to the monograph [Spohn 2004] for a detailed discussion. The Nelson model is the simplest and can be applied to model nucleons interacting with a meson field or, in first approximation, to model the interaction of particles with radiation fields, although the case of the electromagnetic field is typically described through the Pauli–Fierz model. The polaron, on the other hand, provides an effective description of quantum particles in a phonon field, e.g., generated by the vibrational models of a crystal. Note also that the quasiclassical limit $\varepsilon \to 0$ itself can have different interpretations in each model. For instance, in the framework of the polaron model, it can be reformulated as a *strong coupling limit*, which has recently attracted a lot of attention; see, e.g., [Frank and Gang 2020; Griesemer 2017; Leopold et al. 2021; Lieb and Seiringer 2020; Mitrouskas 2021].

In the Nelson and Pauli–Fierz Hamiltonians, there is an ultraviolet regularization, made apparent in the assumptions on λ; we do not consider here the renormalization procedure to remove such ultraviolet cut-off, even if for the Nelson model it is possible to perform it rigorously. We plan to address such a problem in a future work. We also skip at this stage the discussion of the well-posedness of such models (see Sections 4A–4C for further details), but we point out that, with the assumptions made, the operator (1-4) is self-adjoint and bounded from below in each model.

The main problem we study concerns the behavior of the ground state of the microscopic Hamiltonian H_ε in the quasiclassical limit $\varepsilon \to 0$ and, more precisely, we investigate the convergence in the same limit of the bottom of the spectrum

$$E_\varepsilon := \inf \sigma(H_\varepsilon) = \inf_{\Gamma_\varepsilon \in \mathscr{L}^1(\mathscr{H}_\varepsilon), \|\Gamma_\varepsilon\|_1 = 1} \operatorname{tr}(H_\varepsilon \Gamma_\varepsilon) \tag{1-12}$$

of H_ε as well as the limiting behavior of any corresponding *approximate ground state* or *minimizing sequence* $\Psi_{\varepsilon,\delta} \in \mathscr{D}(H_\varepsilon)$ satisfying

$$\langle \Psi_{\varepsilon,\delta} | H_\varepsilon | \Psi_{\varepsilon,\delta} \rangle_{\mathscr{H}_\varepsilon} < E_\varepsilon + \delta, \tag{1-13}$$

for some small $\delta > 0$.

We state our main results with all details in Section 1C. After a brief outlook on the existing literature in Section 1A, we first introduce and discuss the quasiclassical variational problems in Section 1B. In the rest of the paper, we present the proofs.

1A. ***State of the art.*** Our paper fits within the framework of infinite-dimensional semiclassical analysis, which was introduced in the series of works [Ammari and Nier 2008; 2009; 2011; 2015] and further discussed in [Falconi 2018a; 2018b]. Apart from the aforementioned works on quasiclassical analysis, semiclassical techniques have already been used in the study of variational problems, both for systems with creation and annihilation of particles [Ammari and Falconi 2014] and for systems with many bosons, using a slightly different approach called quantum de Finetti theorem; see [Lewin et al. 2014; 2015; 2016]. We also point out that partially classical regimes have already been explored in [Amour and Nourrigat 2015; Amour et al. 2017; 2019; Ginibre et al. 2006], although in other contexts and with different purposes.

The question of the ground state energy convergence in the quasiclassical regime has partially been addressed in [Correggi and Falconi 2018] and [Correggi et al. 2019] for the Nelson and polaron models and the Pauli–Fierz model, respectively. In fact, Theorem 1.3 below completes and extends the corresponding results proven in [Correggi and Falconi 2018, Theorem 2.4] and [Correggi et al. 2019, Theorem 1.9]. More precisely, we develop a more general and self-contained proof strategy, based on the new mathematical structure of *quasiclassical Wigner measures* first introduced in [Correggi et al. 2023], allowing us to relax the assumptions on the microscopic models and taking into account more general settings.

On the other hand, the convergence of microscopic ground states and minimizing sequences in the quasiclassical regime is studied here for the first time; see Theorems 1.7 and 1.15 below. Let us point out that our results *do not require* the existence of a microscopic ground state (and imply the existence of quasiclassical minimizers), although in the presence of the latter they become more transparent. In fact, the problem of the ground state existence in quantum field theory is tricky and has been extensively studied in the past. We refer to [Abdesselam and Hasler 2012; Arai 2001; Arai et al. 1999; Betz et al. 2002; Dereziński 2003; Georgescu et al. 2004; Gérard 2000; Gérard et al. 2011; Griesemer et al. 2001; Hirokawa 2006; Hiroshima 2001; Hiroshima and Matte 2022; Møller 2005; Pizzo 2003] for a detailed discussion of the problem.

1B. ***Quasiclassical variational problems.*** As discussed in detail in [Correggi and Falconi 2018; Correggi et al. 2019; 2023], each of the microscopic models introduced so far admits a quasiclassical counterpart in the limit $\varepsilon \to 0$. More precisely, both their stationary [Correggi and Falconi 2018; Correggi et al. 2019] and dynamical [Correggi et al. 2023] properties can be approximated in such a regime in terms of effective models, where the quantum particle system is driven by a classical field, which in turn is the classical counterpart of the quantized field. In extreme synthesis, the quantum field operator gets replaced by a classical field, which is just a function on $\mathbb{R}^d$, and the interaction term H_I in H_ε gives rise to a potential $\mathcal{V}_z$ depending on the classical field configuration $z \in \mathfrak{h}$. Concretely, the quasiclassical effective Hamiltonian reads

$$\mathcal{H}_z = \mathcal{K}_0 + \sum_{j=1}^{N} \mathcal{V}_z(\boldsymbol{x}_j) + \langle z|\omega|z\rangle_{\mathfrak{h}}, \tag{1-14}$$

and it is self-adjoint on some dense $\mathscr{D} \subset L^2(\mathbb{R}^{dN})$ for any $z \in \mathfrak{h}$; see [Correggi and Falconi 2018, Theorems 2.1–2.3] and [Correggi et al. 2019, Theorem 1.1]. In each model the explicit expression of such an effective potential can be identified explicitly:

(a) In the Nelson model, each particle feels a potential of the form

$$\mathcal{V}_z(\boldsymbol{x}) = 2\mathrm{Re}\langle z|\lambda(\boldsymbol{x})\rangle_{\mathfrak{h}} \in \mathscr{B}(L^2(\mathbb{R}^d)); \tag{1-15}$$

(b) For the polaron, the formal expression of the potential $\mathcal{V}_z$ is the same as in (1-15) above, although, since (1-9) does not belong to $L^\infty(\mathbb{R}^d; \mathfrak{h})$, the expression on the right-hand side must be interpreted in the proper way (see Section 4B); in addition, the obtained potential is no longer bounded but it is infinitesimally form-bounded with respect to $-\Delta$;

(c) In the Pauli–Fierz model, the effective operator is obtained via the replacement of the field $\boldsymbol{A}_\varepsilon$ by its classical counterpart $\boldsymbol{a}_z(\boldsymbol{x}) = 2\mathrm{Re}\langle z|\boldsymbol{\lambda}(\boldsymbol{x})\rangle_{\mathfrak{h}}$, which is continuous and vanishing at ∞ (see [Correggi et al. 2019, Remark 1.5]), and thus, in order to recover the expression (1-14), $\mathcal{V}_z$ must be the operator

$$\mathcal{V}_z(\boldsymbol{x}) = 2\sum_{j=1}^{N} \frac{1}{m_j}[-ie\mathrm{Re}\langle z|\boldsymbol{\lambda}_j(\boldsymbol{x})\rangle_{\mathfrak{h}} \cdot \nabla_j + e^2(\mathrm{Re}\langle z|\boldsymbol{\lambda}_j(\boldsymbol{x})\rangle_{\mathfrak{h}})^2]. \tag{1-16}$$

Note that in case (c) the effective operator can in fact be simply rewritten as[2]

$$\mathcal{H}_z = \sum_{j=1}^{N} \frac{1}{2m_j}(-i\nabla_j + e\boldsymbol{a}_z(\boldsymbol{x}_j))^2 + \mathcal{W}(\boldsymbol{X}) + \langle z|\omega|z\rangle_{\mathfrak{h}}. \tag{1-17}$$

[2] We use the compact notation $\boldsymbol{X} := (\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \in \mathbb{R}^{dN}$.

We can now define the effective quasiclassical ground state energy in terms of the energy functional

$$\mathcal{E}_{\mathrm{qc}}[\psi, z] := \langle \psi | \mathcal{H}_z | \psi \rangle_{L^2(\mathbb{R}^{dN})}, \quad (\psi, z) \in L^2(\mathbb{R}^{dN}) \oplus \mathfrak{h}_\omega, \tag{1-18}$$

as

$$E_{\mathrm{qc}} := \inf_{(\psi,z)\in\mathscr{D}_{\mathrm{qc}}} \mathcal{E}[\psi, z], \tag{1-19}$$

where

$$\mathscr{D}_{\mathrm{qc}} := \{(\psi, z) \in L^2(\mathbb{R}^{dN}) \oplus \mathfrak{h}_\omega : \|\psi\|_2 = 1,\ |\mathcal{E}_{\mathrm{qc}}[\psi, z]| < +\infty\}. \tag{1-20}$$

Here, $\mathfrak{h}_\omega$ is the Hilbert completion of $\bigcap_{k\in\mathbb{N}} \mathscr{D}(\omega^k)$ with respect to the scalar product $\langle \cdot | \cdot \rangle_{\mathfrak{h}_\omega} := \langle \cdot | \omega | \cdot \rangle_{\mathfrak{h}}$, i.e.,

$$\mathfrak{h}_\omega := \overline{\bigcap_{k\in\mathbb{N}} \mathscr{D}(\omega^k)}^{\langle \cdot | \cdot \rangle_{\mathfrak{h}_\omega}}. \tag{1-21}$$

We denote by $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}_{\mathrm{qc}}$ a corresponding minimizing configuration (if any), i.e., such that

$$E_{\mathrm{qc}} = \mathcal{E}_{\mathrm{qc}}[\psi_{\mathrm{qc}}, z_{\mathrm{qc}}]. \tag{1-22}$$

Concretely, the functional $\mathcal{E}_{\mathrm{qc}}$ plays the role of the *quasiclassical energy* of the system under consideration. However, the reader should be careful and be aware that $\mathcal{H}_z$ *is not* the Hamiltonian energy of the whole system: the complete environment-small system evolution is indeed not of Hamiltonian type. For each fixed $z \in \mathfrak{h}_\omega$, the Hamilton–Jacobi equations of $\mathcal{E}_{\mathrm{qc}}[\psi, z]$, with respect to the (complex) ψ variable, yield the dynamics of the small system; the environment on the other hand is stationary in the problems under consideration in this paper; see [Correggi et al. 2023] for a detailed analysis of quasiclassical dynamical systems.

The preliminary questions to address towards the derivation of the above quasiclassical effective models are whether such models are stable and, if this is the case, whether a minimizing configuration does exist: explicitly,

$$\text{“Is } E_{\mathrm{qc}} \text{ greater than } -\infty\text{?” (stability),} \tag{VP1}$$

$$\text{“Does there exist } (\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}_{\mathrm{qc}} \text{ such that } \mathcal{E}_{\mathrm{qc}}(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) = E_{\mathrm{qc}}\text{?” (existence of a ground state).} \tag{VP2}$$

Note that any critical point $(\psi, z) \in \mathscr{D}_{\mathrm{qc}}$ of the functional $\mathcal{E}_{\mathrm{qc}}[\psi, z]$ must satisfy the condition

$$\delta_{(\psi,z)}\big[\mathcal{E}_{\mathrm{qc}}[\psi, z] - \epsilon \|\psi\|_2^2\big] = 0,$$

which yields the Euler–Lagrange equations

$$\begin{cases} \mathcal{H}_z \psi = \epsilon \psi, \\ \omega z + \big\langle \psi \big| \partial_{\bar z} \sum_j \mathcal{V}_z(\boldsymbol{x}_j) \big| \psi \big\rangle_{L^2(\mathbb{R}^{dN})} = 0, \end{cases} \tag{1-23}$$

where the Lagrange multiplier $\epsilon = \langle \psi | H_z | \psi \rangle \in \mathbb{R}$ takes into account the normalization constraint on ψ. We anticipate that a consequence of the convergence of the microscopic ground state, stated in Corollary 1.10, is that, under suitable assumptions on $\mathcal{K}_0$ (for instance if $\mathcal{W}$ is trapping), the answer to both questions in (VP1) and (VP2) is positive and, in particular, the set of minimizers is not empty.

The variational problem above is strictly related to the more general issue of rigorous derivation of effective theories, since, at least for the polaron model, it is known that the minimization of the microscopic energy can be approximated in the limit $\varepsilon \to 0$ in terms of a nonlinear problem on ψ alone. Indeed, focusing on the particle system, one can naturally approach (1-19) in a different and a priori inequivalent way, i.e., *first* one gets rid of the classical field by minimizing over $z \in \mathfrak{h}_\omega$ and *then* investigates the minimization of the remaining functional on ψ, which is obviously nonlinear, since the minimizing z depends on ψ itself. As anticipated, this strategy has been already followed in the literature in the case of the polaron in the strong coupling regime, leading to the *Pekar functional* and the corresponding variational problem [Donsker and Varadhan 1983; Lieb and Thomas 1997; Pekar 1954]. Such a feature is however not exclusive of the polaron and can be observed in all the models mentioned above: we present below a formal derivation of a Pekar-like functional $\mathcal{E}_{\mathrm{Pekar}}[\psi]$ for both the Nelson and polaron model. The Pauli–Fierz case is also discussed below; let us remark however that in this case such a procedure does not yield an explicit nonlinear functional of ψ (see (1-34) below), because it is in general not possible to solve explicitly the variational equation expressing the minimizing z in terms of ψ.

The formal procedure goes as follows: solving the critical point condition $\delta_z \mathcal{E}_{\mathrm{qc}} = 0$ with respect to the variable z for fixed ψ, we find some z_ψ, that we can plug into $\mathcal{E}_{\mathrm{qc}}$, thus obtaining the Pekar energy

$$\mathcal{E}_{\mathrm{Pekar}}[\psi] := \mathcal{E}_{\mathrm{qc}}[\psi, z_\psi].$$

Such a scheme can be made to work rigorously for the polaron (case (b)) with some care, but the variable z is not the right one to consider in cases (a) and (c). Under the assumptions we have made — recall in particular (1-8) and (1-11) — it is indeed more natural to set, since $z \in \mathfrak{h}_\omega$,

$$\eta := \omega^{1/2} z, \tag{1-24}$$

(note however that in case (b) $\eta = z$) and consider the functional $\mathcal{F}_{\mathrm{qc}}[\psi, \eta] := \mathcal{E}_{\mathrm{qc}}[\psi, \omega^{-1/2}\eta]$, which in case (a) reads

$$\begin{aligned}\mathcal{F}_{\mathrm{qc}}[\psi, \eta] &= \left\langle \psi \middle| \mathcal{K}_0 + 2\mathrm{Re} \sum_j \langle \eta | \omega^{-1/2} \lambda(\boldsymbol{x}_j) \rangle_{\mathfrak{h}} \middle| \psi \right\rangle_{L^2(\mathbb{R}^{dN})} + \|\eta\|_{\mathfrak{h}}^2 \\ &= \langle \psi | \mathcal{K}_0 | \psi \rangle_{L^2(\mathbb{R}^{dN})} + 2\mathrm{Re} \big\langle \eta \big| \langle \psi | \Lambda | \psi \rangle_{L^2(\mathbb{R}^{dN})} \big\rangle_{\mathfrak{h}} + \|\eta\|_{\mathfrak{h}}^2,\end{aligned} \tag{1-25}$$

where $\Lambda \in L^\infty(\mathbb{R}^{dN}; \mathfrak{H})$ is given by

$$\Lambda(\boldsymbol{X}) := \sum_{j=1}^{N} (\omega^{-1/2}\lambda)(\boldsymbol{x}_j)$$

(recall the assumption (1-8) on λ) and we have exploited the linearity of the scalar product. Taking the functional derivative with respect to η, we get the Euler–Lagrange equation for the minimization of the above energy with respect to $\eta \in \mathfrak{h}$, i.e.,

$$\eta + \langle \psi | \Lambda(\,\cdot\,) | \psi \rangle_{L^2(\mathbb{R}^{dN})} = 0, \tag{1-26}$$

yielding the minimizing η_{Pekar} written as

$$\eta_{\mathrm{Pekar}}[\psi] = -\sum_{j=1}^{N} \int_{\mathbb{R}^{dN}} \mathrm{d}\boldsymbol{x}_1 \cdots \boldsymbol{x}_N (\omega^{-1/2}\lambda)(\boldsymbol{x}_j) |\psi(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N)|^2, \tag{1-27}$$

which can be easily seen to belong to $\mathfrak{h}$ under the assumptions made. Plugging η_{Pekar} back into (1-25), we get

$$\mathcal{E}_{\mathrm{Pekar}}[\psi] := \inf_{\eta \in \mathfrak{h}} \mathcal{F}_{\mathrm{qc}}[\psi, \eta] = \mathcal{F}_{\mathrm{qc}}[\psi, \eta_{\mathrm{Pekar}}[\psi]] = \langle \psi | \mathcal{K}_0 + \mathcal{V}_{\mathrm{Pekar}} \star |\psi|^2 | \psi \rangle. \tag{1-28}$$

Here we have denoted by $\star$ the action of the integral kernel $\mathcal{V}_{\mathrm{Pekar}}(\boldsymbol{X}, \boldsymbol{Y})$ on $|\psi|^2$, i.e.,

$$(\mathcal{V}_{\mathrm{Pekar}} \star |\psi|^2)(\boldsymbol{X}) := \int_{\mathbb{R}^{dN}} \mathrm{d}\boldsymbol{Y} \, \mathcal{V}_{\mathrm{Pekar}}(\boldsymbol{X}, \boldsymbol{Y}) |\psi(\boldsymbol{Y})|^2, \tag{1-29}$$

and

$$\mathcal{V}_{\mathrm{Pekar}}(\boldsymbol{X}, \boldsymbol{Y}) = -\mathrm{Re} \sum_{i,j=1}^{N} \langle \lambda(\boldsymbol{x}_i) | \omega^{-1} | \lambda(\boldsymbol{y}_j) \rangle_{\mathfrak{h}} \in L^{\infty}(\mathbb{R}^{2dN}). \tag{1-30}$$

Note that in the case of identical particles — either fermionic or bosonic — the above expressions may be conveniently rewritten using the one-particle density $\rho_\psi \in L^1(\mathbb{R}^d)$ associated with ψ, i.e.,

$$\rho_\psi(\boldsymbol{x}) := N \int_{\mathbb{R}^{d(N-1)}} \mathrm{d}\boldsymbol{x}_2 \cdots \mathrm{d}\boldsymbol{x}_N |\Psi(\boldsymbol{x}, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N)|^2. \tag{1-31}$$

Indeed, in this case, (1-27) reads

$$\eta_{\mathrm{Pekar}}[\psi] = -\langle \rho_\psi | (\omega^{-1/2}\lambda)(\,\cdot\,) \rangle_{L^2(\mathbb{R}^d)},$$

and the Pekar energy becomes

$$\mathcal{E}_{\mathrm{Pekar}}[\psi] = \langle \psi | \mathcal{K}_0 | \psi \rangle_{L^2(\mathbb{R}^{dN})} + \langle \rho_\psi | \mathcal{U} | \rho_\psi \rangle_{L^2(\mathbb{R}^d)}, \tag{1-32}$$

where

$$\mathcal{U} = U(\boldsymbol{x}, \boldsymbol{y}) := \langle \lambda(\boldsymbol{x}) | \omega^{-1} | \lambda(\boldsymbol{y}) \rangle_{\mathfrak{h}}, \tag{1-33}$$

which is its typical form in the literature. For instance, in the polaron case, one recovers the self-interacting potential generated by the kernel $\mathcal{U}(\boldsymbol{x} - \boldsymbol{y}) = -\alpha |\boldsymbol{x} - \boldsymbol{y}|^{-1}$.

The above derivation is easily seen to be correct under the assumptions made in case (a). In case (b), however, one cannot apply such a derivation straightforwardly because $\lambda \notin L^{\infty}(\mathbb{R}^{dN}; \mathfrak{h})$, but a simple well-known trick (see Section 4B) allows us to split it into two terms, which can be handled separately as above. In case (c) on the other hand the Pekar functional takes the implicit form

$$\begin{cases} \eta_{\mathrm{Pekar}} + \sum_j \frac{1}{m_j} \langle \psi | e\omega^{-1/2} \boldsymbol{\lambda}_j \cdot (-i\nabla_j) + 2e^2 \omega^{-1/2} \boldsymbol{\lambda}_j \cdot \mathrm{Re} \langle \eta_{\mathrm{Pekar}} | \omega^{-1/2} \boldsymbol{\lambda}_j \rangle_{\mathfrak{h}} | \psi \rangle_{L^2(\mathbb{R}^{3N})} = 0, \\ \mathcal{E}_{\mathrm{Pekar}}[\psi] = \langle \psi | \mathcal{H}_{z_\psi} | \psi \rangle_{L^2(\mathbb{R}^{3N})}, \end{cases} \tag{1-34}$$

where $\mathcal{H}_z$ is given by (1-17), and we set $z_\psi := \omega^{-1/2} \eta_{\mathrm{Pekar}}[\psi]$ for short. As before, all the terms in the first equation belong to $\mathfrak{h}$, thanks to the assumptions on $\boldsymbol{\lambda}_j$ and the fact that any $(\psi, z) \in \mathscr{D}_{\mathrm{qc}}$ is such that

$\psi \in H^1(\mathbb{R}^{3N})$. Furthermore, the last term can be thought of as the action on η_{Pekar} of a linear operator T on $\mathfrak{h}$ whose norm is bounded by

$$2e^2 \sum_{j=1}^{N} \frac{1}{m_j} \|\omega^{-1/2} \boldsymbol{\lambda}_j\|_{\mathfrak{h}}^2,$$

which is smaller than one if e is small enough. In this case, $1+T$ is invertible and there exists a unique solution $\eta_{\text{Pekar}}[\psi] \in \mathfrak{h}$ of the first equation. More generally, existence and uniqueness of $\eta_{\text{Pekar}}[\psi]$ for any value of e follows from the strict convexity of the energy in η; see Remark 1.2 and Lemma 2.4. Note however that unfortunately it is not possible to write explicitly $\mathcal{E}_{\text{Pekar}}$ as a functional of ψ alone, since, due to the presence of an operator — the gradient — one cannot exchange the scalar product in $L^2(\mathbb{R}^{3N})$ with the one in $\mathfrak{h}$, as was done in (1-25). In particular, even for identical particles, the second term in the first equation in (1-34) depends on the reduced density matrix, while the last term is a function of the density alone.

We now define

$$E_{\text{Pekar}} := \inf_{\psi \in \mathscr{D}_{\text{Pekar}}} \mathcal{E}_{\text{Pekar}}[\psi] \tag{1-35}$$

with

$$\mathscr{D}_{\text{Pekar}} := \{\psi \in L^2(\mathbb{R}^{dN}) : \|\psi\|_2 = 1,\ |\mathcal{E}_{\text{Pekar}}[\psi]| < +\infty\}$$

as the ground state energy of the Pekar functionals (1-28) and (1-34), and denote by $\psi_{\text{Pekar}} \in \mathscr{D}_{\text{Pekar}}$ any corresponding minimizer. It is then natural to wonder whether there is any connection between the questions (VP1) and (VP2) and the analogous stability and ground state existence questions for $\mathcal{E}_{\text{Pekar}}$, i.e.,

$$\text{“Is } E_{\text{Pekar}} \text{ greater than } -\infty\text{?”} \tag{VP$'$1}$$

$$\text{“Does there exist } \psi_{\text{Pekar}} \in L^2(\mathbb{R}^{dN}) \text{ such that } \mathcal{E}_{\text{Pekar}}(\psi_{\text{Pekar}}) = E_{\text{Pekar}}\text{?”} \tag{VP$'$2}$$

This is of particular interest for physical applications, since the minimization of the nonlinear functional $\mathcal{E}_{\text{Pekar}}$ may be easier to address also in numerical experiments. A priori however it is not at all obvious that such a relation exists, but in Proposition 1.1 (see Section 2A for the proof) we are going to state that the two variational problems are actually equivalent, which is particularly interesting in case (c) since the explicit form of $\mathcal{E}_{\text{Pekar}}$ is not available.

Proposition 1.1 (equivalence of variational problems). *Under the assumptions made above*,

$$E_{\text{Pekar}} = E_{\text{qc}} > -\infty. \tag{1-36}$$

Furthermore, *if* $(\psi_{\text{qc}}, z_{\text{qc}}) \in \mathscr{D}_{\text{qc}}$ *is a minimizer of* $\mathcal{E}_{\text{qc}}[\psi, z]$, *then*

$$\mathcal{E}_{\text{Pekar}}[\psi_{\text{qc}}] = E_{\text{Pekar}}. \tag{1-37}$$

Conversely, *if* ψ_{Pekar} *is a minimizer of* $\mathcal{E}_{\text{Pekar}}[\psi]$, *then* $\eta_{\text{Pekar}}[\psi_{\text{Pekar}}] \in \mathfrak{h}$ *(given by* (1-26) *and* (1-34) *with* $\psi = \psi_{\text{Pekar}}$, *respectively) and*

$$\mathcal{E}[\psi_{\text{Pekar}}, \eta_{\text{Pekar}}] = E_{\text{qc}}. \tag{1-38}$$

Remark 1.2 (uniqueness of η_{Pekar}). We prove in Lemma 2.4 that the quasiclassical functional $\mathcal{F}_{\mathrm{qc}}[\psi, \eta]$ (or, equivalently, $\mathcal{E}_{\mathrm{qc}}[\psi, z]$) is strictly convex in $\eta \in \mathfrak{h}$ for given $\psi \in L^2(\mathbb{R}^{dN})$. Hence, $\eta_{\mathrm{Pekar}}[\psi]$ is unique (for fixed ψ). Note however that the functional $\mathcal{F}_{\mathrm{qc}}$ is not jointly convex in $(|\psi|^2, \eta)$.

1C. *Ground state in the quasiclassical regime.* We can now state in detail our main results. We work with a minimal set of assumptions on the microscopic models, which are the weakest ones guaranteeing the self-adjointness and boundedness from below of the microscopic Hamiltonians.

Assumptions. The following conditions are satisfied:

(A1) The external potential $\mathcal{W}$ is such that[3]

$$\mathcal{W} \in L^1_{\mathrm{loc}}(\mathbb{R}^{dN}; \mathbb{R}^+); \tag{1-39}$$

(A2) the operator ω is positive and admits a possibly unbounded inverse ω^{-1};

(A3) the form factor λ of the microscopic model must satisfy condition (1-8), (1-9) or (1-11) for the Nelson, polaron or Pauli–Fierz models, respectively.

Observe in particular that the quantum potential $\mathcal{W}$ may not be trapping, so that there might not be a ground state for both the microscopic and the macroscopic problems. In some of the results stated below however we are going to assume this explicitly by requiring an additional property of the unperturbed particle operator:

(A4) The operator $\mathcal{K}_0$ has compact resolvent.

We now consider the microscopic ground state energy E_ε defined in (1-12) and its quasiclassical limit. Recall the definition of the quasiclassical energy E_{qc} in (1-19).

Theorem 1.3 (ground state energy). *Under assumptions* (A1), (A2) *and* (A3), *there exists $C < +\infty$ such that $E_\varepsilon > -C$ and*

$$E_\varepsilon \xrightarrow[\varepsilon \to 0]{} E_{\mathrm{qc}}, \tag{1-40}$$

which in particular implies that (VP1) *holds true.*

The proof of the result above is given in Section 3A. Once the energy convergence has been stated, it is natural to ask whether, in the presence of a microscopic approximate ground state $\Psi_{\varepsilon,\delta}$ or ground state $\Psi_{\varepsilon,\mathrm{gs}}$, one can prove a suitable convergence to quasiclassical minimizing sequences or configurations $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}_{\mathrm{qc}}$, respectively. Let us stress that the question of existence of a ground state of the microscopic energy has been widely studied in the literature and there are more restrictive conditions on the models guaranteeing that $E_\varepsilon \in \sigma_{\mathrm{pp}}(H_\varepsilon)$ (see Sections 4A–4C); our results about approximate ground states apply even if the microscopic ground state does not exist, and whenever it exists we are able to provide its quasiclassical characterization.

[3]As anticipated above, it is sufficient to have an unperturbed particle operator which is self-adjoint and bounded from below. For instance, one could extend the results to potentials with a negative part which is Kato-small with respect to the Laplacian. We stick however to (A1) for the sake of concreteness.

In order to properly formulate the convergence, we first need to introduce a key structure in quasiclassical analysis: the *quasiclassical Wigner measures* and their relative topologies. We preliminarily recall the definition of the space $\mathscr{P}(\mathfrak{h}_\omega; L^2(\mathbb{R}^{dN}))$ of *state-valued probability measures* (see [Correggi et al. 2023, Definition 2.1]), given by measures $\mathfrak{m}$ on $\mathfrak{h}_\omega$ taking values in $\mathscr{L}^1_+(L^2(\mathbb{R}^{dN}))$ — the space of positive trace class operators on $L^2(\mathbb{R}^{dN})$ — such that $\mathfrak{m}(\varnothing) = 0$, the measure is unconditionally σ-additive in the trace class norm and $\|\mathfrak{m}(\mathfrak{h}_\omega)\|_{L^2} = 1$. Starting from such a notion, it is possible to construct a theory of integration of functions with values in the space of bounded operators on $L^2(\mathbb{R}^{dN})$ with respect to state-valued measures, so that, for any measurable $\mathcal{B}(z) \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$,

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{m}(z)\mathcal{B}(z) \in \mathscr{L}^1(L^2(\mathbb{R}^{dN})). \tag{1-41}$$

We refer to the Appendix, or to the existing literature (e.g., [Balazard-Konlein 1985; Fermanian-Kammerer and Gérard 2002; Gérard 1991; Gérard et al. 1991; Teufel 2003]) for further details. In particular, we point out that any such state-valued measure $\mathfrak{m}$ admits a Radon–Nikodým decomposition, i.e., there exists a scalar Borel measure $\mu_\mathfrak{m}$ and a $\mu_\mathfrak{m}$-integrable function $\gamma_\mathfrak{m}(z) \in \mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))$ defined a.e. and with values in normalized density matrices, such that

$$\mathrm{d}\mathfrak{m}(z) = \gamma_\mathfrak{m}(z)\mathrm{d}\mu_\mathfrak{m}(z). \tag{1-42}$$

Hence, (1-41) can be rewritten as

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{m}(z)\mathcal{B}(z) = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_\mathfrak{m}(z)\gamma_\mathfrak{m}(z)\mathcal{B}(z). \tag{1-43}$$

Finally, let us denote by $W_\varepsilon(z)$, $z \in \mathfrak{h}$, the Weyl operator constructed over the creation and annihilation operators $a^\sharp_\varepsilon$, i.e.,

$$W_\varepsilon(z) := e^{i(a^\dagger_\varepsilon(z)+a_\varepsilon(z))}. \tag{1-44}$$

Definition 1.4 (quasiclassical Wigner measures). For any family of normalized microscopic states $\{\Psi_\varepsilon\}_{\varepsilon\in(0,1)} \subset \mathscr{H}_\varepsilon$, the associated set of quasiclassical Wigner measures

$$\mathscr{W}(\Psi_\varepsilon, \varepsilon \in (0,1)) \subset \mathscr{P}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))$$

is the subset of all probability measures $\mathfrak{m}$ such that there exists $\{\varepsilon_n\}_{n\in\mathbb{N}}$, $\varepsilon_n \xrightarrow[n\to\infty]{} 0$, so that

$$\Psi_{\varepsilon_n} \xrightarrow[n\to\infty]{\mathrm{qc}} \mathfrak{m}, \tag{1-45}$$

where the above convergence yields, for all $\eta \in \mathscr{D}(\omega^{-1/2})$ and all compact operators $\mathcal{K} \in \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))$,

$$\begin{aligned}\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathcal{K} \otimes W_{\varepsilon_n}(\eta)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} &= \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_\mathfrak{m}(z) e^{2i\mathrm{Re}\langle\eta|z\rangle_\mathfrak{h}} \operatorname{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_\mathfrak{m}(z)\mathcal{K}] \\ &= \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_\mathfrak{m}(z) e^{2i\mathrm{Re}\langle\omega^{-1/2}\eta|\omega^{1/2}z\rangle_\mathfrak{h}} \operatorname{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_\mathfrak{m}(z)\mathcal{K}].\end{aligned} \tag{1-46}$$

Remark 1.5 (measures on $\mathfrak{h}_\omega$ and test functions). A reader familiar with infinite dimensional semiclassical analysis or quasiclassical analysis will find the definition of Wigner measures given here differs slightly from the usual definition [Ammari and Nier 2008; Correggi et al. 2023]. Typically, one considers microscopic states that satisfy a number operator estimate, namely for which the expectation of $\mathrm{d}\mathcal{G}_\varepsilon(1)^c$ is ε-uniformly bounded for some $c > 0$. The corresponding Wigner measures are concentrated on $\mathfrak{h}$ [Ammari and Nier 2008], and it is natural to test the convergence with Weyl operators having arguments $\eta \in \mathfrak{h}$. However, in studying variational problems the number operator estimate may not always be available, in particular whenever the field is massless, such as in electromagnetism (Pauli–Fierz model). In that case, only energy estimates, i.e., involving $\mathrm{d}\mathcal{G}_\varepsilon(\omega)$, are available. The Wigner measures of states satisfying such an energy estimate are concentrated in $\mathfrak{h}_\omega$, and it is natural to test convergence with Weyl operators having arguments $\eta \in \mathscr{D}(\omega^{-1/2})$ belonging to a dense subset of the continuous dual space [Falconi 2018a]. If both the number estimate and the free energy estimate are available, then the measure is concentrated in $\mathfrak{h} \cap \mathfrak{h}_\omega$; this happens for massive fields, where in addition $\mathfrak{h} \cap \mathfrak{h}_\omega = \mathfrak{h}_\omega$. Finally, let us remark as well that in all concrete applications $\mathfrak{h}_\omega$ is in fact the natural domain of definition of the quasiclassical energy $\mathcal{E}_{\mathrm{qc}}$.

The above notion of quasiclassical convergence, defined in (1-46), is however not the only meaningful topology one can consider for sequences of microscopic states. More precisely, the test in (1-46) may be extended to bounded operators, which means that one is considering the weak* topology on $\mathscr{B}(L^2(\mathbb{R}^{dN}))'$ instead of $\mathscr{L}^1(L^2(\mathbb{R}^{dN})) = \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))'$. In this case, the cluster points belong to a larger space than $\mathscr{P}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))$, namely the space of *generalized state-valued measures*; see [Falconi 2018b] for a detailed and more general discussion. We thus introduce the set of positive states $\overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$ in the closure with respect to the weak* topology of the space of trace class operators on $L^2(\mathbb{R}^{dN})$: we denote the action of a functional $F \in \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$ on a bounded operator $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$ by $F[\mathcal{B}] \in \mathbb{C}$ and its norm by

$$\|F\|_{\mathscr{B}'} := \sup_{\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN})),\, \|\mathcal{B}\|=1} |F[\mathcal{B}]|. \tag{1-47}$$

Definition 1.6 (generalized quasiclassical Wigner measures). For any family of normalized microscopic states $\{\Psi_\varepsilon\}_{\varepsilon\in(0,1)} \subset L^2(\mathbb{R}^{dN})_\varepsilon$, the associated set of generalized quasiclassical Wigner measures

$$\mathscr{GW}(\Psi_\varepsilon, \varepsilon \in (0,1)) \subset \mathscr{P}(\mathfrak{h}_\omega; \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN})))$$

is the subset of all probability measures $\mathfrak{n}$ such that there exists $\{\varepsilon_n\}_{n\in\mathbb{N}}$, $\varepsilon_n \xrightarrow[n\to\infty]{} 0$, so that

$$\Psi_{\varepsilon_n} \xrightarrow[n\to\infty]{\mathrm{gqc}} \mathfrak{n}, \tag{1-48}$$

where the above convergence means that, for all $\eta \in \mathscr{D}(\omega^{-1/2})$ and all bounded operators $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$,

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathcal{B} \otimes W_{\varepsilon_n}(\eta) \Psi_{\varepsilon_n} \rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{B}] e^{2i\mathrm{Re}\langle \omega^{-1/2}\eta | \omega^{1/2} z\rangle_{\mathfrak{h}}}. \tag{1-49}$$

We can now formulate the results about the convergence of microscopic minimizing sequences $\Psi_{\varepsilon,\delta}$ and microscopic minimizers $\Psi_{\varepsilon,\mathrm{gs}}$ (for the proofs see Section 3B). We start by stating a stronger result with some additional assumptions on the microscopic models. Without such assumptions we are still able to prove a weaker convergence, but it requires the introduction of a generalized variational problem.

Theorem 1.7 (convergence of approximate ground states (I)). *Under assumptions* (A1), (A2), (A3) *and* (A4), *for any* $\delta > 0$ *and for any family of approximate ground states* $\Psi_{\varepsilon,\delta}$ *satisfying* (1-13), *we have*

$$\mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1)) \neq \varnothing.$$

Moreover, any family of quasiclassical Wigner measures $\{\mathfrak{m}_\delta\}_{\delta>0}$, *with* $\mathfrak{m}_\delta \in \mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1))$ *for any* δ, *is such that, for all* $\delta > 0$, *we have that* $\mathrm{tr}_{L^2(\mathbb{R}^{dN})} \mathfrak{m}_\delta(\mathfrak{h}_\omega) = 1$ *and* $\mathfrak{m}_\delta$ *is an approximate ground state of* $\mathcal{E}_{\mathrm{qc}}[\psi, z]$, *i.e.*,

$$\mathcal{E}_{\mathrm{svm}}[\mathfrak{m}_\delta] := \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}_\delta}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}(\gamma_{\mathfrak{m}_\delta}(z)\mathcal{H}_z) < E_{\mathrm{qc}} + \delta. \tag{1-50}$$

Remark 1.8 (concentration in probability). The result stated in Theorem 1.7 does not imply that the energy $E(z) := \mathrm{tr}_{L^2(\mathbb{R}^{dN})}(\gamma_{\mathfrak{m}_\delta}(z)\mathcal{H}_z)$ is smaller than $E_{\mathrm{qc}}+\delta$ for any $z \in \mathfrak{h}_\omega$. Roughly speaking, there might be a nonzero probability that $\mathfrak{m}_\delta$ is concentrated on pairs $(\psi(z), z)$ with large $\mathcal{E}_{\mathrm{qc}}$ energy. However, $E(z)$ can be much larger than $E_{\mathrm{qc}} + \delta$ only with small $\mu_{\mathfrak{m}_\delta}$-probability. More precisely, for any $k \geq 1$,

$$\mathbb{P}_{\mu_{\mathfrak{m}_\delta}}\{E(z) \geq E_{\mathrm{qc}} + k\delta\} < \frac{1}{k}. \tag{1-51}$$

Corollary 1.9 (convergence to ground states (I)). *If* (A4) *holds, then any quasiclassical Wigner measure* $\mathfrak{m} \in \mathscr{W}(\Psi_{\varepsilon,o_\varepsilon(1)}, \varepsilon \in (0, 1))$, *corresponding to approximate ground states* $\Psi_{\varepsilon,o_\varepsilon(1)}$ *satisfying* (1-13) *with* $\delta = o_\varepsilon(1)$, *is such that* $\mathrm{tr}_{L^2(\mathbb{R}^{dN})} \mathfrak{m}(\mathfrak{h}_\omega) = 1$ *and* $\mathfrak{m}$ *is concentrated on the set of ground states* $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}_{\mathrm{qc}}$ *of* $\mathcal{E}_{\mathrm{qc}}[\psi, z]$. *Consequently,* $\mathcal{E}_{\mathrm{qc}}[\psi, z]$ *has at least one ground state and both* (VP2) *and* (VP′2) *hold true.*

Corollary 1.10 (convergence of ground states (I)). *If* (A4) *holds and* H_ε *has a ground state* $\Psi_{\varepsilon,\mathrm{gs}}$, *then any corresponding quasiclassical Wigner measure* $\mathfrak{m} \in \mathscr{W}(\Psi_{\varepsilon,\mathrm{gs}}, \varepsilon \in (0, 1))$ *is such that* $\mathrm{tr}_{L^2(\mathbb{R}^{dN})} \mathfrak{m}(\mathfrak{h}_\omega) = 1$ *and* $\mathfrak{m}$ *is concentrated on the set of ground states* $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}_{\mathrm{qc}}$ *of* $\mathcal{E}_{\mathrm{qc}}[\psi, z]$.

Remark 1.11 (uniqueness and gauge invariance). Concerning uniqueness, we point out that both the microscopic and the quasiclassical variational problems are gauge invariant, namely the multiplication by a constant phase factor of Ψ or ψ does not change the energy. Hence, even if one could prove uniqueness of the quasiclassical minimizer $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ up to gauge transformations, one could not conclude that the set of limit points $\mathscr{W}(\Psi_{\varepsilon,o_\varepsilon(1)}, \varepsilon \in (0, 1))$ or $\mathscr{W}(\Psi_{\varepsilon,\mathrm{gs}}, \varepsilon \in (0, 1))$ are just given by a Dirac delta measure centered at $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$. Indeed, because of gauge invariance, the quasiclassical Wigner measures would be supported over the unit one-dimensional sphere generated by the configurations $(e^{i\vartheta}\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ with $\vartheta \in \mathbb{R}$.

Remark 1.12 (condition on $\mathcal{K}_0$). The assumption that $\mathcal{K}_0$ has compact resolvent is reasonable, since that is typically the case in which one can also prove the existence of a microscopic minimizer at least for massive systems (see Remark 1.13 below), e.g., in the presence of a trapping potential. However, it is also needed in a technical step in the proof to ensure that there is no loss of mass along the convergence (1-46), i.e., $\mathrm{tr}_{L^2(\mathbb{R}^{dN})} \mathfrak{m}(\mathfrak{h}_\omega) = 1$. Similar assumptions are present also in [Correggi et al. 2023]; see in particular the discussion in [Correggi et al. 2023, Remarks 1.9–1.10 and Section 1.6].

Remark 1.13 (existence of $\Psi_{\varepsilon,\mathrm{gs}}$). In all three cases (a)–(c), if the Bose field is *massive*, i.e., there exists $m > 0$ such that $\omega \geq m > 0$ (which is always the case for the polaron), then it is known [Dereziński and Gérard 1999, Theorem 4.1] that the microscopic Hamiltonian H_ε admits a ground state $\Psi_{\varepsilon,\mathrm{gs}} \in \mathscr{H}_\varepsilon$, if $\mathcal{K}_0$

has compact resolvent. Hence, in the massive case, one can remove the assumption on the existence of $\Psi_{\varepsilon,\mathrm{gs}}$. When the field is *massless*, on the other hand, it is also known that microscopic ground states might not exist or belong to a non-Fock representation of the algebra of observables [Pizzo 2003]. This second case is not covered by Corollary 1.10, but it may be treated with our techniques. We plan to come back to such a question in a future work.

Remark 1.14 (existence of quasiclassical minimizers). Our analysis shows that the quasiclassical energy functionals $\mathcal{E}_{\mathrm{qc}}[\psi, z]$ *always* have at least one minimizer, provided that $\mathcal{K}_0$ has compact resolvent, i.e., provided that the quantum subsystem is trapped. This gives additional evidence that the behavior of the ground state in quantum field theories can differ quite dramatically (nonexistence or non-Fock-representability, see Remark 1.13) from that of their classical and quantum finite-dimensional counterparts.

As anticipated, if we drop the assumption on the operator $\mathcal{K}_0$ there is still convergence, but the variational problem (1-19) has to be generalized: we thus set, for any pure state $\rho \in \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$ and any $z \in \mathfrak{h}_\omega$,

$$\mathcal{E}_{\mathrm{gqc}}[\rho, z] := \rho[\mathcal{H}_z]. \tag{1-52}$$

We consider the corresponding variational problem: setting (recall the definition (1-47))

$$\mathscr{D}_{\mathrm{gqc}} := \{(\rho, z) \in \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN})) \oplus \mathfrak{h}_\omega : \|\rho\|_{\mathscr{B}'} = 1,\ |\rho[\mathcal{H}_z]| < +\infty\}, \tag{1-53}$$

we define

$$E_{\mathrm{gqc}} := \inf_{(\rho,z)\in\mathscr{D}_{\mathrm{gqc}}} \mathcal{E}_{\mathrm{gqc}}[\rho, z], \tag{1-54}$$

and we denote by $(\rho_\delta, z_\delta) \in \mathscr{D}_{\mathrm{gqc}}$ a minimizing sequence satisfying

$$\mathcal{E}_{\mathrm{gqc}}[\rho_\delta, z_\delta] < E_{\mathrm{gqc}} + \delta$$

and by $(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) \in \mathscr{D}_{\mathrm{gqc}}$ any corresponding minimizing configuration.

Theorem 1.15 (convergence of approximate ground states (II)). *Under assumptions* (A1), (A2) *and* (A3), *for any* $\delta > 0$ *and for any family of approximate ground states* $\Psi_{\varepsilon,\delta}$ *satisfying* (1-13), *we have that* $\mathscr{G}\mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0,1)) \neq \varnothing$. *Moreover, any family of generalized quasiclassical Wigner measures* $\{\mathfrak{n}_\delta\}_{\delta>0}$, *with* $\mathfrak{n}_\delta \in \bigcup_{\delta>0} \mathscr{G}\mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0,1))$ *for any* δ, *is such that, for all* $\delta > 0$, *we have that* $\|\mathfrak{n}_\delta(\mathfrak{h}_\omega)\|_{\mathscr{B}'} = 1$ *and* $\mathfrak{n}_\delta$ *is an approximate ground state of* $\mathcal{E}_{\mathrm{gqc}}[\rho, z]$, *i.e.*,

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_\delta(z)[\mathcal{H}_z] < E_{\mathrm{gqc}} + \delta. \tag{1-55}$$

Corollary 1.16 (convergence to ground states (II)). *Any generalized quasiclassical Wigner measure* $\mathfrak{n} \in \mathscr{G}\mathscr{W}(\Psi_{\varepsilon,o_\varepsilon(1)}, \varepsilon \in (0,1))$, *corresponding to approximate ground states* $\Psi_{\varepsilon,o_\varepsilon(1)}$ *satisfying* (1-13) *with* $\delta = o_\varepsilon(1)$, *is such that* $\|\mathfrak{n}(\mathfrak{h}_\omega)\|_{\mathscr{B}'} = 1$ *and* $\mathfrak{n}$ *is concentrated on the set of ground states* $(\varrho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) \in \mathscr{D}_{\mathrm{gqc}}$ *of* $\mathcal{E}_{\mathrm{gqc}}[\varrho, z]$. *Consequently, the functional* $\mathcal{E}_{\mathrm{gqc}}[\rho, z]$ *admits at least one ground state in* $\mathscr{D}_{\mathrm{gqc}}$.

Corollary 1.17 (convergence of ground states (II)). *If* H_ε *has a ground state* $\Psi_{\varepsilon,\mathrm{gs}}$, *then any generalized Wigner measure* $\mathfrak{n} \in \mathscr{G}\mathscr{W}(\Psi_{\varepsilon,\mathrm{gs}}, \varepsilon \in (0,1))$ *is such that* $\|\mathfrak{n}(\mathfrak{h}_\omega)\|_{\mathscr{B}'} = 1$ *and* $\mathfrak{n}$ *is concentrated on the set of ground states* $(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) \in \mathscr{D}_{\mathrm{gqc}}$ *of* $\mathcal{E}_{\mathrm{gqc}}[\rho, z]$.

Remark 1.18 (quasiclassical energy and generalized quasiclassical energy). As proved in Section 2 (see Proposition 2.8),

$$E_{\mathrm{qc}} = E_{\mathrm{gqc}},$$

which is in fact crucial to prove convergence of the ground state energy for systems without trapping on the quantum particles.

2. Quasiclassical minimization problems

Here we consider minimization problems in the quasiclassical setting: we study the functionals introduced in Section 1B and the relative minimizations, but also define and investigate more general problems.

2A. *Quasiclassical functionals, states and related minimization problems.* A quasiclassical system behaves like an open system in which a *classical environment* (of infinite dimension) drives a quantum *small system*, described by a Hilbert space $L^2(\mathbb{R}^{dN})$. The classical environment is described by a space of configurations $\mathfrak{h}_\omega$, usually a complex Hilbert space identifiable with the complex phase space of the environment's degrees of freedom. A probability distribution μ on $\mathfrak{h}_\omega$ tells how probable each environment's configuration is, while a state-valued function $\mathfrak{h}_\omega \ni z \mapsto \gamma(z) \in \mathscr{L}^1_+(L^2(\mathbb{R}^{dN}))$ tells how each environment's configuration drives the small system's quantum state. Analogously, both the value of observables $\mathcal{F}(z)$ and the small system's dynamics $\mathcal{U}_t(z)$ are driven by the environment.

A quasiclassical minimization problem consists of finding the lowest energy and possibly the ground states of a suitable functional $\mathcal{E}[\psi, z] : L^2(\mathbb{R}^{dN}) \oplus \mathfrak{h}_\omega \to \mathbb{R}$ depending on the configuration of both the small system and the environment. The first energy functional to consider is $\mathcal{E}_{\mathrm{qc}}[\psi, z]$, defined in (1-18):

$$\mathcal{E}_{\mathrm{qc}}[\psi, z] := \langle \psi | \mathcal{H}_z | \psi \rangle_{L^2(\mathbb{R}^{dN})}, \qquad (\psi, z) \in \mathscr{D}_{\mathrm{qc}},$$

where $\mathcal{H}_z$ and $\mathscr{D}_{\mathrm{qc}}$ are given in (1-14) and (1-20), respectively. We also recall that the ground state energy and minimizer of $\mathcal{E}_{\mathrm{qc}}$ are denoted by E_{qc} and $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$, respectively.

Although the above is the foremost functional coming to mind in this context, another minimization problem emerges naturally in studying the quasiclassical limit. To this purpose, we recall the notion of a state-valued measure [Correggi et al. 2023; Falconi 2018b], already mentioned in Section 1C: a state-valued *probability* measure $\mathfrak{m} \in \mathscr{P}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))$ is a vector Borel Radon measure on $\mathfrak{h}_\omega$, taking values in the density matrices $\mathscr{L}^1_+(L^2(\mathbb{R}^{dN}))$ of the small system, such that

$$\|\mathfrak{m}(\mathfrak{h}_\omega)\|_{\mathscr{L}^1} = 1. \tag{2-1}$$

Thanks to the Radon–Nikodým property enjoyed by the separable dual space $\mathscr{L}^1(L^2(\mathbb{R}^{dN}))$, it is possible to decompose $\mathfrak{m}$ in a scalar Borel Radon probability measure $\mu_{\mathfrak{m}} \in \mathscr{P}(\mathfrak{h}_\omega)$ such that $\mu_{\mathfrak{m}}(\mathfrak{h}) = 1$, and in an a.e.-defined function (the Radon–Nikodým derivative)

$$\mathfrak{h}_\omega \ni z \mapsto \gamma_{\mathfrak{m}}(z) \in \mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))$$

taking values in the normalized density matrices of the small system:

$$\mathrm{d}\mathfrak{m}(z) = \gamma_{\mathfrak{m}}(z)\mathrm{d}\mu_{\mathfrak{m}}(z).$$

The quasiclassical energy $\mathcal{E}_{\mathrm{qc}}$, constrained to $\|\psi\|_{L^2(\mathbb{R}^{dN})} = 1$, is the expectation of the quasiclassical Hamiltonian $\mathcal{H}_z$. Therefore, its generalization to state-valued measures obviously reads

$$\mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] := \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{H}_z]. \tag{2-2}$$

This leads to the following minimization problem: setting

$$\mathscr{D}_{\mathrm{svm}} := \{\mathfrak{m} \in \mathscr{P}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN}))) : \mathrm{tr}_{L^2(\mathbb{R}^{dN})}\, \mathfrak{m}(\mathfrak{h}_\omega) = 1,\ |\mathcal{E}_{\mathrm{svm}}[\mathfrak{m}]| < +\infty\}, \tag{2-3}$$

we ask (stability)

$$\text{“Is } E_{\mathrm{svm}} := \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] \text{ greater than } -\infty\text{?”} \tag{vp1}$$

and (existence of a ground state)

$$\text{“Does there exist } \mathfrak{m}_{\mathrm{svm}} \in \mathscr{D}_{\mathrm{svm}} \text{ such that } \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}_{\mathrm{svm}}] = E_{\mathrm{svm}}\text{?”} \tag{vp2}$$

A variant of the above problem is obtained by assuming that $\gamma_{\mathfrak{m}}(z) = |\psi\rangle\langle\psi|$ for some $\psi \in L^2(\mathbb{R}^{dN})$ independent of z, in which case the functional depends only on a wave function ψ and a probability measure μ over $\mathfrak{h}_\omega$. We thus set

$$\mathcal{E}_{\mathrm{pm}}[\psi, \mu] := \int_{\mathfrak{h}_\omega} \mathrm{d}\mu(z) \langle\psi|\mathcal{H}_z|\psi\rangle_{L^2(\mathbb{R}^{dN})}. \tag{2-4}$$

The variational problem (stability) reads

$$\text{“Is } E_{\mathrm{pm}} := \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}}} \mathcal{E}_{\mathrm{pm}}[\psi, \mu] \text{ greater than } -\infty\text{?”} \tag{vp$'$1}$$

where

$$\mathscr{D}_{\mathrm{pm}} := \{(\psi, \mu) \in L^2(\mathbb{R}^{dN}) \oplus \mathscr{P}(\mathfrak{h}_\omega) : \|\psi\|_2 = 1,\ \mu(\mathfrak{h}_\omega) = 1,\ |\mathcal{E}_{\mathrm{pm}}[\psi, \mu]| < +\infty\}, \tag{2-5}$$

and (existence of a ground state)

$$\text{“Does there exist } (\psi_{\mathrm{pm}}, \mu_{\mathrm{pm}}) \in \mathscr{D}_{\mathrm{pm}} \text{ such that } \mathcal{E}_{\mathrm{pm}}[(\psi_{\mathrm{pm}}, \mu_{\mathrm{pm}})] = E_{\mathrm{pm}}\text{?”} \tag{vp$'$2}$$

Note that the functional $\mathcal{E}_{\mathrm{qc}}$ and the corresponding variational problems (VP1) and (VP2) are recovered by simply imposing in $\mathcal{E}_{\mathrm{pm}}$ above that μ is a Dirac delta, i.e., there exists $z_0 \in \mathfrak{h}_\omega$ such that $\mu = \delta_{z_0}$. Yet another minimization problem can be formulated by substituting the minimization over $\mathscr{P}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))$ and $\mathscr{P}(\mathfrak{h}_\omega)$ in (2-2) and (2-4) with the one over atomic measures $\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega; \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))$ and $\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)$, respectively.

Finally, in the spirit of derivation of effective functionals of ψ or z alone, as the Pekar-like functionals defined in (1-28) and (1-34), we can also define the effective energy

$$\mathcal{I}[z] := \inf_{\psi\in L^2(\mathbb{R}^{dN}),\, \|\psi\|_2=1} \mathcal{E}_{\mathrm{qc}}[\psi, z]. \tag{2-6}$$

The rest of this section is devoted to proving equivalences between the minimization problems defined above. In fact, the natural variational problem emerging in the quasiclassical limit is the one involving state-valued measures (see (vp1) and (vp2)), however the most relevant from the physical and practical point of view is the one formulated in terms of wave functions and classical fields (see (VP1) and (VP2)). Therefore, the fact that all the infima turn out to be equal (Propositions 2.1 and 2.8) and that the existence of the various minimizers are related (Propositions 2.3 and 2.9) allow us to derive a more concrete physical statement.

Proposition 2.1 (quasiclassical energies). *Under assumptions* (A1), (A2) *and* (A3),

$$E_{\mathrm{qc}} = E_{\mathrm{svm}} = \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] = E_{\mathrm{pm}} = \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\,\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] = E_{\mathrm{Pekar}} = \inf_{z\in\mathfrak{h}_\omega}\mathcal{I}[z]. \tag{2-7}$$

Proof. We use the weak density of atomic scalar measures, supported on a finite number of points, in the space of all finite measures, that holds for $\mathfrak{h}_\omega$ separable [Parthasarathy 1967]. Thanks to that it is possible to prove the following (see [Correggi and Falconi 2018, Lemma 3.20] for a detailed proof):

$$E_{\mathrm{svm}} = \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] = \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}],$$

$$E_{\mathrm{pm}} = \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}}} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] = \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\,\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu].$$

Now, let us prove that

$$\inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] = \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu]. \tag{2-8}$$

Let $\delta > 0$, and let $\mathfrak{m}_\delta = \sum_{k=1}^K \lambda_k\gamma_k\delta_{z_k}$ — with $\lambda_k \geq 0$ (recall that $\mathfrak{m}_\delta$ takes values in positive operators), $\sum_{k=1}^K \lambda_k = 1$ and $\gamma_k \in \mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))$ — be an atomic state-valued measure such that

$$\mathcal{E}_{\mathrm{svm}}[\mathfrak{m}_\delta] = \sum_{k=1}^K \lambda_k \operatorname{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_k\mathcal{H}_{z_k}] < \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] + \delta.$$

For fixed k, since γ_k is a normalized density matrix,

$$\inf_{\psi\in L^2(\mathbb{R}^{dN}),\,\|\psi\|_2=1} \langle\psi|\mathcal{H}_{z_k}|\psi\rangle_{L^2(\mathbb{R}^{dN})} \leq \operatorname{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_k\mathcal{H}_{z_k}].$$

Therefore,

$$\begin{aligned}\inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\,\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] &= \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\,\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \int_{\mathfrak{h}_\omega} \mathrm{d}\mu\langle\psi|\mathcal{H}_z|\psi\rangle_{L^2(\mathbb{R}^{dN})}\\ &\leq \sum_{k=1}^K \lambda_k \inf_{\psi\in L^2(\mathbb{R}^{dN}),\,\|\psi\|_2=1} \langle\psi|\mathcal{H}_{z_k}|\psi\rangle_{L^2(\mathbb{R}^{dN})} \leq \sum_{k=1}^K \lambda_k \operatorname{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_k\mathcal{H}_{z_k}]\\ &< \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] + \delta.\end{aligned} \tag{2-9}$$

Since $\delta > 0$ is arbitrary, we conclude that

$$\inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\,\mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] \leq \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}]. \tag{2-10}$$

To prove the opposite inequality, we follow a similar reasoning. Let $\delta > 0$ and $\mu_\delta = \sum_{k=1}^K \lambda_k\delta_{z_k}$ be a scalar atomic measure and $\psi_{\delta,z_k} \in L^2(\mathbb{R}^{dN})$ a family of normalized wave functions such that $\mu_\delta(\mathfrak{h}_\omega) = 1$

and

$$\sum_{k=1}^{K} \lambda_k \langle \psi_{\delta,z_k} | \mathcal{H}_{z_k} | \psi_{\delta,z_k} \rangle_{L^2(\mathbb{R}^{dN})} < \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] + \delta.$$

Now, $\mathfrak{m}_\delta := \sum_{k=1}^{K} \lambda_k |\psi_{\delta,z_k}\rangle\langle\psi_{\delta,z_k}| \delta_{z_k}$ is an atomic state-valued measure belonging to $\mathscr{D}_{\mathrm{svm}}$. Therefore,

$$\begin{aligned} \inf_{\mathfrak{m}\in\mathscr{D}_{\mathrm{svm}}\cap\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega;\mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))} \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}] \le \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}_\delta] &= \sum_{k=1}^{K} \lambda_k \langle \psi_{\delta,z_k} | \mathcal{H}_{z_k} | \psi_{\delta,z_k} \rangle_{L^2(\mathbb{R}^{dN})} \\ &< \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] + \delta, \end{aligned} \tag{2-11}$$

which yields the desired inequality.

To complete the proof, we show that

$$\inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] = \inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] = E_{\mathrm{Pekar}} = E_{\mathrm{qc}}. \tag{2-12}$$

Let us prove the first equality beforehand. Let $\mu_\delta = \sum_{k=1}^{K} \lambda_k \delta_{z_k}$ be the atomic minimizing family of measures defined before and ψ_{δ,z_k} the corresponding minimizing vectors. Then

$$\begin{aligned} \sum_{k=1}^{K} \lambda_k \inf_{\psi\in L^2(\mathbb{R}^{dN}),\, \|\psi\|_2=1} \langle \psi | \mathcal{H}_{z_k} | \psi \rangle_{L^2(\mathbb{R}^{dN})} &\le \sum_{k=1}^{K} \lambda_k \langle \psi_{\delta,z_k} | \mathcal{H}_{z_k} | \psi_{\delta,z_k} \rangle_{L^2(\mathbb{R}^{dN})} \\ &< \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] + \delta. \end{aligned} \tag{2-13}$$

Since the left-hand side is a convex combination and δ is arbitrary, we immediately deduce that

$$\inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] \le \inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu]. \tag{2-14}$$

On the other hand, since a measure concentrated in a single point is atomic,

$$\inf_{(\psi,\mu)\in\mathscr{D}_{\mathrm{pm}},\, \mu\in\mathscr{P}_{\mathrm{atom}}(\mathfrak{h}_\omega)} \mathcal{E}_{\mathrm{pm}}[\psi,\mu] \le \inf_{z\in\mathfrak{h}_\omega} \inf_{\psi\in L^2(\mathbb{R}^{dN}),\, \|\psi\|_2=1} \mathcal{E}_{\mathrm{qc}}[\psi,z] = \inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z],$$

which implies the first identity in (2-12).

Now, let us prove the second equality above, namely

$$\inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] = E_{\mathrm{Pekar}}. \tag{2-15}$$

Let again $\delta > 0$ and let z_δ be a minimizing family of vectors for $\mathcal{I}$, i.e., such that $\mathcal{I}[z_\delta] < \inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] + \delta$. For each z_δ, let ψ_{δ,z_δ} be a minimizing vector for $\mathcal{E}_{\mathrm{qc}}[\,\cdot\,, z_\delta]$, i.e., such that

$$\mathcal{E}_{\mathrm{qc}}[\psi_{\delta,z_\delta}, z_\delta] < \mathcal{I}[z_\delta] + \delta.$$

Now,

$$E_{\mathrm{Pekar}} \le \mathcal{E}_{\mathrm{Pekar}}[\psi_{\delta,z_\delta}] \le \mathcal{E}_{\mathrm{qc}}[\psi_{\delta,z_\delta}, z_\delta],$$

therefore

$$E_{\mathrm{Pekar}} \le \inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z]. \tag{2-16}$$

On the other hand, let ψ_δ be a minimizing family of states for E_{Pekar}, and, after fixing ψ_δ, let z_{δ,ψ_δ} be a minimizing family for $\mathcal{E}_{\mathrm{qc}}[\psi_\delta, \cdot\,]$:

$$\mathcal{E}_{\mathrm{qc}}[\psi_\delta, z_{\delta,\psi_\delta}] < E_{\mathrm{Pekar}} + \delta. \tag{2-17}$$

As above, we then get

$$\inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] \le \inf_{\psi\in L^2(\mathbb{R}^{dN}),\,\|\psi\|_2=1} \mathcal{E}_{\mathrm{qc}}[\psi, z_{\delta,\psi_\delta}] \le \mathcal{E}_{\mathrm{qc}}[\psi_\delta, z_{\delta,\psi_\delta}] < E_{\mathrm{Pekar}} + \delta,$$

which yields

$$\inf_{z\in\mathfrak{h}_\omega} \mathcal{I}[z] \le E_{\mathrm{Pekar}}. \tag{2-18}$$

Finally, we prove that

$$E_{\mathrm{Pekar}} = E_{\mathrm{qc}}. \tag{2-19}$$

Now, let $(\psi_\delta, z_{\delta,\psi_\delta})$ be as above, i.e., such that (2-17) holds true. Hence,

$$E_{\mathrm{qc}} \le \mathcal{E}_{\mathrm{qc}}[\psi_\delta, z_{\delta,\psi_\delta}] < E_{\mathrm{Pekar}} + \delta,$$

and thus $E_{\mathrm{qc}} \le E_{\mathrm{Pekar}}$. On the other hand, let (ψ_δ, z_δ) be a minimizing family of configurations for $\mathcal{E}_{\mathrm{qc}}$:

$$\mathcal{E}_{\mathrm{qc}}[\psi_\delta, z_\delta] < E_{\mathrm{qc}} + \delta.$$

Clearly, now one has

$$E_{\mathrm{Pekar}} \le \mathcal{E}_{\mathrm{Pekar}}[\psi_\delta] \le \mathcal{E}_{\mathrm{qc}}[\psi_\delta, z_\delta] < E_{\mathrm{qc}} + \delta,$$

yielding the opposite inequality, i.e., $E_{\mathrm{Pekar}} \le E_{\mathrm{qc}}$. □

Remark 2.2 (stability). In the above proof we have implicitly assumed that the energies under considerations are bounded from below, but in fact it is easy to see that, if one of the functionals is unbounded from below, then all the others must be unstable as well. We do not provide any detail of such an argument, because our main result (Theorem 1.3) implies that (VP1) holds true, so that (VP′1), (vp1) and (vp′1) immediately follow.

The other important result concerns equivalences for the existence of minimizers in the variational problems above.

Proposition 2.3 (quasiclassical minimizers). *Under assumptions* (A1), (A2) *and* (A3),

$$\text{(VP2)} \iff \text{(VP}'2) \iff \text{(vp2)} \iff \text{(vp}'2). \tag{2-20}$$

Furthermore, any minimizer $\mathfrak{m}_{\mathrm{svm}}$ *of* (vp2) *is concentrated on the set of minimizers* $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ *of* (VP2).

Proof. Some implications are easy to prove. Let us first prove that (VP2) $\Longrightarrow$ (vp′2). Let $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ be a minimizer of $\mathcal{E}_{\mathrm{qc}}$ in $\mathscr{D}_{\mathrm{qc}}$. Then, evaluating the energy $\mathcal{E}_{\mathrm{pm}}$ on the configuration $(\psi_{\mathrm{qc}}, \mu_0)$, with $\mu_0 = \delta_{z_{\mathrm{qc}}}$, we get

$$\mathcal{E}_{\mathrm{pm}}[\psi_{\mathrm{qc}}, \mu_0] = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_0(z) \mathcal{E}_{\mathrm{qc}}[\psi_{\mathrm{qc}}, z] = \mathcal{E}_{\mathrm{qc}}[\psi_{\mathrm{qc}}, z_{\mathrm{qc}}] = E_{\mathrm{qc}}.$$

By Proposition 2.1, $(\psi_{\mathrm{qc}}, \mu_0)$ thus solves (vp′2). Analogously, let us prove (vp′2) $\Longrightarrow$ (vp2): let $(\psi_{\mathrm{pm}}, \mu_{\mathrm{pm}})$ be a minimizer for (vp′2); then, the state-valued measure $\mathfrak{m}_0$, with $\mu_{\mathfrak{m}_0} = \mu_{\mathrm{pm}}$ and $\gamma_{\mathfrak{m}_0}(z) = |\psi_{\mathrm{pm}}\rangle\langle\psi_{\mathrm{pm}}|$, solves (VP2) by Proposition 2.1.

We prove now that (vp2) $\Longrightarrow$ (VP2). Given a minimizer $\mathfrak{m}_{\mathrm{svm}}$ of $\mathcal{E}_{\mathrm{svm}}$, for $\mu_{\mathfrak{m}_{\mathrm{svm}}}$-a.e. $z \in \mathfrak{h}_\omega$ there exists $\{\lambda_k(z)\}_{k\in\mathbb{N}}$, with $\lambda_k(z) \geq 0$ and $\sum_{k\in\mathbb{N}} \lambda_k(z) = 1$, and $\{\psi_k(z)\}_{k\in\mathbb{N}}$, with $\|\psi_k(z)\|_{L^2(\mathbb{R}^{dN})} = 1$, such that

$$E_{\mathrm{svm}} = \mathcal{E}_{\mathrm{svm}}[\mathfrak{m}_{\mathrm{svm}}] = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}_{\mathrm{svm}}}(z) \sum_{k\in\mathbb{N}} \lambda_k(z) \mathcal{E}_{\mathrm{qc}}[\psi_k(z), z].$$

The above is due to the fact that $\gamma_{\mathfrak{m}_{\mathrm{svm}}}(z)$ is a density matrix on $L^2(\mathbb{R}^{dN})$ for $\mu_{\mathfrak{m}_{\mathrm{svm}}}$-a.e. z. The measure $\mu_{\mathfrak{m}_{\mathrm{svm}}} \in \mathscr{P}(\mathfrak{h}_\omega)$ is a probability measure, hence the right-hand side of the above equation is a (double) convex combination of numerical values of the real-valued function $\mathcal{E}_{\mathrm{qc}}$. However, a convex combination of values of a function equals its infimum, if and only if the infimum is a minimum, and all variables appearing in the convex combination are minimizers. Therefore, $\mathcal{E}_{\mathrm{qc}}$ admits at least one minimizer. Actually, the measure $\mathfrak{m}_{\mathrm{svm}}$ is concentrated on the set of minimizers $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$, in the above sense.

Finally, we consider the Pekar-like variational problem (VP′2) and its equivalence with (VP2). Let us first prove that (VP′2) $\Longrightarrow$ (VP2): given a Pekar minimizer $\psi_{\mathrm{Pekar}} \in L^2(\mathbb{R}^{dN})$, we immediately deduce that $\psi_{\mathrm{Pekar}} \in H^1(\mathbb{R}^{dN})$ by boundedness from above of the energy and regularity of the classical field $\boldsymbol{a}(\boldsymbol{x})$, which is continuous and vanishing at infinity [Correggi et al. 2019, Remark 1.5]. Furthermore, Lemma 2.4 guarantees the existence (and uniqueness) of $\eta_{\mathrm{Pekar}}[\psi_{\mathrm{Pekar}}] \in \mathfrak{h}$ minimizing $\mathcal{E}_{\mathrm{qc}}[\psi_{\mathrm{Pekar}}, z]$ with respect to z. Therefore, the configuration $(\psi_{\mathrm{Pekar}}, \eta_{\mathrm{Pekar}}[\psi_{\mathrm{Pekar}}])$ is admissible for $\mathcal{E}_{\mathrm{qc}}$ and we deduce from Proposition 2.1 that $\mathcal{E}_{\mathrm{qc}}[\psi_{\mathrm{Pekar}}, \eta_{\mathrm{Pekar}}[\psi_{\mathrm{Pekar}}]] = E_{\mathrm{qc}}$.

Conversely, given a minimizer $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}}) \in \mathscr{D}$ of $\mathcal{E}_{\mathrm{qc}}$, we know that the configuration must satisfy the Euler–Lagrange equations (1-23) at least in the weak sense. However, the second equation in (1-23) is easily seen to coincide with (1-27) or the first equation in (1-34), when the change of variable $\eta = \omega^{1/2} z$ has been performed. Furthermore, any weak solution η of such equations is in fact a strong solution, i.e., $\eta \in \mathfrak{h}$, under the assumptions made. Hence, by strict convexity of $\mathcal{F}_{\mathrm{qc}}[\psi, \eta]$ in η proven in Lemma 2.4 and then uniqueness of η_{Pekar}, we deduce that $\eta_{\mathrm{Pekar}}[\psi_{\mathrm{qc}}] = \omega^{1/2} z_{\mathrm{qc}}$, and the equivalence (VP2) $\Longrightarrow$ (VP′2) is readily proven via Proposition 2.1. □

The next result about the quasiclassical functional defined in (1-18) or, more precisely, about its variant $\mathcal{F}_{\mathrm{qc}}$ introduced in (1-25) is important to explore the connection with the Pekar-like functionals (1-28) and (1-34).

Lemma 2.4. *For any fixed ψ, the functional $\mathcal{F}_{\mathrm{qc}}[\psi, \eta]$ is strictly convex in $\eta \in \mathfrak{h}_\omega$.*

Proof. In cases (a) and (b) the proof is trivial, since $\mathcal{F}_{\mathrm{qc}}$ contains only two terms depending on η: one is quadratic in η (the free field energy) and therefore strictly convex, while the other (the interaction) is linear and thus convex.

So we have to investigate in detail only case (c), namely the Pauli–Fierz quasiclassical energy, and, specifically, only the kinetic part of the energy involving the interaction, which reads

$$\sum_{j=1}^{N} \frac{1}{2m_j} \big(-i\nabla_j + 2\mathrm{Re}\langle \eta | (\omega^{-1/2} \boldsymbol{\lambda}_j)(\boldsymbol{x}_j) \rangle_{\mathfrak{h}}\big)^2.$$

Let us then set $\eta = \beta\eta_1 + (1-\beta)\eta_2$ for some $\eta_1, \eta_2 \in \mathfrak{h}$ and $\beta \in (0,1)$. Expanding the square and setting $\boldsymbol{\xi}_j(\boldsymbol{x}) := \omega^{-1/2}\lambda_j(\boldsymbol{x})$ for short, we get (for any nonzero ψ)

$$\begin{aligned}\big\langle\psi\big|(-i\nabla_j + 2\mathrm{Re}\langle\eta|\boldsymbol{\xi}_j(\boldsymbol{x}_j)\rangle_{\mathfrak{h}})^2\big|\psi\big\rangle_{L^2(\mathbb{R}^{3N})} \\ < \langle\psi|-\Delta_j|\psi\rangle_{L^2(\mathbb{R}^{3N})} - 2\big\langle\psi\big|i\beta\mathrm{Re}\langle\eta_1|\boldsymbol{\xi}_j(\boldsymbol{x}_j)\rangle_{\mathfrak{h}}\cdot\nabla_j + i(1-\beta)\mathrm{Re}\langle\eta_2|\boldsymbol{\xi}_j(\boldsymbol{x}_j)\rangle_{\mathfrak{h}}\cdot\nabla_j\big|\psi\big\rangle_{L^2(\mathbb{R}^{3N})} \\ + 4\big\langle\psi\big|\beta(\mathrm{Re}\langle\eta_1|\boldsymbol{\xi}_j(\boldsymbol{x}_j)\rangle_{\mathfrak{h}})^2 + (1-\beta)(\mathrm{Re}\langle\eta_2|\boldsymbol{\xi}_j(\boldsymbol{x}_j)\rangle_{\mathfrak{h}})^2\big|\psi\big\rangle_{L^2(\mathbb{R}^{3N})},\end{aligned} \tag{2-21}$$

again by the strict convexity of the square, i.e., the bound $(\beta a + (1-\beta)b)^2 < \beta a^2 + (1-\beta)b^2$, valid for any $a, b \in \mathbb{R}$ and $\beta \in (0,1)$. The result easily follows, since the remaining term in the functional depending on η is the free field energy, which is quadratic in η and thus strictly convex as well. □

Remark 2.5 (minimizers for (vp′2)). The existence of a solution for (vp′2) obtained here is trivial, i.e., it involves a measure concentrated in a single point $z_{\mathrm{qc}} \in \mathfrak{h}_\omega$ and a $\psi_{z_{\mathrm{qc}}}$ dependent on such a point. It would be interesting, but outside the scope of this paper, to know whether there are nontrivial minimizers in which μ_0 is not concentrated at a single point. This is obviously related to the question of uniqueness of the minimizing configuration $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$. Note that this would not be in contradiction with Lemma 2.4, since we prove there strict convexity of $\mathcal{F}_{\mathrm{qc}}[\psi,\eta]$ only in η, while the full functional $\mathcal{E}_{\mathrm{qc}}[\psi, z]$ is in general not jointly convex in ψ and z nor in $|\psi|^2$ and z (see also Remark 1.2).

Proof of Proposition 1.1. Combining Proposition 2.1 with Proposition 2.3 one obtains the equivalence of the variational problems. □

2B. ***Minimization problem for generalized state-valued measures.*** We discuss now the generalization of the concepts introduced above needed to deal with the minimization (1-52), which is particularly useful to treat small systems consisting of unconfined particles. Taking the double dual, it is well known that $\mathscr{L}^1(L^2(\mathbb{R}^{dN}))$ can be continuously embedded in $\mathscr{B}(L^2(\mathbb{R}^{dN}))'$, the dual of bounded operators, in a positivity preserving way. By an abuse of notation, we will write $\mathscr{L}^1(L^2(\mathbb{R}^{dN})) \subset \mathscr{B}(L^2(\mathbb{R}^{dN}))'$. We recall that we denoted by $\overline{\mathscr{L}^1}(L^2(\mathbb{R}^{dN}))$ the closure of $\mathscr{L}^1(L^2(\mathbb{R}^{dN}))$ with respect to the weak* topology $\sigma(\mathscr{B}(L^2(\mathbb{R}^{dN}))', \mathscr{B}(L^2(\mathbb{R}^{dN})))$ on $\mathscr{B}(L^2(\mathbb{R}^{dN}))'$. Also, $\overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$ and $\overline{\mathscr{L}^1}_{+,1}(L^2(\mathbb{R}^{dN}))$ stand for the subsets of positive and normalized positive elements, respectively. A generalized state-valued measure is then a measure on $\mathfrak{h}_\omega$ with values in the space of generalized states $\overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$. Properties of generalized state-valued measures are discussed in the Appendix. Since the dual space $\mathscr{B}(L^2(\mathbb{R}^{dN}))'$ is not separable, it does not have the Radon–Nikodým property, therefore integration of functions $\mathcal{F} : \mathfrak{h}_\omega \to \mathscr{B}(L^2(\mathbb{R}^{dN}))$ is restricted only to those with separable range.

Such integration can be extended to functions valued in unbounded operators in the following sense.

Definition 2.6 (domains of generalized Wigner measures). Let $\mathcal{T}$ be a strictly positive unbounded operator on $L^2(\mathbb{R}^{dN})$. A generalized state-valued measure $\mathfrak{n}$ is *in the domain of* $\mathcal{T}$ if and only if there exists a measure $\mathfrak{n}_{\mathcal{T}} \in \mathscr{P}(\mathfrak{h}_\omega, \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN})))$ such that for all $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$ and all Borel sets $S \subseteq \mathfrak{h}_\omega$,

$$\mathfrak{n}_{\mathcal{T}}(S)[\mathcal{T}^{-1/2}\mathcal{B}\mathcal{T}^{-1/2}] = \mathfrak{n}(S)[\mathcal{B}]. \tag{2-22}$$

Therefore, if $\mathfrak{n}$ is in the domain of $\mathcal{T}$, with a little abuse of notation we may write

$$\mathfrak{n}(S)[\mathcal{T}^{1/2} \cdot \mathcal{T}^{1/2}] = \mathfrak{n}_{\mathcal{T}}(S)[\,\cdot\,] \tag{2-23}$$

as a state-valued measure "absorbing a singularity" of order $\mathcal{T}$. Now, let $\mathcal{F}(z)$ be a function with values in unbounded operators such that for all $z \in \mathfrak{h}_\omega$,

- $\mathcal{T}^{-1/2}\mathcal{F}(z)\mathcal{T}^{-1/2} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$,
- the range of $z \mapsto \mathcal{T}^{-1/2}\mathcal{F}(z)\mathcal{T}^{-1/2}$ is separable,
- $\mathcal{T}^{-1/2}\mathcal{F}(z)\mathcal{T}^{-1/2}$ is $\mathfrak{n}_{\mathcal{T}}$-absolutely integrable.

Then, it follows that we can define the integral of $\mathcal{F}$ with respect to $\mathfrak{n}$ as

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{F}(z)] := \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_{\mathcal{T}}(z)[\mathcal{T}^{-1/2}\mathcal{F}(z)\mathcal{T}^{-1/2}]. \tag{2-24}$$

A simple but useful example of such $\mathcal{F}(z)$ is the following: let $\mathcal{S}$ be a self-adjoint operator, and let $\mathfrak{n}$ be in the domain of $\mathcal{T} = |\mathcal{S}| + 1$; then the function $\mathcal{F}(z) = \mathcal{S}$ satisfies all above hypotheses and thus it makes sense to write, for all Borel set $S \subseteq \mathfrak{h}_\omega$,

$$\int_S \mathrm{d}\mathfrak{n}(z)[\mathcal{S}] = \mathfrak{n}(S)[\mathcal{S}] := \mathfrak{n}_{\mathcal{T}}(S)[\mathcal{T}^{-1/2}\mathcal{S}\mathcal{T}^{-1/2}] \in \mathbb{R}. \tag{2-25}$$

The other cases useful for our analysis are discussed in Section 3.

We are now in a position to define another quasiclassical minimization problem. Recall the definition of the domain $\mathscr{D}_{\mathrm{gqc}}$ (1-53), the ground state energy E_{gqc} given by (1-54) and any corresponding minimizing configuration $(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) \in \mathscr{D}_{\mathrm{gqc}}$; then the analogues of (VP1) and (VP2) are (stability)

$$\text{"Is } E_{\mathrm{gqc}} \text{ greater than } -\infty\text{?"} \tag{GVP1}$$

and (existence of a ground state)

$$\text{"Does there exist } (\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) \in \mathscr{D}_{\mathrm{gqc}} \text{ such that } \mathcal{E}_{\mathrm{gqc}}(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}}) = E_{\mathrm{gqc}}\text{?"} \tag{GVP2}$$

The functional $\mathcal{E}_{\mathrm{gqc}}$ can indeed be seen as the generalized quasiclassical energy: let H_z be the abstract realization of $\mathcal{H}_z$ as an operator affiliated to the abstract C^*-algebra $\mathscr{B}(L^2(\mathbb{R}^{dN}))$. Then, given a normalized pure state $\rho \in \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN}))$, we define the corresponding irreducible GNS representation by $(\mathscr{K}_\rho, \pi_\rho, \psi_\rho)$, where $\mathscr{K}_\rho$ is a suitable Hilbert space, $\pi_\varrho : \mathscr{B}(L^2(\mathbb{R}^{dN})) \to \mathscr{B}(\mathscr{K}_\rho)$ is a C^*-homomorphism (that can be extended to operators affiliated to the algebra) and $\psi_\rho \in \mathscr{K}_\varrho$ is the normalized cyclic vector associated to ρ. Therefore, it follows that

$$\mathcal{E}_{\mathrm{gqc}}[\rho, z] = \langle \psi_\rho | \pi_\rho(H_z) | \psi_\rho \rangle_{\mathscr{K}_\rho}.$$

This expression is analogous to the one for $\mathcal{E}_{\mathrm{qc}}$ (see (1-18)) and it reduces exactly to the latter whenever ρ is a pure state belonging to $\mathscr{L}^1(L^2(\mathbb{R}^{dN}))$ (see Remark 2.7).

The generalization of the variational problems for state-valued measures (vp1) and (vp2) is obtained as follows: setting

$$\mathscr{D}_{\mathrm{gsvm}} := \left\{ \mathfrak{n} \in \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN})) : \|\mathfrak{n}(\mathfrak{h}_\omega)\|_{\mathscr{B}'} = 1, \ \left| \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{H}_z] \right| < +\infty \right\}, \tag{2-26}$$

we consider the questions (stability)

$$\text{“Is } E_{\mathrm{gsvm}} := \inf_{\mathfrak{n}\in\mathscr{D}_{\mathrm{gsvm}}} \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{H}_z] \text{ greater than } -\infty\text{?”} \tag{gvp1}$$

and (existence of a ground state)

$$\text{“Does there exists } \mathfrak{n}_{\mathrm{gsvm}} \in \mathscr{D}_{\mathrm{gsvm}} \text{ such that } \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_{\mathrm{gsvm}}(z)[\mathcal{H}_z] = E_{\mathrm{gsvm}}\text{?”} \tag{gvp2}$$

Remark 2.7 (state-valued and generalized state-valued measures). We point out that, if a generalized state-valued measure $\mathfrak{n} \in \mathscr{D}_{\mathrm{gsvm}}$ is actually a state-valued measure, i.e., such that, for all Borel sets $S \subseteq \mathfrak{h}_\omega$,

$$\mathfrak{n}(S) \in \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})),$$

then $\mathfrak{n} \in \mathscr{D}_{\mathrm{svm}}$ and

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{H}_z] = \mathcal{E}_{\mathrm{svm}}[\mathfrak{n}].$$

Proposition 2.8 (generalized quasiclassical ground state energy). *Under assumptions* (A1), (A2) *and* (A3),

$$E_{\mathrm{qc}} = E_{\mathrm{gqc}} = E_{\mathrm{gsvm}}. \tag{2-27}$$

Proof. Firstly, let us prove that

$$E_{\mathrm{qc}} = E_{\mathrm{gqc}}.$$

Since ρ belongs to the weak* closure of $\mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))$, there exists a filter base $\mathfrak{S} \subset 2^{\mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))}$ such that $\mathfrak{S} \to \rho$ in the weak* topology. Hence, for any fixed $z \in \mathfrak{h}_\omega$,[4]

$$\lim_{\mathfrak{S}\to\rho} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\mathfrak{S}(\mathcal{H}_z)] = \rho[\mathcal{H}_z].$$

Now, on one hand, each $|\psi\rangle\langle\psi|$, $\psi \in L^2(\mathbb{R}^{dN})$, is also a pure generalized state and therefore

$$E_{\mathrm{gqc}} \le \inf_{(\psi,z)\in\mathscr{D}_{\mathrm{qc}}} \mathcal{E}_{\mathrm{qc}}[\psi, z] = E_{\mathrm{qc}}. \tag{2-28}$$

On the other hand, let $(\rho_\delta, z_\delta) \in \mathscr{D}_{\mathrm{gqc}}$ be a minimizing sequence:

$$\mathcal{E}_{\mathrm{gqc}}[\rho_\delta, z_\delta] = \rho_\delta[\mathcal{H}_{z_\delta}] < E_{\mathrm{gqc}} + \delta,$$

for some $\delta > 0$ and let $\mathfrak{S}_\delta \subset 2^{\mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))}$ be the corresponding approximating filter base for ρ_δ. Then,

$$\begin{aligned} E_{\mathrm{qc}} = \inf_{(\psi,z)\in\mathscr{D}_{\mathrm{qc}}} \mathcal{E}_{\mathrm{qc}}[\psi, z] &= \inf_{(\gamma,z)\in\mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}))\oplus\mathfrak{h}_\omega} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma\mathcal{H}_z] \le \sup_{X\in\mathfrak{S}_\delta} \inf_{\gamma\in X} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma\mathcal{H}_{z_\delta}] \\ &= \liminf_{\mathfrak{S}_\delta} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\mathfrak{S}_\delta(\mathcal{H}_{z_\delta})] = \lim_{\mathfrak{S}_\delta\to\rho_\delta} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\mathfrak{S}_\delta(\mathcal{H}_{z_\delta})] = \rho_\delta[\mathcal{H}_{z_\delta}] < E_{\mathrm{gqc}} + \delta. \end{aligned} \tag{2-29}$$

[4]The notation $\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\mathfrak{S}(\mathcal{H}_z)]$ stands for the filter base that is the image of $\mathfrak{S}$ on $\mathbb{R}$ via the map $\gamma \mapsto \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma\mathcal{H}_z]$; given any $X \in \mathfrak{S}$, we have that $\{\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma\mathcal{H}_z], \gamma \in X\} \in \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\mathfrak{S}(\mathcal{H}_z)]$.

Since the above chain of inequalities is valid for all $\delta > 0$, it follows that the opposite inequality of (2-28) holds true, i.e.,

$$E_{\mathrm{qc}} \leq E_{\mathrm{gqc}}, \tag{2-30}$$

which implies the claim.

The proof of the identity $E_{\mathrm{gsvm}} = E_{\mathrm{qc}}$ is perfectly analogous, where we remind the reader that it is possible to approximate any measure $\mathfrak{n} \in \mathscr{P}(\mathfrak{h}_\omega, \overline{\mathscr{L}^1}_+(L^2(\mathbb{R}^{dN})))$ with a filter base $\mathfrak{T} \subset 2^{\mathscr{P}(\mathfrak{h}_\omega, \mathscr{L}^1_+(L^2(\mathbb{R}^{dN})))}$ with respect to the product of weak* topologies

$$\prod_{S \subset \mathfrak{h}_\omega \text{ Borel}} \sigma(\mathcal{B}(L^2(\mathbb{R}^{dN}))', \mathcal{B}(L^2(\mathbb{R}^{dN}))),$$

which implies the convergence of integrals[5]

$$\lim_{\mathfrak{T} \to \mathfrak{n}} \mathrm{tr}_{L^2(\mathbb{R}^{dN})}\left[\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{T}(z) \mathcal{H}_z\right] = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{H}_z]. \qquad \square$$

Finally, also for the generalized minimization problems, it is possible to prove equivalence of existence of minimizers.

Proposition 2.9 (generalized quasiclassical minimizers). *Under assumptions* (A1), (A2) *and* (A3),

$$\text{(GVP2)} \iff \text{(gvp2)}. \tag{2-31}$$

Furthermore, any minimizer $\mathfrak{n}_{\mathrm{gsvm}}$ *of* (gvp2) *is concentrated on the set of minimizers* $(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}})$ *of* (GVP2).

Proof. The forward implication is trivial: let $(\rho_{\mathrm{gqc}}, z_{\mathrm{gqc}})$ be a minimizer for (GVP2). Then, evaluating the energy of the generalized state-valued measure $\mathfrak{n}_0 = \delta_{z_{\mathrm{gqc}}} \rho_{\mathrm{gqc}}$, we get

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_0(z)[\mathcal{H}_z] = \rho_{\mathrm{gqc}}[\mathcal{H}_{z_{\mathrm{gqc}}}] = E_{\mathrm{gqc}}. \tag{2-32}$$

By Proposition 2.8, $\mathfrak{n}_0$ is thus a minimizer for (gvp2).

To prove the reverse implication, note that the integral with respect to a generalized state-valued probability measure is a convex combination of expectations over possibly mixed generalized states. Since the mixed states are themselves convex combinations of pure states, it follows that the measure $\mathfrak{n}_{\mathrm{gsvm}}$ must be concentrated on the set of minimizers for (gvp2), and thus the latter is not empty. $\square$

3. Ground state energies and ground states in the quasiclassical regime

In this section we study the quasiclassical limit of ground state energies and ground states of the microscopic models introduced in Section 1.

The microscopic interaction is described by a fully quantum system, in which both the small system and the environment are quantum. The Hilbert space is thus (see (1-2)) given by $\mathscr{H}_\varepsilon = L^2(\mathbb{R}^{dN}) \otimes \mathcal{G}_\epsilon(\mathfrak{h})$, where $\mathcal{G}_\epsilon(\mathfrak{h}) = \bigoplus_{n \in \mathbb{N}} \mathfrak{h}^{\otimes_s n}$ is the symmetric Fock space over $\mathfrak{h}$ and ε is the quasiclassical parameter whose dependence is given by a semiclassical choice of canonical commutation relations (1-3), i.e.,

[5] As before, the integral with respect to $\mathrm{d}\mathfrak{T}$ is just a short-hand notation to denote the integral over elements belonging to the filter $\mathfrak{T}$.

$[a_\varepsilon(z), a_\varepsilon^\dagger(w)] = \varepsilon\langle z|w\rangle_{\mathfrak{h}}$, with $a_\varepsilon^\sharp$ the annihilation and creation operators on the Fock space. A state of the whole system is given by a density matrix

$$\Gamma_\varepsilon \in \mathscr{L}^1_{+,1}(L^2(\mathbb{R}^{dN}) \otimes \mathcal{G}_\varepsilon(\mathfrak{h})),$$

the positive trace-class operators with unit trace.

The dynamics of the system is described by a self-adjoint Hamiltonian operator H_ε whose general form is given in (1-4). Such an operator is the partial Wick quantization of the quasiclassical Schrödinger energy operator $\mathcal{H}_z$ provided in (1-14). Wick quantization consists in substituting each z appearing in $\mathcal{H}$ with a_ε and each $\bar{z}$ with $a_\varepsilon^\dagger$, and of ordering all the $a_\varepsilon^\dagger$ to the left of all the a_ε. Such a quantization procedure is well-defined for symbols $\mathcal{F}_z$ that are polynomial in z and z^*, as is the case in the concrete models we are considering; see Section 4 for additional details and [Ammari and Nier 2008] for the rigorous procedure. Hence, we write

$$H_\varepsilon = \mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{H}_z), \tag{3-1}$$

and, more precisely, $\mathcal{H}_z$ can be split into three terms, at least in the sense of quadratic forms, i.e.,

$$\mathcal{H}_z = \mathcal{K}_0 + \sum_{i=1}^{N} \mathcal{V}_z(\boldsymbol{x}_i) + \langle z|\omega|z\rangle_{\mathfrak{h}} \tag{3-2}$$

with $\mathcal{K}_0$ self-adjoint and bounded from below, yielding

$$H_\varepsilon = \mathcal{K}_0 \otimes 1 + 1 \otimes \mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\langle z|\omega|z\rangle_{\mathfrak{h}}) + \sum_{i=1}^{N} \mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{V}_z(\boldsymbol{x}_i)) \tag{3-3}$$

as a quadratic form. The first and second terms on the right-hand side are the free energies of the small system and environment, respectively, and the third term is the *small system-environment* interaction.

The minimization problem for the quantum system described by H_ε is defined in (1-12): the microscopic ground state energy is $E_\varepsilon := \inf \sigma(H_\varepsilon)$, while $\Psi_{\varepsilon,\mathrm{gs}}$ stands for any corresponding minimizer. Such a minimization problem has been thoroughly studied for the concrete models under consideration in this paper; see Section 1A. A crucial ingredient of our proof is the uniform boundedness from below of the spectrum of H_ε. Note again that we do not need the existence of a microscopic ground state $\Psi_{\varepsilon,\mathrm{gs}}$.

Proposition 3.1 (stability and existence of the ground state). *Under assumptions* (A1), (A2) *and* (A3), *there exist finite constants* $c, C > 0$ *independent of* ε *such that*

$$-c \le E_\varepsilon \le C. \tag{3-4}$$

The proof of the above result is model-dependent and therefore it is postponed to Section 4.

We now investigate the link between the microscopic ground state problem and the quasiclassical minimization problems described in Section 2, starting from the proof of Theorem 1.3. The strategy of proof can be outlined as follows:

- Derive an energy upper bound (Proposition 3.2) by means of a suitable trial state.
- Prove a matching lower bound (Proposition 3.3) by showing the convergence of the expectation of each term in the energy over a suitable minimizing sequence.

Although both cases could be treated at once, we provide a separate discussion of the main results for trapped and nontrapped particle systems, whose difference is apparent in the statements of Corollary 1.10 and Corollary 1.17. The convergence of minimizing sequences and ground states (Theorem 1.7), if present, is then obtained as a direct consequence of the above arguments.

3A. ***Proof of Theorem 1.3.*** The proof of Theorem 1.3 is obtained by putting together the energy upper bound (Proposition 3.2) and lower bound (Proposition 3.3).

In the following, we denote by $\Psi_{\varepsilon,\delta} \in \mathscr{D}(H_\varepsilon)$, $\delta > 0$, a minimizing sequence for H_ε:

$$\langle \Psi_{\varepsilon,\delta} | H_\varepsilon | \Psi_{\varepsilon,\delta} \rangle_{\mathscr{H}_\varepsilon} < E_\varepsilon + \delta. \tag{3-5}$$

Proposition 3.2 (energy upper bound). *Under assumptions* (A1), (A2) *and* (A3),

$$\limsup_{\varepsilon \to 0} E_\varepsilon \leq E_{\mathrm{qc}}. \tag{3-6}$$

Proof. In order to prove the upper bound we use a coherent trial state: let us denote by $\Omega_\varepsilon \in \mathcal{G}_\varepsilon(\mathfrak{h})$ the Fock vacuum and let

$$\Xi_\varepsilon[\psi, z] := \psi \otimes W_\varepsilon\Big(\frac{z}{i\varepsilon}\Big)\Omega_\varepsilon \tag{3-7}$$

be a coherent product state constructed over the particle state ψ and the classical configuration $z \in \mathfrak{h}$. We shall restrict to $\psi \in \mathscr{Q}(\mathcal{K}_0)$, where $\mathscr{Q}(\mathcal{K}_0)$ is the form domain of $\mathcal{K}_0$, and $z \in \mathfrak{h}$ such that $\omega^{1/2} z \in \mathfrak{h}$. As discussed in Section 4, this is sufficient to make $\Xi_\varepsilon[\psi, z] \in \mathscr{Q}(H_\varepsilon)$ and $(\psi, z) \in \mathscr{D}_{\mathrm{qc}}$. The energy of the above trial state is

$$\langle \Xi_\varepsilon[\psi, z] | H_\varepsilon | \Xi_\varepsilon[\psi, z] \rangle_{\mathscr{H}_\varepsilon} = \mathcal{E}_{\mathrm{qc}}[\psi, z] + o_\varepsilon(1). \tag{3-8}$$

The proof of the above estimate depends on the microscopic model involved. The computation of the expectation over the trial states (3-7) can be found in [Correggi and Falconi 2018, Proposition 3.11 and Section 3.6] for the Nelson and polaron models, and in [Correggi et al. 2019, Proof of Theorem 1.9] for the Pauli–Fierz model. Hence, we have that

$$E_\varepsilon \leq \inf_{(\psi,z) \in \mathscr{D}_{\mathrm{qc}}} \langle \Xi_\varepsilon[\psi, z] | H_\varepsilon | \Xi_\varepsilon[\psi, z] \rangle_{\mathscr{H}_\varepsilon} = \inf_{(\psi,z) \in \mathscr{D}_{\mathrm{qc}}} \mathcal{E}_{\mathrm{qc}}[\psi, z] + o_\varepsilon(1) = E_{\mathrm{qc}} + o_\varepsilon(1). \tag{3-9}$$

The result is then obtained by taking the $\limsup_{\varepsilon \to 0}$ on both sides. □

The symmetric result of Proposition 3.2 is stated in the following proposition.

Proposition 3.3 (energy lower bound). *Under assumptions* (A1), (A2) *and* (A3),

$$\liminf_{\varepsilon \to 0} E_\varepsilon \geq E_{\mathrm{qc}}. \tag{3-10}$$

Although not necessary in principle, we find it convenient to present two different proofs of (3-10), one valid only when $\mathcal{K}_0$ has compact resolvent, e.g., when the small system is trapped, and one valid for nontrapped small systems as well. The main reason is that the former does not require the use of generalized Wigner measures, since conventional state-valued measures are sufficient, resulting in a more accessible proof.

3A1. *Energy lower bound*: *trapped particle systems.* If $\mathcal{K}_0$ has compact resolvent, the set of quasiclassical Wigner measures (as in Definition 1.4) associated with minimizing sequences for H_ε is not empty. In addition, the expectation of $\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{V}_z)$ converges to the quasiclassical integral of $\mathcal{V}_z$. Let us formulate some preliminary results about the convergence of the expectation values of the operators involved. Such results rely on suitable a priori bounds on the family of states $\Psi_\varepsilon \in \mathscr{H}_\varepsilon$, as ε varies in $(0, 1)$. Lemma 3.7 guarantees that there exists a minimizing sequence $\Psi_{\varepsilon,\delta}$ in the sense of (3-5) satisfying such bounds.

Lemma 3.4. *If* (A4) *holds and there exists $C < +\infty$ such that*, *uniformly with respect to $\varepsilon \in (0, 1)$*,

$$\left|\langle \Psi_\varepsilon | (\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega) + 1) | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon}\right| \le C, \tag{3-11}$$

then $\mathscr{W}(\Psi_\varepsilon, \varepsilon \in (0, 1)) \neq \varnothing$. Furthermore, if $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n \to 0]{\mathrm{qc}} \mathfrak{m}$, then $\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{K}_0]$ is $\mu_{\mathfrak{m}}$-a.e. finite and $\mu_{\mathfrak{m}}$-absolutely integrable, *and*

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathcal{K}_0 | \Psi_{\varepsilon_n} \rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{K}_0]. \tag{3-12}$$

Proof. For $\omega = 1$ this proposition is proved in [Correggi et al. 2023, Propositions 2.3 and 2.6]. For a generic $\omega \ge 0$, the proof (in the presence of semiclassical degrees of freedom only) can be found in [Falconi 2018a, Theorem 3.3]; the extension to the quasiclassical setting is straightforward, testing with compact observables of the small system, as in the aforementioned [Correggi et al. 2023, Propositions 2.3 and 2.6]. Let us stress that the fact that all Wigner measures are probability measures, i.e., there is no loss of mass and $\mathfrak{m}(\mathfrak{h}_\omega) = 1$, is due to the fact that $\mathcal{K}_0$ has compact resolvent. Otherwise, there may be a loss of probability mass due to the interplay between the particle system and the environment; see [Correggi et al. 2023, Corollary 1.7 and Remark 1.9] for additional details. □

In order to control the convergence of the free field energy, we first have to regularize it: we pick a sequence of positive self-adjoint compact operators $\{\mathbb{1}_r\}_{r\in\mathbb{N}} \subset \mathscr{B}(\mathfrak{h})$ approximating the identity: for all $r \in \mathbb{N}$, $\mathbb{1}_r \le \mathbb{1}$, and for all $z \in \mathfrak{h}_\omega$,

$$\lim_{r\to\infty} \langle z | \omega_r | z \rangle_{\mathfrak{h}} = \lim_{r\to\infty} \langle z | \mathbb{1}_r | z \rangle_{\mathfrak{h}_\omega} = \|z\|^2_{\mathfrak{h}_\omega} = \langle z | \omega | z \rangle_{\mathfrak{h}}, \tag{3-13}$$

where we have written $\omega_r := \omega^{1/2}\mathbb{1}_r\omega^{1/2}$. Recall also that $\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\langle z|\omega|z\rangle_{\mathfrak{h}}) = 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega)$, where $\mathrm{d}\mathcal{G}_\varepsilon(\omega)$ stands for the second quantization of ω as above.

Lemma 3.5. *If* (A4) *holds and there exist $C < +\infty$ and $\delta > 1$ such that*, *uniformly with respect to $\varepsilon \in (0, 1)$*,

$$\left|\langle \Psi_\varepsilon | (\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega)^\delta + 1) | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon}\right| \le C, \tag{3-14}$$

then, *if $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n \to 0]{\mathrm{qc}} \mathfrak{m} \in \mathscr{W}(\Psi_\varepsilon, \varepsilon \in (0, 1))$, it follows that for any $\eta \le \delta$*,

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z) \langle z|\omega|z\rangle_{\mathfrak{h}}^\eta \le C, \tag{3-15}$$

and, *for all $r \in \mathbb{N}$*,

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | 1 \otimes \mathrm{d}\mathcal{G}_{\varepsilon_n}(\omega_r) | \Psi_{\varepsilon_n} \rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z) \langle z|\omega_r|z\rangle_{\mathfrak{h}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z) \langle z|\mathbb{1}_r|z\rangle_{\mathfrak{h}_\omega}. \tag{3-16}$$

Proof. The proof of $\mu_{\mathfrak{m}}$-integrability of $\langle z|\omega|z\rangle_{\mathfrak{h}}^{\eta}$ (and the relative bound) is a consequence of the corresponding result for semiclassical (scalar) Wigner measures proved in [Ammari and Nier 2008; Falconi 2018a]. Analogously, the convergence holds because $\langle z|\mathbb{1}_r|z\rangle_{\mathfrak{h}_\omega}$ is a compact scalar symbol; see [Falconi 2018a] for the convergence of compact symbols in $\mathfrak{h}_\omega$, and [Correggi et al. 2023, Propositions 2.3 and 2.6] for additional details on the generalization of results in semiclassical analysis to the quasiclassical case. □

Lemma 3.6. *If* (A4) *holds and there exists* $C < +\infty$ *such that*, *uniformly with respect to* $\varepsilon \in (0, 1)$,

$$\left|\langle \Psi_\varepsilon|(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega)^2 + 1)|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \le C, \tag{3-17}$$

then, *if* $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n\to 0]{\mathrm{qc}} \mathfrak{m}$, *for any* $i = 1, \dots, N$,

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n}|\mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_i))|\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{V}_z(\boldsymbol{x}_i)]. \tag{3-18}$$

Lemma 3.7. *Under assumptions* (A1), (A2) *and* (A3), *there exists a minimizing sequence* $\{\Psi_{\varepsilon,\delta}\}_{\varepsilon,\delta\in(0,1)}$ *such that*, *for all fixed* $\delta \in (0, 1)$, (3-5) *holds true and there exists* $C_\delta < +\infty$ *such that*

$$\left|\langle \Psi_{\varepsilon,\delta}|(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega)^2 + 1)|\Psi_{\varepsilon,\delta}\rangle_{\mathscr{H}_\varepsilon}\right| \le C_\delta. \tag{3-19}$$

The proofs of Lemma 3.6 and Lemma 3.7, like the form of the quasiclassical potential $\mathcal{V}_z$, depend on the model considered. We thus provide them in Section 4.

Remark 3.8. Observe that if Lemma 3.7 holds, then the assumptions of Lemmas 3.4–3.6 are verified for the minimizing sequence $\Psi_{\varepsilon,\delta}$.

We are now in a position to prove the lower bound in the trapped case.

Proof of Proposition 3.3. Let $\Psi_{\varepsilon,\delta}$ be the minimizing sequence for H_ε of Lemma 3.7. Since for any $r \in \mathbb{N}$, $\omega_r \le \omega$, it follows that $\mathrm{d}\mathcal{G}_\varepsilon(\omega_r) \le \mathrm{d}\mathcal{G}_\varepsilon(\omega)$. Hence,

$$\left\langle \Psi_{\varepsilon,\delta}\middle|\left(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega_r) + \mathrm{Op}^{\mathrm{Wick}}_\varepsilon\left(\sum_i \mathcal{V}_z(\boldsymbol{x}_i)\right)\right)\middle|\Psi_{\varepsilon,\delta}\right\rangle_{\mathscr{H}_\varepsilon} \le \langle \Psi_{\varepsilon,\delta}|H_\varepsilon|\Psi_{\varepsilon,\delta}\rangle_{\mathscr{H}_\varepsilon} < E_\varepsilon + \delta. \tag{3-20}$$

Now, let us recall that, by Lemmas 3.4–3.7,

- for any $\delta > 0$, $\mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1)) \ne \varnothing$;
- the expectation value of each term in the Hamiltonian converges as $\varepsilon \to 0$ or, more precisely, there exists $\mathfrak{m} \in \mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1))$ such that

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}\left[\gamma_{\mathfrak{m}}\left(\mathcal{K}_0 + \langle z|\omega_r|z\rangle_{\mathfrak{h}} + \sum_i \mathcal{V}_z(\boldsymbol{x}_i)\right)\right] \\ \le \liminf_{\varepsilon\to 0}\left\langle \Psi_{\varepsilon,\delta}\middle|\left(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega_r) + \mathrm{Op}^{\mathrm{Wick}}_\varepsilon\left(\sum_i \mathcal{V}_z(\boldsymbol{x}_i)\right)\right)\middle|\Psi_{\varepsilon,\delta}\right\rangle_{\mathscr{H}_\varepsilon}. \tag{3-21}$$

Hence, we deduce that

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}\Big[\gamma_{\mathfrak{m}}\Big(\mathcal{K}_0 + \langle z|\omega_r|z\rangle_{\mathfrak{h}} + \sum_i \mathcal{V}_z(\boldsymbol{x}_i)\Big)\Big] < \liminf_{\varepsilon\to 0} E_\varepsilon + \delta. \tag{3-22}$$

Now, $\langle z|\omega_r|z\rangle_{\mathfrak{h}} \xrightarrow[r\to\infty]{} \langle z|\omega|z\rangle_{\mathfrak{h}}$ for any $z \in \mathfrak{h}_\omega$ by construction, and any $\mathfrak{m} \in \mathscr{W}(\Psi_\varepsilon, \varepsilon \in (0,1))$ is concentrated on $\mathfrak{h}_\omega$ by Lemma 3.4. Furthermore,

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\langle z|\omega_r|z\rangle_{\mathfrak{h}} \le \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\langle z|\omega|z\rangle_{\mathfrak{h}} \le C < +\infty.$$

Hence, by dominated convergence,

$$\lim_{r\to\infty}\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\langle z|\omega_r|z\rangle_{\mathfrak{h}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\langle z|\omega|z\rangle_{\mathfrak{h}}. \tag{3-23}$$

Thus, one gets

$$\inf_{\mathfrak{m}\in\mathscr{W}(\Psi_{\varepsilon,\delta},\varepsilon\in(0,1))}\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}\mathcal{H}_z] < \liminf_{\varepsilon\to 0} E_\varepsilon + \delta, \tag{3-24}$$

which, via Proposition 2.1, implies that

$$E_{\mathrm{qc}} \le \inf_{\mathfrak{m}\in\mathscr{W}(\Psi_{\varepsilon,\delta},\varepsilon\in(0,1))}\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}\mathcal{H}_z] < \liminf_{\varepsilon\to 0} E_\varepsilon + \delta.$$

Since $\delta > 0$ is arbitrary, the claim follows. □

3A2. *Energy lower bound*: *nontrapped particle systems.* In the nontrapped case, the strategy of proof is very similar, however it is not ensured that the set of quasiclassical Wigner measures for the minimizing sequence is not empty. It is then necessary to use generalized Wigner measures (recall Definition 1.6).

We first generalize the preparatory lemmas that we needed in the trapped case to the general situation. Note that for Lemma 3.7 it is not necessary that $\mathcal{K}_0$ has compact resolvent and therefore we can use it directly also in the nontrapped case. We also use the same notation as in the trapped case; in particular, we make use of the same compact approximation ω_r of ω we introduced in (3-13).

Lemma 3.9. *If there exists $C < +\infty$ such that*, *uniformly with respect to $\varepsilon \in (0,1)$*,

$$\big|\langle\Psi_\varepsilon|(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega) + 1)|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\big| \le C, \tag{3-25}$$

then $\mathscr{GW}(\Psi_\varepsilon, \varepsilon \in (0,1)) \neq \varnothing$. Furthermore, if $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n\to 0]{\mathrm{gqc}} \mathfrak{n}$, then $\mathfrak{n}$ is in the domain of $\mathcal{K}_0 + 1$ in the sense of Definition 2.6 and

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}|\mathcal{K}_0|\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{K}_0]. \tag{3-26}$$

In addition, *it follows that*

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[1]\langle z|\omega|z\rangle_{\mathfrak{h}} \le C, \tag{3-27}$$

and, *for all $r \in \mathbb{N}$*,

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}|1\otimes \mathrm{d}\mathcal{G}_{\varepsilon_n}(\omega_r)|\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[1]\langle z|\omega_r|z\rangle_{\mathfrak{h}}. \tag{3-28}$$

Proof. These lemmas extend to generalized Wigner measures Lemmas 3.4 and 3.5, respectively. The proof is, *mutatis mutandis*, completely analogous to those of the latter. Contrary to Lemma 3.4, since now $\mathcal{K}_0$ has a noncompact resolvent, the set of Wigner measures of Ψ_ε may be empty and there might be a loss of mass along the quasiclassical convergence. The set of generalized Wigner measures is, however, always nonempty: no mass is lost due to the fact that

$$\|\Psi_\varepsilon\|^2_{\mathscr{H}_\varepsilon} = \langle \Psi_\varepsilon | 1 \otimes W_\varepsilon(0) | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon} = 1,$$

and the identity operator belongs to $\mathscr{B}(L^2(\mathbb{R}^{dN}))$ but is not compact. More precisely, the above quantity can be immediately identified, in the limit $\varepsilon \to 0$, with the total mass of all generalized Wigner measures associated to Ψ_ε, as defined in Definition 1.6, whereas it is a priori only bigger than or equal to the total mass of measures defined by the convergence in Definition 1.4 (if all cluster points for the aforementioned convergence have total mass strictly less than one, the set of Wigner measures associated to Ψ_ε, which are required by Definition 1.4 to have total mass 1, is thus empty). ☐

Lemma 3.10. *If there exists $C < +\infty$ such that, uniformly with respect to $\varepsilon \in (0, 1)$,*

$$\left| \langle \Psi_\varepsilon | (\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega)^2 + 1) | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon} \right| \le C, \tag{3-29}$$

then, if $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n \to 0]{\mathrm{gqc}} \mathfrak{n}$, for any $i = 1, \dots, N$,

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_i)) | \Psi_{\varepsilon_n} \rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{V}_z(\boldsymbol{x}_i)]. \tag{3-30}$$

Like its analogue Lemma 3.6, the proof of Lemma 3.10 is model-dependent and thus given in Section 4.

The proof of the lower bound for the nontrapped case is now equivalent to the one in the trapped case, using generalized Wigner measures.

Proof of Proposition 3.3. Let $\Psi_{\varepsilon,\delta}$ be the minimizing sequence for H_ε of Lemma 3.7 satisfying (3-20). By Lemmas 3.7–3.10,

- for any $\delta > 0$, we have that $\mathscr{GW}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1)) \neq \varnothing$;
- for Wigner measures, there exists $\mathfrak{n} \in \mathscr{GW}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0, 1))$ such that

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z) \left[\mathcal{K}_0 + \langle z | \omega_r | z \rangle_{\mathfrak{h}} + \sum_i \mathcal{V}_z(\boldsymbol{x}_i) \right] \le \liminf_{\varepsilon\to 0} \left\langle \Psi_{\varepsilon,\delta} \middle| \left(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega_r) + \mathrm{Op}^{\mathrm{Wick}}_\varepsilon\left(\sum_i \mathcal{V}_z(\boldsymbol{x}_i) \right) \right) \middle| \Psi_{\varepsilon,\delta} \right\rangle_{\mathscr{H}_\varepsilon},$$

and therefore

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z) \left[\mathcal{K}_0 + \langle z | \omega_r | z \rangle_{\mathfrak{h}} + \sum_i \mathcal{V}_z(\boldsymbol{x}_i) \right] < \liminf_{\varepsilon\to 0} E_\varepsilon + \delta. \tag{3-31}$$

However, by dominated convergence, see Theorem A.18 in the Appendix,

$$\lim_{r\to\infty} \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[1] \langle z | \omega_r | z \rangle_{\mathfrak{h}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[1] \langle z | \omega | z \rangle_{\mathfrak{h}}.$$

Hence,

$$E_{\mathrm{gqc}} \le \inf_{\mathfrak{n} \in \mathscr{GW}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0,1))} \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}(z)[\mathcal{H}_z] < \liminf_{\varepsilon\to 0} E_\varepsilon + \delta,$$

and the result follows from the arbitrariness of $\delta > 0$, via Proposition 2.8. ☐

3B. ***Convergence of minimizing sequences and minimizers.*** Once the energy convergence is proven, we investigate the behavior of minimizing sequences and minimizers, if any.

Proof of Theorem 1.7. Let $\Psi_{\varepsilon,\delta} \in \mathscr{D}(H_\varepsilon)$ be a minimizing sequence. Then by Lemmas 3.4–3.7, any $\mathfrak{m}_\delta \in \mathscr{W}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0,1))$, corresponding to a sequence $\{\Psi_{\varepsilon_n,\delta}\}_{n\in\mathbb{N}}$, $\varepsilon_n \to 0$, satisfies

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}_\delta}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}_\delta}(z)\mathcal{H}_z] = \lim_{n\to\infty} \langle \Psi_{\varepsilon_n,\delta} | H_{\varepsilon_n} | \Psi_{\varepsilon_n,\delta}\rangle_{\mathscr{H}_{\varepsilon_n}} < \lim_{n\to\infty} E_{\varepsilon_n} + \delta = E_{\mathrm{qc}} + \delta,$$

as proven in Theorem 1.3. □

Proof of Corollary 1.9. If $\delta = o_\varepsilon(1)$, then considering $\mathfrak{m}_0 \in \mathscr{W}(\Psi_{\varepsilon,o_\varepsilon(1)}, \varepsilon \in (0,1))$, corresponding to a sequence $\{\Psi_{\varepsilon_n,\delta}\}_{n\in\mathbb{N}}$, $\varepsilon_n \to 0$, we have

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}_0}(z)\, \mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}_0}(z)\mathcal{H}_z] \le \lim_{n\to\infty} (E_{\varepsilon_n} + o_{\varepsilon_n}(1)) = E_{\mathrm{qc}}.$$

By Proposition 2.1 it follows that $\mathfrak{m}_0$ is a minimizer of (vp2) and, by Proposition 2.3, is concentrated on the set $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ of minimizers of (VP2). □

Proof of Corollary 1.10. Let $\Psi_{\varepsilon,\mathrm{gs}}$ be a ground state of H_ε. Then it is also an (exact) minimizing sequence with $\delta = 0$, and thus as above $\mathfrak{m}_0$ is a minimizer of (vp2) and is concentrated on the set $(\psi_{\mathrm{qc}}, z_{\mathrm{qc}})$ of minimizers of (VP2). □

The proof of Theorem 1.15 is also completely analogous to the proof of Theorem 1.7 for trapped systems.

Proof of Theorem 1.15. If $\mathcal{K}_0$ does not have compact resolvent, then by Lemmas 3.7, 3.9 and 3.10, any $\mathfrak{n}_\delta \in \mathscr{GW}(\Psi_{\varepsilon,\delta}, \varepsilon \in (0,1))$ satisfies

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_\delta(z)[\mathcal{H}_z] < \lim_{\varepsilon_n\to 0} E_{\varepsilon_n} + \delta = E_{\mathrm{qc}} + \delta = E_{\mathrm{gqc}} + \delta, \tag{3-32}$$

by Theorem 1.3 and Proposition 2.8. □

Proof of Corollary 1.16. If $\delta = o_\varepsilon(1)$, it follows that $\mathfrak{n}_0 \in \mathscr{GW}(\Psi_{\varepsilon,o_\varepsilon(1)}, \varepsilon \in (0,1))$ satisfies

$$\int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}_0(z)[\mathcal{H}_z] = \lim_{\varepsilon_n\to 0} E_{\varepsilon_n} = E_{\mathrm{gqc}}.$$

Therefore $\mathfrak{n}_0$ solves (gvp2), and thus it is concentrated on minimizers solving (GVP2). □

Proof of Corollary 1.17. This proof is completely analogous to that of Corollary 1.10. □

4. Concrete models

In this section we discuss the concrete models introduced in Section 1, and in particular we provide the proofs of results used in Section 3 that require a model-dependent treatment.

4A. ***The Nelson model.*** The simplest model under consideration is the so-called Nelson model [1964]. It consists of a small system of N nonrelativistic particles coupled with a scalar bosonic field, both moving in d spatial dimensions.

We recall the explicit expression of the quasiclassical energy (1-14) in the Nelson model:

$$\mathcal{H}_z = \sum_{j=1}^{N} \{-\Delta_j + \mathcal{V}_z(\boldsymbol{x}_j)\} + \mathcal{W}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) + \langle z|\omega|z\rangle_{\mathfrak{h}},$$

acting on $L^2(\mathbb{R}^{dN})$ and dependent on $z \in \mathfrak{h}$, where $\mathcal{V}_z$ is the potential (1-15), i.e., $\mathcal{V}_z(\boldsymbol{x}) = 2\mathrm{Re}\langle z|\lambda(\boldsymbol{x})\rangle_{\mathfrak{h}}$, $\mathcal{W} \in L^1_{\mathrm{loc}}(\mathbb{R}^{dN}; \mathbb{R}_+)$ is a field-independent potential,[6] e.g., a trap or an interaction between the particles, $\omega \geq 0$ is a self-adjoint operator on $\mathfrak{h}$ with an inverse that is possibly unbounded and λ, $\omega^{-1/2}\lambda \in L^\infty(\mathbb{R}^d, \mathfrak{h})$. Both $\mathcal{W}$ and $\mathcal{V}_z$ are multiplication operators and $\mathcal{H}_z$ is self-adjoint on $\mathscr{D}(-\Delta + \mathcal{W})$ and bounded from below for all $z \in \mathfrak{h}_\omega$. The associated quasiclassical energy of the system is the quadratic form $\mathcal{E}_{\mathrm{qc}}$, whose form domain is thus contained in $\mathscr{Q}(-\Delta + \mathcal{W}) \oplus \mathscr{Q}(\omega)$, where we recall that $\mathscr{Q}(A)$ stands for the quadratic form domain associated with the self-adjoint operator A.

The quasiclassical Wick quantization of $\mathcal{H}_z$ yields the quantum field Hamiltonian

$$H_\varepsilon = \sum_{j=1}^{N} \{-\Delta_j \otimes 1 + a_\varepsilon(\lambda(\boldsymbol{x}_j)) + a_\varepsilon^\dagger(\lambda(\boldsymbol{x}_j))\} + \mathcal{W}(\boldsymbol{x}_1, \dots, \boldsymbol{x}_N) \otimes 1 + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega)$$

acting on $\mathscr{H}_\varepsilon = L^2(\mathbb{R}^{dN}) \otimes \mathcal{G}_\varepsilon(\mathfrak{h})$, where we have explicitly highlighted the trivial action of some terms of H_ε on either the particle's or the field's degrees of freedom. Whenever $\lambda \in L^\infty(\mathbb{R}^d; \mathfrak{h})$, the operator H_ε is self-adjoint, with domain of essential self-adjointness

$$\mathscr{D}(-\Delta + \mathcal{W} + \mathrm{d}\mathcal{G}_\varepsilon(\omega)) \cap \mathscr{C}_0^\infty(\mathrm{d}\mathcal{G}_\varepsilon(1)),$$

where the latter is the set of vectors with a finite number of field excitations [Falconi 2015], but it may be unbounded from below if $0 \in \sigma(\omega)$. It is however well known that, if for a.e. $\boldsymbol{x} \in \mathbb{R}^d$ we have $\lambda(\boldsymbol{x}) \in \mathscr{D}(\omega^{-1/2})$, that we assume in (1-8), then H_ε is bounded from below by Kato–Rellich's theorem. Nonetheless, it may still not have a ground state if $0 \in \sigma(\omega)$ or if $\mathcal{W}$ is not regular enough. We simply remark here that the ground state exists if $0 \notin \sigma(\omega)$ and $-\Delta + \mathcal{W}$ has compact resolvent (trapped particle system), or if $0 \in \sigma(\omega)$ and λ and $\mathcal{W}$ satisfy suitable conditions, irrespective of compactness of the resolvent of $-\Delta + \mathcal{W}$.

Proof of Proposition 3.1. The upper and lower bounds in (3-4) are well known; see, e.g., [Ammari and Falconi 2014; Correggi and Falconi 2018; Ginibre et al. 2006]. The lower bound is a direct consequence of Kato–Rellich's inequality, while the upper bound is proved using coherent states for the field. We provide some details for the sake of completeness.

[6] Of course we may allow for a negative part of the potential $\mathcal{W}$, provided it is bounded, but we choose a positive potential for the sake of simplicity.

Setting[7]

$$H_{\mathrm{free}} := \mathcal{K}_0 \otimes 1 + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega), \tag{4-1}$$

we get, for all $\alpha > 0$ and all $\Psi_\varepsilon \in \mathscr{D}(H_{\mathrm{free}})$,

$$\begin{aligned}\Big\| \sum_{j=1}^{N} (a_\varepsilon(\lambda(\boldsymbol{x}_j)) + a_\varepsilon^\dagger(\lambda(\boldsymbol{x}_j)))\Psi_\varepsilon \Big\|_{\mathscr{H}_\varepsilon} & \\ &\le 2N \|\omega^{-1/2}\lambda\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})} \|\mathrm{d}\mathcal{G}_\varepsilon(\omega)^{1/2}\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon} + \sqrt{\varepsilon}\|\lambda\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})}\|\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon} \\ &\le \alpha\langle\Psi_\varepsilon|\mathrm{d}\mathcal{G}_\varepsilon(\omega)|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} + \Big[\frac{N^2}{\alpha}\|\omega^{-1/2}\lambda\|^2_{L^\infty(\mathbb{R}^d;\mathfrak{h})} + \sqrt{\varepsilon}\|\lambda\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})}\Big]\|\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}. \end{aligned} \tag{4-2}$$

Therefore, choosing $\alpha = 1$, we deduce that (recall that $\varepsilon \in (0, 1)$)

$$E_\varepsilon \ge -N^2\|\omega^{-1/2}\lambda\|^2_{L^\infty(\mathbb{R}^d;\mathfrak{h})} - \|\lambda\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})}. \tag{4-3}$$

The upper bound is trivial to show by exploiting (4-2) and evaluating the energy on any state such that $\langle\Psi_\varepsilon|\mathrm{d}\mathcal{G}_\varepsilon(\omega)|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \le C < +\infty$, e.g., a product state $\Psi_\varepsilon = \psi \otimes \Omega_\varepsilon$, with $\psi \in \mathscr{D}(\mathcal{K}_0)$ and Ω_ε the field vacuum. Note that the uniform boundedness of E_ε from above could as well be deduced by the boundedness of E_0, which in turn follows from the evaluation of $\mathcal{E}_{\mathrm{qc}}$ on, e.g., a configuration $(\psi, 0)$, with $\psi \in \mathscr{D}(\mathcal{K}_0)$. □

We now prove Lemmas 3.6 and 3.7 for the Nelson model. We have however to state first a technical result, which generalizes the convergence of expectation values proven in [Correggi et al. 2023]: indeed, in [Correggi et al. 2023, Proposition 2.6] it is shown that,[8] if

$$\langle\Psi_\varepsilon, (\mathrm{d}\mathcal{G}_\varepsilon(\omega)+1)^\delta\Psi_\varepsilon\rangle_{L^2(\mathbb{R}^{dN})\otimes\mathscr{H}_\varepsilon} \le C,$$

for any $\delta > \frac{1}{2}$, and $\Psi_{\varepsilon_n} \xrightarrow[n\to\infty]{\mathrm{qc}} \mathfrak{m}$, then, for all $\mathcal{K} \in \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))$,

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}|\mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z)\mathcal{K}\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{V}_z\mathcal{K}], \tag{4-4}$$

but our goal is to apply the above convergence to the identity, which is not compact. We have then to approximate it with compact operators.

Lemma 4.1. *If* (A4) *holds and there exist $C < +\infty$ and $\delta \ge 1$ such that, uniformly with respect to $\varepsilon \in (0, 1)$,*

$$\big|\langle\Psi_\varepsilon|(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega)^\delta + 1)|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\big| \le C \tag{4-5}$$

and $\Psi_{\varepsilon_n} \xrightarrow[\varepsilon_n\to 0]{\mathrm{qc}} \mathfrak{m}$, then, for all $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$ and any $j = 1, \dots, N$,

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}|\mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))\mathcal{B}\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{V}_z(\boldsymbol{x}_j)\mathcal{B}]. \tag{4-6}$$

[7] Even if not stated explicitly, we use the notation H_{free} also in Sections 4B and 4C with the same meaning.

[8] In [Correggi et al. 2023, Proposition 2.6] the result is proved for $\omega = 1$. The extension to a generic ω is done straightforwardly by combining the proof of Proposition 2.6 with the techniques introduced in [Falconi 2018a].

Proof. Let us introduce compact approximate identities $\{1_m\}_{m\in\mathbb{N}} \subset \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))$ as follows:

$$1_m := \mathbb{1}_{[-m,m]}(\mathcal{K}_0),$$

where $\mathbb{1}_{[-m,m]} : \mathbb{R} \to \{0, 1\}$ is the characteristic function of the interval $[-m, m]$, so that the right-hand side of the above expression is the usual spectral projector of $\mathcal{K}_0$ constructed via spectral theory. For later convenience, let us also define $\mathcal{B}_m := \mathcal{B}1_m$. Therefore, we have

$$\begin{aligned}\langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))\mathcal{B}\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} \\ = \langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))\mathcal{B}_m\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} + \langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))(\mathcal{B}-\mathcal{B}_m)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}. \end{aligned} \tag{4-7}$$

The first term on the right-hand side converges when $n \to \infty$ for any fixed $m \in \mathbb{N}$, since we have that $\mathcal{B}_m \in \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))$ (see (4-4)), i.e.,

$$\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))\mathcal{B}_m\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{V}_z(\boldsymbol{x}_j)\mathcal{B}_m].$$

By dominated convergence, we can then take the limit $m \to \infty$, to obtain

$$\lim_{m\to\infty}\lim_{n\to\infty} \langle \Psi_{\varepsilon_n} | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon_n}(\mathcal{V}_z(\boldsymbol{x}_j))\mathcal{B}_m\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mu_{\mathfrak{m}}(z)\,\mathrm{tr}_{L^2(\mathbb{R}^{dN})}[\gamma_{\mathfrak{m}}(z)\mathcal{V}_z(\boldsymbol{x}_j)\mathcal{B}]. \tag{4-8}$$

It remains to prove that

$$\lim_{m\to\infty}\sup_{\varepsilon\in(0,1)} \left|\langle \Psi_\varepsilon | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon}(\mathcal{V}_z(\boldsymbol{x}_j))(\mathcal{B}-\mathcal{B}_m)\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| = 0. \tag{4-9}$$

For any $0 < s \le \frac{1}{2}$ and for any $c_0 > |\inf \sigma(\mathcal{K}_0)|$,

$$\begin{aligned}&\left|\langle \Psi_\varepsilon | \mathrm{Op}^{\mathrm{Wick}}_{\varepsilon}(\mathcal{V}_z(\boldsymbol{x}_j))(\mathcal{B}-\mathcal{B}_m)\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \\ &\quad\le 2\|(\mathcal{B}-\mathcal{B}_m)(\mathcal{K}_0+c_0)^{-s/2}\|_{\mathscr{B}(L^2(\mathbb{R}^{dN}))}\|(\mathrm{d}\mathcal{G}_\varepsilon(\omega)^{1/2}+1)^{-1/2}a_\varepsilon(\lambda(\boldsymbol{x}_j))(\mathrm{d}\mathcal{G}_\varepsilon(\omega)^{1/2}+1)^{-1/2}\|_{\mathscr{B}(\mathscr{H}_\varepsilon)} \\ &\qquad\qquad \times \|(\mathrm{d}\mathcal{G}_\varepsilon(\omega)^{1/2}+1)^{1/2}(\mathcal{K}_0+c_0)^{s/2}\Psi_\varepsilon\|^2_{\mathscr{H}_\varepsilon} \\ &\quad\le C\|\mathcal{B}\|_{\mathscr{B}}\|(1-1_m)(\mathcal{K}_0+c_0)^{-s/2}\|_{\mathscr{B}}\|\omega^{-1/2}\lambda\|_{L^\infty(\mathbb{R}^d,\mathfrak{h})}\langle\Psi_\varepsilon|\mathcal{K}_0^{2s}+\mathrm{d}\mathcal{G}_\varepsilon(1)+1|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \\ &\quad\le C \sup_{\eta\in[(-\infty,-m)\cup(m,+\infty)]\cap\sigma(\mathcal{K}_0)} \frac{1}{(\eta+c_0)^{s/2}} \le Cm^{-s/2}\end{aligned}$$

for m large enough, e.g., larger than $|\inf\sigma(\mathcal{K}_0)|$. Therefore, since the above quantity vanishes as $m \to \infty$ uniformly with respect to $\varepsilon \in (0, 1)$, we conclude that (4-9) holds true and the result follows. □

Proof of Lemma 3.6. The result follows by taking $\mathcal{B} = 1$ in Lemma 4.1. Again, this makes crucial use of the fact that $\mathcal{K}_0 = -\Delta + \mathcal{W}$ has compact resolvent, and that Ψ_ε is regular enough with respect to $\mathcal{K}_0$. □

Proof of Lemma 3.7. The proof of Lemma 3.7 stems from a known result that allows us to compare the expectation of the square of the free energy H^2_{free} with the expectation of the square of the full Hamiltonian H^2_ε. This is a consequence of Kato–Rellich's inequality: there exists $C > 0$ (independent of ε) such that

$$\langle\Psi_\varepsilon|H^2_{\mathrm{free}}|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \le C\langle\Psi_\varepsilon|H^2_\varepsilon+1|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}. \tag{4-10}$$

The idea of the proof of this standard inequality goes as follows: From the triangular inequality we get

$$\langle\Psi_\varepsilon|H^2_{\mathrm{free}}|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \le 2\langle\Psi_\varepsilon|H^2_\varepsilon|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} + 2\langle\Psi_\varepsilon|(H_\varepsilon - H_{\mathrm{free}})^2|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}.$$

Now, using inequality (4-2), we get that for any $\alpha < 1/\sqrt{2}$,

$$(1-2\alpha^2)\langle\Psi_\varepsilon|H_{\text{free}}^2|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \le 2\langle\Psi_\varepsilon|H_\varepsilon^2|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} + C_\alpha\|\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}^2,$$

with C_α independent of ε. The result then easily follows.

It remains to prove that there exists a minimizing sequence $\{\Psi_{\varepsilon,\delta}\}_{\varepsilon,\delta\in(0,1)} \subset \mathscr{D}(H_\varepsilon)$ for H_ε such that

$$\langle\Psi_\varepsilon|H_\varepsilon^2|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \le \max\{E_\varepsilon^2, (E_\varepsilon+\delta)^2\} \le C, \tag{4-11}$$

with the last inequality given by Proposition 3.1. Indeed, combining the above estimate with (4-10), we immediately deduce that (3-17) holds true. Let us denote by $\mathbb{1}_{(a,b)}(H_\varepsilon)$ the spectral projections of H_ε, and by $\mathscr{P}_{(a,b)} := \mathbb{1}_{(\alpha,\beta)}(H_\varepsilon)\mathscr{H}_\varepsilon$ the associated spectral subspaces. Let us now choose, for any $\delta > 0$,

$$\Psi_{\varepsilon,\delta} \in \{\Psi \in \mathscr{P}_{(E_\varepsilon-\delta, E_\varepsilon+\delta)} : \|\Psi\|_{\mathscr{H}_\varepsilon} = 1\}.$$

Each spectral subspace above is not empty by definition of $E_\varepsilon = \inf\sigma(H_\varepsilon)$. Therefore, on one hand,

$$\langle\Psi_{\varepsilon,\delta}|H_\varepsilon|\Psi_{\varepsilon,\delta}\rangle_{\mathscr{H}_\varepsilon} \le E_\varepsilon + \delta,$$

and, on the other,

$$\|H_\varepsilon\Psi_{\varepsilon,\delta}\|_{\mathscr{H}_\varepsilon}^2 \le \max\{E_\varepsilon^2, (E_\varepsilon+\delta)^2\}. \qquad \square$$

It remains only to prove Lemma 3.10, used in the nontrapped case.

Proof of Lemma 3.10. To prove the result, it is sufficient to show that, if Ψ_ε is such that

$$\left|\langle\Psi_\varepsilon|(\mathrm{d}\mathcal{G}_\varepsilon(\omega)+1)^\delta|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \le C,$$

for some $\delta > \frac{1}{2}$ and some finite constant C, and if $\Psi_{\varepsilon_n} \xrightarrow[n\to\infty]{\text{gqc}} \mathfrak{n}$, then (3-30) holds true, i.e., for all $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$,

$$\lim_{n\to\infty}\langle\Psi_{\varepsilon_n}|\mathrm{Op}_{\varepsilon_n}^{\text{Wick}}(\mathcal{V}_z))\mathcal{B}\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_\varepsilon} = \int_{\mathfrak{h}_\omega} \mathrm{d}\mathfrak{n}[\mathcal{V}_z\mathcal{B}].$$

Such a result is however a special case of [Correggi et al. 2023, Proposition 2.6], if in that statement Wigner measures are substituted by generalized Wigner measures, the test with compact operators of the small system is replaced with the test with bounded operators, and $\mathrm{d}\mathcal{G}_\varepsilon(1)$ is replaced by $\mathrm{d}\mathcal{G}_\varepsilon(\omega)$. The proof given there is generalized to this setting straightforwardly, recalling the properties of generalized Wigner measures outlined in the Appendix. There is only one thing we need to mention explicitly: the integration of operator-valued functions with respect to generalized Wigner measures makes sense only if $\mathrm{Ran}(z \mapsto \mathcal{V}_z) \subset \mathscr{B}(L^2(\mathbb{R}^{dN}))$ is separable in the norm topology of $\mathscr{B}(L^2(\mathbb{R}^{dN}))$. Let us check explicitly that $\mathrm{Ran}(z \mapsto \mathcal{V}_z)$ is indeed separable: Since $\mathfrak{h}_\omega$ is separable, let us denote by $\mathfrak{k} \subset \mathfrak{h}_\omega$ a countable dense subset and denote by

$$\mathcal{V}_\mathfrak{k} := \{\mathcal{V}_\zeta(\boldsymbol{x}) \in \mathscr{B}(L^2(\mathbb{R}^{dN})) : \zeta \in \mathfrak{k}\}$$

the image of $\mathfrak{k}$ by means of $z \mapsto \mathcal{V}_z$. Now, for any $z \in \mathfrak{h}_\omega$, $\zeta \in \mathfrak{k}$, we have that

$$\|\mathcal{V}_z - \mathcal{V}_\zeta\|_{\mathscr{B}(L^2(\mathbb{R}^{dN}))} \le 2\|\omega^{-1/2}\lambda\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})}\|z-\zeta\|_{\mathfrak{h}_\omega},$$

which implies that $\mathcal{V}_\mathfrak{k}$ is dense in $\mathrm{Ran}(z \mapsto \mathcal{V}_z)$ with respect to the $\mathscr{B}(L^2(\mathbb{R}^{dN}))$-norm topology. $\square$

4B. ***The polaron model.*** The polaron model, introduced in [Fröhlich 1937], describes N electrons (spinless for simplicity) subjected to the vibrational (phonon) field of a lattice. This model is similar to Nelson's, however the coupling is slightly more singular. The one-excitation space is $\mathfrak{h} = L^2(\mathbb{R}^d)$, while the form factor is given by (1-9): the quasiclassical energy has the same form as in the Nelson model, as well as the effective potential $\mathcal{V}_z$ (see (1-15)), although now

$$\lambda(\boldsymbol{x};\boldsymbol{k}) = \sqrt{\alpha}\frac{e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}}{|\boldsymbol{k}|^{(d-1)/2}}, \quad \omega = 1,$$

where $\alpha > 0$ is a constant measuring the coupling's strength. The assumptions on $\mathcal{K}_0 = -\Delta + \mathcal{W}$ are the same as in the Nelson model. Let us remark that in this case since $\omega = 1$, we have that $\mathfrak{h}_\omega = \mathfrak{h}$.

The key difference with the aforementioned Nelson model is thus that there exists $z \in \mathfrak{h}$ such that

$$\mathcal{V}_z(\,\cdot\,) \notin L^\infty(\mathbb{R}^d),$$

due to the fact that $\lambda \notin L^\infty(\mathbb{R}^d;\mathfrak{h})$. However, it is possible to write $\mathcal{V}_z$ as the sum of an L^∞ function and the commutator between an L^∞ vector function and the momentum operator $-i\nabla_{\boldsymbol{x}}$:

$$\mathcal{V}_z(\boldsymbol{x}) = \sqrt{\alpha}(\mathcal{V}_{<,z}(\boldsymbol{x}) + [-i\nabla_{\boldsymbol{x}}, \boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x})]), \tag{4-12}$$

where

$$\mathcal{V}_{<,z}(\boldsymbol{x}) = 2\mathrm{Re}\mathscr{F}^{-1}[\lambda_< z](\boldsymbol{x}), \quad \lambda_<(\boldsymbol{k}) := \mathbb{1}_{|\boldsymbol{k}|\le\varrho}|\boldsymbol{k}|^{-(d-1)/2},$$
$$\boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x}) = 2\mathrm{Re}\mathscr{F}^{-1}[\boldsymbol{\lambda}_> z](\boldsymbol{x}), \quad \boldsymbol{\lambda}_>(\boldsymbol{k}) := \mathbb{1}_{|\boldsymbol{k}|>\varrho}|\boldsymbol{k}|^{-(d+1)/2}\hat{\boldsymbol{k}},$$

where $\hat{\boldsymbol{k}} := \boldsymbol{k}/|\boldsymbol{k}|$ and $\mathscr{F}$ stands for the Fourier transform in $\mathbb{R}^d$. Note that, for any $\varrho > 0$, we have that $\lambda_< \in \mathfrak{h}$ and $\boldsymbol{\lambda}_> \in \mathfrak{h} \otimes \mathbb{C}^d$. By the KLMN theorem, it then follows that $\mathcal{H}_z$ is self-adjoint and bounded from below for all $z \in \mathfrak{h}$, with z-independent form domain $\mathscr{Q}(\mathcal{H}_z) = \mathscr{Q}(\mathcal{K}_0)$. Let us remark that, choosing ρ suitably large (independent of z) in the above decomposition, it is possible to make the operator $\mathcal{H}_z$ bounded from below uniformly with respect to $z \in \mathfrak{h}$; see, e.g., [Correggi and Falconi 2018, Proposition 3.21].

The quasiclassical Wick quantization of $\mathcal{H}_z$ formally yields the same expression as in the Nelson model (with $\omega = 1$ and λ as above). Such a formal operator gives rise to a closed and bounded from below quadratic form, via the decomposition (4-12) (this can also be proved by the KLMN theorem, choosing ϱ sufficiently large; see, e.g., [Frank and Schlein 2014; Lieb and Thomas 1997]). We still denote the corresponding self-adjoint operator by H_ε with a little abuse of notation. The polaron Hamiltonian H_ε has a ground state, if $-\Delta + \mathcal{W}$ has compact resolvent by an application of the HVZ theorem analogous to the one for the Nelson model (see the aforementioned result in [Dereziński and Gérard 1999]). It is known that ground states exist also for nonconfining but suitably regular external potentials $\mathcal{W}$.

Proof of Proposition 3.1. These lower and upper bounds are well known; see, e.g., [Correggi and Falconi 2018; Lieb and Thomas 1997]. The lower bound is a direct consequence of the KLMN theorem, while the upper bound is proved using coherent states for the field in a fashion that is completely analogous to the one discussed for the Nelson model. Thus here we focus on the lower bound.

Let us introduce the unperturbed operator $H_{\mathrm{free}} = \mathcal{K}_0 \otimes 1 + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(1)$, as in the Nelson model. Then, for any $\Psi_\varepsilon \in \mathscr{Q}(H_{\mathrm{free}})$, for all $\varrho > 0$ and for all $\beta > 0$, we can bound the interaction term in the polaron quadratic form via

$$\begin{aligned}\left|\langle \Psi_\varepsilon | \mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\mathcal{V}_{<,z}(\boldsymbol{x})) - i\nabla_{\boldsymbol{x}} \cdot \mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x})) + i\mathrm{Op}_\varepsilon^{\mathrm{Wick}}(\boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x})) \cdot \nabla_{\boldsymbol{x}} | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \\ \leq 2\|\lambda_<\|_{\mathfrak{h}} \langle \Psi_\varepsilon | H_{\mathrm{free}}^{1/2} | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} + 4\|\boldsymbol{\lambda}_>\|_{\mathfrak{h}} \langle \Psi_\varepsilon | H_{\mathrm{free}} | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} \\ \leq \frac{1}{\beta}\|\lambda_<\|_{\mathfrak{h}}^2 \|\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}^2 + (\beta + 4\|\boldsymbol{\lambda}_>\|_{\mathfrak{h}}) \langle \Psi_\varepsilon | H_{\mathrm{free}} | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}.\end{aligned} \tag{4-13}$$

Obviously, the norms of $\lambda_<$ and $\boldsymbol{\lambda}_>$ depend on ϱ. However, since the norm of $\boldsymbol{\lambda}_>$ diverges as $\varrho \to 0$ and vanishes as $\varrho \to +\infty$, we can always choose $\varrho = \varrho(\beta)$ such that

$$4\|\boldsymbol{\lambda}_>\|_{\mathfrak{h}} = \beta. \tag{4-14}$$

Hence, we can bound

$$\left|\langle \Psi_\varepsilon | H_I | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \leq \sqrt{\alpha} N \Big[2\beta \langle \Psi_\varepsilon | H_{\mathrm{free}} | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon} + \frac{1}{\beta}\|\lambda_<\|_{\mathfrak{h}}^2 \|\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}^2\Big],$$

and therefore, taking $\beta = (2\sqrt{\alpha}N)^{-1}$, we conclude that

$$E_\varepsilon \geq -2\alpha N^2 \|\lambda_<\|_{\mathfrak{h}}^2, \tag{4-15}$$

where the last norm is evaluated at $\varrho((2\sqrt{\alpha}N)^{-1})$. □

Let us now prove Lemmas 3.6 and 3.7. The assumption in the former takes the following simplified form for the polaron model: assuming that there exists a finite constant C such that

$$\left|\langle \Psi_\varepsilon | (\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(1)^2 + 1) | \Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}\right| \leq C, \tag{4-16}$$

the convergence (3-18) holds true for any limit point in $\mathscr{W}(\Psi_\varepsilon, \varepsilon \in (0, 1))$.

Proof of Lemma 3.6. Using again the splitting (4-12), we see that the term involving the quantization of $\mathcal{V}_{<,z}$ converges by Lemma 4.1. Let us consider then the other term. Analogously to the proof of Lemma 4.1, we define compact approximate identities $\{1_m\}_{m\in\mathbb{N}} \subset \mathscr{L}^\infty(L^2(\mathbb{R}^{dN}))$ as

$$1_m := \mathbb{1}_{[-m,m]}(\mathcal{K}_0).$$

We can now rewrite explicitly the term involving the quantization of $\boldsymbol{\mathcal{V}}_{>,z}$, by introducing $\boldsymbol{\xi} \in L^\infty(\mathbb{R}^d; \mathfrak{h})$ given by

$$\boldsymbol{\xi}(\boldsymbol{x}; \boldsymbol{k}) := \boldsymbol{\lambda}_> e^{-i\boldsymbol{k}\cdot\boldsymbol{x}}, \tag{4-17}$$

as

$$\begin{aligned}\sqrt{\alpha} \sum_{j=1}^N \langle \Psi_{\varepsilon_n} | [-i\nabla_j, \mathrm{Op}_{\varepsilon_n}^{(\mathrm{Wick})}(\boldsymbol{\mathcal{V}}_>(\boldsymbol{x}_j))] | \Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}} \\ = 2\sqrt{\alpha} \sum_{j=1}^N \mathrm{Re}\langle -i\nabla_j \Psi_{\varepsilon_n} | [a_{\varepsilon_n}^\dagger(\boldsymbol{\xi}(\boldsymbol{x}_j)) + a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))] \Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}.\end{aligned} \tag{4-18}$$

In order to prove its convergence, we estimate

$$\begin{aligned}\left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))]\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right| &\\ \le \left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))]1_m\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right| &\\ + \left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))](1-1_m)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right|. &\quad (4\text{-}19)\end{aligned}$$

The first term on the right-hand side converges when $n\to\infty$ and $m\in\mathbb{N}$ is fixed, thanks to [Correggi et al. 2023, Proposition 7.1]; then, a dominated convergence argument allows us to take the limit $m\to\infty$, yielding the desired result. It remains therefore to prove that the second term on the right-hand side converges to zero as $m\to\infty$, uniformly with respect to $\varepsilon\in(0,1)$. This is done as follows:

$$\begin{aligned}\left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))](1-1_m)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right| &\\ \le \|\nabla_j\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}\|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))](1-1_m)\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon} &\\ \le 2(\varepsilon+\|\boldsymbol{\xi}\|_{L^\infty(\mathbb{R}^d;\mathfrak{h})})\|\nabla_j\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}\|(\mathrm{d}\mathcal{G}_\varepsilon(1)+1)^{1/2}(1-1_m)\Psi_\varepsilon\|_{\mathscr{H}_\varepsilon}. &\quad (4\text{-}20)\end{aligned}$$

Thus, for all $\beta>0$, $\varepsilon\in(0,1)$ and $s>0$ and for any $c_0>|\inf\sigma(\mathcal{K}_0)|$,

$$\begin{aligned}&\left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))](1-1_m)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right|\\ &\le (1+\|\boldsymbol{\xi}\|_{L^\infty})\Big[\beta\|\mathcal{K}_0^{1/2}\Psi_\varepsilon\|^2_{\mathscr{H}_\varepsilon}\\ &\qquad+\frac{1}{\beta}\|(1-1_m)(\mathcal{K}_0+c_0)^{-s/2}\|^2_{\mathscr{B}(L^2(\mathbb{R}^{dN}))}\|(\mathrm{d}\mathcal{G}_\varepsilon(1)+1)^{1/2}(\mathcal{K}_0+c_0)^{s/2}\Psi_\varepsilon\|^2_{\mathscr{H}_\varepsilon}\Big]\\ &\le 2(1+\|\boldsymbol{\xi}\|_{L^\infty})\Big(\beta+\frac{1}{\beta}\|(1-1_m)(\mathcal{K}_0+c_0)^{-s/2}\|^2_{\mathscr{B}}\Big)\langle\Psi_\varepsilon|\mathcal{K}_0+\mathcal{K}_0^{2s}+\mathrm{d}\mathcal{G}_\varepsilon(1)^2+1|\Psi_\varepsilon\rangle_{\mathscr{H}_\varepsilon}. \qquad (4\text{-}21)\end{aligned}$$

Hence, using (4-16), for any $s\le\frac{1}{2}$, we get

$$\left|\langle -i\nabla_j\Psi_{\varepsilon_n}|[a^\dagger_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))+a_{\varepsilon_n}(\boldsymbol{\xi}(\boldsymbol{x}_j))](1-1_m)\Psi_{\varepsilon_n}\rangle_{\mathscr{H}_{\varepsilon_n}}\right|\le C\beta_m, \qquad (4\text{-}22)$$

where we have chosen

$$\beta=\beta_m:=\|(1-1_m)(\mathcal{K}_0+c_0)^{-s/2}\|_{\mathscr{B}}=\sup_{\eta\in[(-\infty,-m)\cup(m,+\infty)]\cap\sigma(\mathcal{K}_0)}\frac{1}{(\eta+c_0)^{s/2}}\xrightarrow[m\to\infty]{}0.$$

Since the right-hand side of (4-22) is independent of ε and converges to zero as $m\to\infty$, the result is proven. □

Proof of Lemma 3.7. The proof is analogous to the one for the Nelson model. The expectation of the number operator squared is bounded via the *pull-through formula* by means of the expectation of H_ε^2. As discussed in [Correggi et al. 2023], the pull-through formula was originally proved for the renormalized Nelson Hamiltonian with a bound that is ε-dependent in [Ammari 2000]; the uniformity of such bound with respect to $\varepsilon\in(0,1)$ has been proved in [Ammari and Falconi 2017]. Since the renormalized Nelson model "contains" all type of terms appearing in the polaron model, the proof of the formula extends to the polaron model immediately, see [Olivieri 2020] for additional details.

The pull-through formula reads as follows: there exists a finite constant C (independent of ε) such that

$$\langle \Psi_\varepsilon | \mathrm{d}\mathcal{G}_\varepsilon(1)^2 | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon} \le C \langle \Psi_\varepsilon | (H_\varepsilon + 1)^2 | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon}. \tag{4-23}$$

The expectation of H_{free} is bounded by means of the expectation of H_ε, using the KLMN inequality, already discussed in the proof of Proposition 3.1, in the very same way we used the Kato–Rellich inequality for the Nelson model. The fact that there exists a minimizing sequence such that the expectation of H_ε^2 is bounded uniformly with respect to $\varepsilon \in (0, 1)$ is also discussed in the proof for the Nelson model and it does not depend on the model at hand. We omit further details for the sake of brevity. □

It remains only to prove Lemma 3.10 for nontrapping potentials.

Proof of Lemma 3.10. The proof uses the following fact: if Ψ_ε is such that there exists $\delta \ge 1$ and a finite constant C such that

$$\left| \langle \Psi_\varepsilon | (\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(1)^\delta + 1) | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon} \right| \le C, \tag{4-24}$$

then, if $\mathfrak{n} \in \mathscr{GW}(\Psi_\varepsilon, \varepsilon \in (0, 1))$ and $\Psi_{\varepsilon_n} \xrightarrow[n\to\infty]{\text{gqc}} \mathfrak{n}$, one has that (3-30) holds true.

Such a result is proved by a combination of [Correggi et al. 2023, Propositions 2.6 and 7.1], if in these propositions Wigner measures are substituted by generalized Wigner measures and the test with compact operators of the small system is substituted by the test with the identity operator. The proof given there is generalized to this setting straightforwardly, recalling the properties of generalized Wigner measures outlined in the Appendix.

As in the proof for the Nelson model, let us check explicitly that $\mathrm{Ran}(z \mapsto \mathcal{V}_z)$ is separable in the norm operator topology.[9] By using the decomposition (4-12), we see that the term containing $\mathcal{V}_{<,z}$ has separable range, since it is equivalent to the one appearing in the Nelson model. Let us focus then on the remaining term containing the expectation of the operator $[-i\nabla_x, \boldsymbol{\mathcal{V}}_{>,z}]$. Such an operator is not bounded. Nonetheless, it is $\mathfrak{n}_{\mathcal{T}}$-integrable with $\mathcal{T} = \mathcal{K}_0 + 1$ by (4-24), provided that

$$\mathfrak{h} \ni z \mapsto \sum_{j=1}^{N} \mathcal{T}^{-1/2} [-i\nabla_j, \boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x}_j)] \mathcal{T}^{-1/2} \in \mathscr{B}(L^2(\mathbb{R}^{dN})) \tag{4-25}$$

has separable range. Since $\mathfrak{h}$ is separable, let us denote by $\mathfrak{k} \subset \mathfrak{h}$ a countable dense subset and denote by

$$\mathcal{T}^{-1/2} \widetilde{\mathcal{V}}_{\mathfrak{k}} \mathcal{T}^{-1/2} := \left\{ \sum_j \mathcal{T}^{-1/2} [-i\nabla_j, \boldsymbol{\mathcal{V}}_{>,\zeta(\boldsymbol{x}_j)}] \mathcal{T}^{-1/2} \in \mathscr{B}(L^2(\mathbb{R}^{dN})) : \zeta \in \mathfrak{k} \right\}$$

the image of $\mathfrak{k}$ through $\mathcal{T}^{-1/2} \sum_j [-i\nabla_j, \boldsymbol{\mathcal{V}}_{>,\,\cdot\,}(\boldsymbol{x}_j)] \mathcal{T}^{-1/2}$. Now, for any $z \in \mathfrak{h}$, $\zeta \in \mathfrak{k}$ and $j = 1, \ldots, N$, we have that (recall (4-17))

$$\| \mathcal{T}^{-1/2} [-i\nabla_j, \boldsymbol{\mathcal{V}}_{>,z}(\boldsymbol{x}_j)] \mathcal{T}^{-1/2} - \mathcal{T}^{-1/2} [-i\nabla_j, \boldsymbol{\mathcal{V}}_{>,\zeta}(\boldsymbol{x}_j)] \mathcal{T}^{-1/2} \|_{\mathscr{B}(L^2(\mathbb{R}^{dN}))} \le 4 \|\boldsymbol{\xi}\|_{L^\infty} \|z - \zeta\|_{\mathfrak{h}},$$

which implies that $\mathcal{T}^{-1/2} \widetilde{\mathcal{V}}_{\mathfrak{k}} \mathcal{T}^{-1/2}$ is dense in the image of the map (4-25) with respect to the norm topology in $\mathscr{B}(L^2(\mathbb{R}^{dN}))$. □

[9] More precisely, we prove that $\mathrm{Ran}(z \mapsto (\mathcal{K}_0 + 1)^{-1/2} \mathcal{V}_z (\mathcal{K}_0 + 1)^{-1/2})$ has separable range. This is sufficient to prove that $\mathcal{V}_{(\,\cdot\,)}$ is integrable with respect to $\mathfrak{n}$, since the latter is in the domain of $\mathcal{K}_0 + 1$.

4C. ***The Pauli–Fierz model.*** The Pauli–Fierz model describes N spinless charges (with an extended and sufficiently smooth charge distribution) interacting with the electromagnetic field in the Coulomb gauge, in three dimensions. Generalizations to other gauges, to particles with spin or to two dimensions are possible without much effort. The one-excitation Hilbert space is thus $\mathfrak{h} = L^2(\mathbb{R}^3; \mathbb{C}^2)$. Let the charge density of each particle be given by $\lambda_j(\boldsymbol{x})$, with $\lambda_j \in L^\infty(\mathbb{R}^3; L^2(\mathbb{R}^3))$, $j = 1, \ldots, N$, such that $-i\nabla_j \lambda_j(\boldsymbol{x}; \boldsymbol{k}) = \boldsymbol{k}\lambda_j(\boldsymbol{x}; \boldsymbol{k})$ and let the polarization vectors be denoted $\boldsymbol{e}_p \in L^\infty(\mathbb{R}^3; \mathbb{R}^3)$, $p = 1, 2$, such that for a.e. $\boldsymbol{k} \in \mathbb{R}^3$ and $\boldsymbol{e}_p(\boldsymbol{k}) \cdot \boldsymbol{e}_{p'}(\boldsymbol{k}) = \delta_{pp'}$, $\boldsymbol{k} \cdot \boldsymbol{e}_p(\boldsymbol{k}) = 0$ (Coulomb gauge). The quasiclassical energy functional is then given by (1-17), i.e.,[10]

$$\mathcal{H}_z = \sum_{j=1}^{N} \frac{1}{2m_j} (-i\nabla_j + \boldsymbol{a}_{z,j}(\boldsymbol{x}_j))^2 + \mathcal{W}(\boldsymbol{X}) + \langle z|\omega|z\rangle_{\mathfrak{h}},$$

where the classical field is

$$\boldsymbol{a}_{z,j}(\boldsymbol{x}) = 2\mathrm{Re}\langle z|\boldsymbol{\lambda}_j(\boldsymbol{x})\rangle_{\mathfrak{h}} = 2\mathrm{Re} \sum_{p=1}^{2} \langle z_p|\lambda_j(\boldsymbol{x})\boldsymbol{e}_p\rangle_{L^2(\mathbb{R}^3)} \in \mathbb{C}^3$$

and, as usual, $\mathcal{W}$ is an external positive potential acting on the particles. Note that the field free energy is

$$\langle z|\omega|z\rangle_{\mathfrak{h}} = \sum_{p=1}^{2} \langle z_p|\omega|z_p\rangle_{L^2(\mathbb{R}^3)}.$$

The operator $\mathcal{H}_z$ is self-adjoint for all $z \in \mathfrak{h}_\omega$, with domain of self-adjointness $\mathscr{D}(\mathcal{K}_0)$, where we recall that $\mathcal{K}_0 = -\Delta + \mathcal{W}$, where in this case we adopt the notation

$$-\Delta = \sum_{j=1}^{N} -\frac{\Delta_j}{2m_j}.$$

The quasiclassical Wick quantization of $\mathcal{H}_z$ yields the Pauli–Fierz Hamiltonian in (1-10):

$$H_\varepsilon = \sum_{j=1}^{N} \frac{1}{2m_j} (-i\nabla_j + \boldsymbol{A}_{\varepsilon,j}(\boldsymbol{x}_j))^2 + \mathcal{W}(\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N) + 1 \otimes \mathrm{d}\mathcal{G}_\varepsilon(\omega),$$

where

$$\boldsymbol{A}_{\varepsilon,j}(\boldsymbol{x}) = a_\varepsilon^\dagger(\boldsymbol{\lambda}_j(\boldsymbol{x})) + a_\varepsilon(\boldsymbol{\lambda}_j(\boldsymbol{x})) = \sum_{p=1}^{2} (a_{\varepsilon,p}^\dagger(\lambda_j(\boldsymbol{x})\boldsymbol{e}_p) + a_{\varepsilon,p}(\lambda_j(\boldsymbol{x})\boldsymbol{e}_p))$$

is the quantized magnetic potential. The Pauli–Fierz Hamiltonian is self-adjoint on $\mathscr{D}(\mathcal{K}_0 + \mathrm{d}\mathcal{G}_\varepsilon(\omega))$, provided that for almost all $\boldsymbol{x} \in \mathbb{R}^3$ and for all $j = 1, \ldots, N$, we have $\lambda_j(\boldsymbol{x}) \in \mathscr{Q}(\omega + \omega^{-1})$ (see [Falconi 2015; Hasler and Herbst 2008; Hiroshima 2000; 2002; Matte 2017]), that we assumed in (1-11). The Pauli–Fierz Hamiltonian has a ground state for suitable choices of the potential $\mathcal{W}$, e.g., if it is the sum of single particle and pair potentials with suitable properties (clustering, binding, etc.); see, e.g., [Arai et al. 1999; Gérard 2000; Griesemer et al. 2001; Hiroshima 2001]. In particular, this holds true when the field is massive [Gérard 2000], i.e., for $\omega > 0$. As for the other models, we refrain from giving a detailed

[10] Without loss of generality, we fix the charge $e = 1$ since it does not play any relevant role in these arguments.

description of the conditions allowing them to have a ground state, since for our purposes it is sufficient that a ground state does exist in some cases.

Proof of Proposition 3.1. The lower bound follows from the diamagnetic inequality [Matte 2017]:

$$\langle \Psi_\varepsilon | -\Delta_j | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon} \leq \langle \Psi_\varepsilon | (-i\nabla_j + \boldsymbol{A}_{\varepsilon,j}(\boldsymbol{x}_j))^2 | \Psi_\varepsilon \rangle_{\mathscr{H}_\varepsilon}, \tag{4-26}$$

which in particular implies that H_ε is positive. The upper bound is proved using coherent states for the field, analogously to the Nelson model and the polaron. □

Let us now prove Lemmas 3.6 and 3.7 for the Pauli–Fierz model. The former takes the following form.

Proof of Lemma 3.6. The "potential" (1-16) is composed of two parts:

$$\mathcal{V}_z(\boldsymbol{x}) = 2\sum_{j=1}^{N} \frac{1}{m_j}[-i\mathrm{Re}\langle z|\boldsymbol{\lambda}_j(\boldsymbol{x})\rangle_{\mathfrak{h}} \cdot \nabla_j + (\mathrm{Re}\langle z|\boldsymbol{\lambda}_j(\boldsymbol{x})\rangle_{\mathfrak{h}})^2]$$

as well as its Wick quantization. The convergence of the quantization of the second term is perfectly analogous to the one given for the Nelson model in Lemma 4.1. The proof of convergence for the quantization of the term involving the gradient is given in the proof of Lemma 3.6 for the polaron. □

Proof of Lemma 3.7. The proof follows from the next estimate, due to F. Hiroshima, and whose detailed proof will be given in [Ammari et al. 2022]. There exists a finite constant $C > 0$ such that, for all $\Psi_\varepsilon \in \mathscr{D}(H_{\mathrm{free}})$,

$$\| H_{\mathrm{free}} \Psi_\varepsilon \|_{\mathscr{H}_\varepsilon} \leq C \| H_\varepsilon \Psi_\varepsilon \|_{\mathscr{H}_\varepsilon}. \tag{4-27}$$

Let us remark that the expectation of

$$\mathcal{K}_0 = -\sum_j (1/(2m_j))\Delta_j + \mathcal{W}$$

could also be bounded by means of the expectation of H_ε using the diamagnetic inequality (4-26). Hence if $\omega > 0$, (3-19) could be proved combining the diamagnetic inequality and the pull-through formula (4-23).

Finally, the fact that there exists a minimizing sequence such that the expectation of H_ε^2 is bounded uniformly with respect to $\varepsilon \in (0, 1)$ is also discussed in the proof of Lemma 3.7 for the Nelson model. □

It remains only to prove Lemma 3.10 for nontrapped systems.

Proof of Lemma 3.10. The proof here is obtained combining the proofs given for the Nelson and polaron models. In fact, the quadratic terms can be treated exactly as the linear terms in the Nelson model, and the gradient terms are equivalent to those appearing in the polaron. □

Appendix: Algebraic state-valued measures

The quasiclassical Wigner measures are state-valued by construction [Correggi et al. 2023; Falconi 2018b]. In other words, quasiclassical measures are countably additive (in a sense to be clarified below) measures on the measurable phase space of classical fields, taking values in quantum states, or, more generally, in the Banach cone $\mathfrak{A}'_+$ of positive elements in the dual of a C*-algebra $\mathfrak{A}$. In addition, the quasiclassical symbols are measurable functions from the phase space to a W*-algebra $\mathfrak{B} \supseteq \mathfrak{A}$ of observables (operators), where $\mathfrak{A}$ is supposed to be an ideal of $\mathfrak{B}$. It is therefore necessary to properly define integration of operator-valued symbols with respect to a state-valued measure. In this appendix we collect some technical properties of state-valued measures and integration, from a general algebraic standpoint that includes both state-valued and generalized state-valued measures, as used throughout the paper. The ideas developed here in great generality are particularly suited for what we called generalized state-valued measures, and they are mostly taken from [Bartle 1956; Neeb 1998]. In fact, if state-valued measures have been already studied in semiclassical analysis and adiabatic theories (see [Balazard-Konlein 1985; Fermanian-Kammerer and Gérard 2002; Gérard 1991; Gérard et al. 1991; Teufel 2003]), the reader might not be so familiar with generalized state-valued measures. Since for the latter there is no Radon–Nikodým property, their description is more abstract, and there are some limitations, especially concerning integration of operator-valued functions. This justifies the abstract approach followed in this appendix.

A1. *Algebraic state-valued measures.* Let $\mathfrak{A}$ be a C*-algebra and denote by $\mathfrak{A}'_+$ the cone of positive elements in the dual of $\mathfrak{A}$. In addition, let (X, Σ) be a measurable space. There are two *equivalent* ways of defining an $\mathfrak{A}'_+$-valued measure on (X, Σ).

Definition A.1 (state-valued measure [Neeb 1998]). A family of real-valued measures $(\mu_A)_{A\in\mathfrak{A}_+}$ defines a weak* σ-additive measure $\mathfrak{m} : \Sigma \to \mathfrak{A}'_+$ as

$$[\mathfrak{m}(S)](A_1 - A_2 + iA_3 - iA_4) = \mu_{A_1}(S) - \mu_{A_2}(S) + i\mu_{A_3}(S) - i\mu_{A_4}(S),$$

for any $S \in \Sigma$ and $A_1, A_2, A_3, A_4 \in \mathfrak{A}_+$, if and only if for any $A, B \in \mathfrak{A}_+$ and $\lambda \in \mathbb{R}_+$, we have $\mu_{\lambda A+B} = \lambda\mu_A + \mu_B$.

Definition A.2 (algebraic state-valued measure [Bartle 1956]). An application $\mathfrak{m} : \Sigma \to \mathfrak{A}'_+$ is a measure if and only if $\mathfrak{m}(\varnothing) = 0$, and for any family $(S_n)_{n\in\mathbb{N}} \subset \Sigma$ of mutually disjoint measurable sets,

$$\mathfrak{m}\Bigl(\bigcup_{n\in\mathbb{N}} S_n\Bigr) = \sum_{n\in\mathbb{N}} \mathfrak{m}(S_n),$$

where the right-hand side converges unconditionally in the norm of $\mathfrak{A}'$.

It is clear that any $\mathfrak{m}$ satisfying Definition A.2 satisfies also Definition A.1, since σ-additivity in norm implies weak* σ-additivity. The converse, i.e., that an $\mathfrak{m}$ satisfying Definition A.1 also satisfies Definition A.2 is nontrivial, and follows from properties of uniform boundedness in Banach spaces, as proved in [Dunford 1938, Chapter II]. We use these two definitions interchangeably, depending on the context. Let us remark that with the definitions above, any state-valued measure is automatically finite, since $\mathfrak{m}(X) \in \mathfrak{A}'_+$. Actually, in the main body of the paper, we consider probability measures, i.e., $\|\mathfrak{m}(X)\|_{\mathfrak{A}'} = 1$.

Remark A.3 (state-valued and generalized state-valued measures). The state-valued measures used in the paper correspond to choosing $\mathfrak{A} = \mathscr{L}^\infty(\mathscr{H})$; generalized state-valued measures are in a subset of the measures obtained by picking $\mathfrak{A} = \mathscr{L}^1(\mathscr{H})$.

For algebraic state-valued (cylindrical) measures on vector spaces, Bochner's theorem holds, and the Fourier transforms are completely positive maps that are weak* continuous when restricted to any finite-dimensional subspace; see [Falconi 2018b] for additional details. An algebraic state-valued measure is also *monotone*:

Lemma A.4. *For any* $S_1 \subseteq S_2 \in \Sigma$,

$$\mathfrak{m}(S_1) \leq \mathfrak{m}(S_2),$$

i.e., $\mathfrak{m}(S_2) - \mathfrak{m}(S_1) \in \mathfrak{A}'_+$.

Proof. The scalar measures $\mu_A,\ A \in \mathfrak{A}_+$, are monotonic. Therefore, for all $A \in \mathfrak{A}_+$,

$$[\mathfrak{m}(S_2)](A) := \mu_A(S_2) \geq \mu_A(S_1) =: [\mathfrak{m}(S_1)](A). \tag{A-1}$$

Hence, for all $A \in \mathfrak{A}_+$,

$$[\mathfrak{m}(S_2) - \mathfrak{m}(S_1)](A) \geq 0. \qquad \square$$

We can now introduce the scalar norm measure m, satisfying $\mu_A(S) \leq \|A\|_{\mathfrak{A}} m(S)$, for any $S \in \Sigma$, that proves to be a very useful tool to compare vector integrals with scalar integrals.

Definition A.5 (norm measure). Let $\mathfrak{m}$ be an algebraic state-valued measure. Then, its norm measure $m : \Sigma \to \mathbb{R}_+$ is defined as

$$m(S) := \|\mathfrak{m}(S)\|_{\mathfrak{A}'}, \tag{A-2}$$

for any measurable set S.

Using the cone properties of positive states in a C*-algebra, it is possible to prove that m is a finite measure. Let us recall that the C*-algebra $\mathfrak{A}$ may not be unital, so from now on we assume that there exists a W*-algebra $\mathfrak{B} \supseteq \mathfrak{A}$. If $\mathfrak{A} = \mathscr{L}^\infty(\mathscr{K})$ — the compact operators on a separable Hilbert space $\mathscr{K}$ — and $\mathfrak{B} = \mathscr{B}(\mathscr{K})$, it is well known that the aforementioned property is satisfied: $\mathfrak{A}$ is actually in this case a two-sided ideal of $\mathfrak{B}$. Let us denote by $e \in \mathfrak{B}$ the identity element.

Proposition A.6 (properties of the norm measure). *Let* $\mathfrak{m}$ *be an algebraic state-valued measure. Then its norm measure m is a finite measure on* (X, Σ) *and* $\mathfrak{m} \ll m$.

Proof. The proof that $m(\varnothing) = 0$ and $m(X) < +\infty$ follows immediately from the definition, while σ-additivity is proved as follows: Let $(S_n)_{n\in\mathbb{N}} \subset \Sigma$ be a family of mutually disjoint measurable sets. We are going to prove that, for any $N \in \mathbb{N}$,

$$m\biggl(\bigcup_{n=1}^{N} S_n\biggr) = \sum_{n=1}^{N} m(S_n). \tag{A-3}$$

Indeed, let $(e_\alpha)_{\alpha\in I} \subset \mathfrak{A}_+$ be an approximate identity of $e \in \mathfrak{B}$. It is well known that for any $\omega \in \mathfrak{A}'_+$ we have $\|\omega\|_{\mathfrak{A}'} = \lim_{\alpha\in I} \omega(w_\alpha)$. Hence, by Definition A.1 and Definition A.5,

$$m\biggl(\bigcup_{n=1}^{N} S_n\biggr) = \lim_{\alpha\in I} \mathfrak{m}\biggl(\bigcup_{n=1}^{N} S_n\biggr)(e_\alpha) = \lim_{\alpha\in I} \mu_{e_\alpha}\biggl(\bigcup_{n=1}^{N} S_n\biggr) = \lim_{\alpha\in I} \sum_{n=1}^{N} \mu_{e_\alpha}(S_n) = \sum_{n=1}^{N} m(S_n).$$

Next, we show

$$\lim_{N\to\infty} m\Bigl(\bigcup_{n\in\mathbb{N}} S_n\Bigr) - \sum_{n=1}^{N} m(S_n) = 0, \tag{A-4}$$

which directly implies σ-additivity: Using again the approximate identity on the left-hand side, we obtain

$$\lim_{N\to\infty} \lim_{\alpha\in I} m\Bigl(\bigcup_{n\in\mathbb{N}} S_n\Bigr) - \sum_{n=1}^{N} \mu_{e_\alpha}(S_n).$$

We know that every μ_{e_α}, $\alpha \in I$, is σ-additive, and therefore that $\lim_{N\to\infty} \sum_{n=1}^{N} \mu_{e_\alpha}(S_n) = \mu_{e_\alpha}\bigl(\bigcup_{n\in\mathbb{N}} S_n\bigr)$ and $\lim_{\alpha\in I} \mu_{e_\alpha}\bigl(\bigcup_{n\in\mathbb{N}} S_n\bigr) = m\bigl(\bigcup_{n\in\mathbb{N}} S_n\bigr)$. Hence, it remains to show that the limits in N and α can be exchanged. In order to do that, it suffices to show that the limit in α exists uniformly with respect to N:

$$\begin{aligned}\lim_{\alpha\in I} \sup_{N\in\mathbb{N}} \Bigl| m\Bigl(\bigcup_{n=1}^{N} S_n\Bigr) - \sum_{n=1}^{N} \mu_{e_\alpha}(S_n)\Bigr| &= \lim_{\alpha\in I} \sup_{N\in\mathbb{N}} \Bigl| m\Bigl(\bigcup_{n=1}^{N} S_n\Bigr) - \mu_{e_\alpha}\Bigl(\bigcup_{n=1}^{N} S_n\Bigr)\Bigr| \\ &= \lim_{\alpha\in I} \sup_{N\in\mathbb{N}} (m - \mu_{e_\alpha})\Bigl(\bigcup_{n=1}^{N} S_n\Bigr) \\ &\le \lim_{\alpha\in I} (m - \mu_{e_\alpha})(X) = 0, \end{aligned} \tag{A-5}$$

where we have used finite additivity of m and $m - \mu_{e_\alpha}$ and the fact that for any $S \in \Sigma$, $\mu_{e_\alpha}(S) \le m(S)$.

It remains to prove that $\mathfrak{m}$ is absolutely continuous with respect to m. For absolute continuity of a vector measure with respect to a scalar measure, we adopt the definition of [Diestel and Uhl 1977, Section I.2, Definition 3]. Since both $\mathfrak{m}$ and m are countably additive, it suffices to prove that, for any $S \in \Sigma$, $m(S) = 0$ implies $\mathfrak{m}(S) = 0$. However, since $m(S) = \|\mathfrak{m}(S)\|_{\mathfrak{A}'}$ and $\|\cdot\|_{\mathfrak{A}'}$ is a norm, then the aforementioned implication follows directly by the properties of norms. □

A2. ***Integration of scalar functions.*** The theory of integration for algebraic state-valued measures could be done in a unified way for scalar- and operator-valued functions. However, it is instructive to deal with scalar functions first. Let us recall that a function $g : X \to \mathbb{R}^+$ is simple if there exist a number $N \in \mathbb{N}$, mutually disjoint measurable sets $S_1, \ldots, S_N \in \Sigma$ and nonnegative numbers $c_1, \ldots, c_N \in \mathbb{R}^+$, such that, for all $x \in X$,

$$g(x) = \sum_{j=1}^{N} c_j \mathbb{1}_{S_j}(x), \tag{A-6}$$

where $\mathbb{1}_{S_j}$ is the characteristic function of the set S_j. Integration of simple functions with respect to an algebraic state-valued measure μ is straightforwardly defined as

$$\int_X d\mathfrak{m}(x) g(x) = \sum_{j=1}^{N} c_j \mathfrak{m}(S_j) \in \mathfrak{A}'_+. \tag{A-7}$$

The integral of a nonsimple function can be defined again in two equivalent ways.

Definition A.7 (integrability I [Neeb 1998, Lemma I.12]). We say that a measurable function $f : X \to \mathbb{R}^+$ is $\mathfrak{m}$-integrable if and only if f is μ_A-integrable for any $A \in \mathfrak{A}_+$. Furthermore, its integral belongs to $\mathfrak{A}'_+$ and is uniquely defined by the integral with respect to μ_A, i.e.,

$$\Bigl(\int_S \mathrm{d}\mathfrak{m}(x) f(x)\Bigr)(A_1 - A_2 + iA_3 - iA_4) = \int_S \mathrm{d}\mu_{A_1}(x) f(x) - \int_S \mathrm{d}\mu_{A_2}(x) f(x) + i \int_S \mathrm{d}\mu_{A_3}(x) f(x) - i \int_S \mathrm{d}\mu_{A_4}(x) f(x), \quad \text{(A-8)}$$

for any $A_1, A_2, A_3, A_4 \in \mathfrak{A}_+$.

Definition A.8 (integrability II [Bartle 1956, Definition 1]). We say that a measurable function $f : X \to \mathbb{R}^+$ is $\mathfrak{m}$-integrable if and only if for any $S \in \Sigma$ the sequence of simple integrals

$$\Bigl\{\int_X \mathrm{d}\mathfrak{m}(x) f_n(x) \mathbb{1}_S(x)\Bigr\}_{n\in\mathbb{N}} \in \mathfrak{A}'$$

is Cauchy, where $(f_n)_{n\in\mathbb{N}}$ is any approximation of f in terms of simple functions. The integral is then defined as

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) = \lim_{n\to\infty} \int_X \mathrm{d}\mathfrak{m}(x) f_n(x) \mathbb{1}_S(x), \quad \text{(A-9)}$$

and it is independent of the chosen approximation.

In both cases one says that a complex function $f : X \to \mathbb{C}$ is μ-integrable if and only if $|f|$ is $\mathfrak{m}$-integrable and, in this case, its integral is given by the complex combination of the integrals of its real positive, real negative, imaginary positive and imaginary negative parts.

Since the weak* and strong limits coincide if they both exist, it follows that the integrals of a function that is $\mathfrak{m}$-integrable with respect to Definitions A.7 and A.8 coincide. In addition, if f is $\mathfrak{m}$-integrable in the "strong" sense of Definition A.8, then it is also $\mathfrak{m}$-integrable in the weak* sense of Definition A.7. It remains to show that if f is $\mathfrak{m}$-integrable in the sense of Definition A.7, then it is $\mathfrak{m}$-integrable in the sense of Definition A.8, but this can be done by exploiting the norm measure m.

Lemma A.9. *If a measurable function $f : X \to \mathbb{R}^+$ is $\mathfrak{m}$-integrable in the sense of Definition A.7, then it is m-integrable as well.*

Proof. If f is $\mathfrak{m}$-integrable, then for any $S \in \Sigma$, $\int_S \mathrm{d}\mu_A(x) f(x)$ is finite and nonnegative for any $A \in \mathfrak{A}_+$. Applying [Neeb 1998, Lemma I.5], we deduce that there exists a finite constant C, depending only on S, $\mathfrak{m}$, and f, such that

$$\int_S \mathrm{d}\mu_A(x) f(x) \le C \|A\|_{\mathfrak{A}}. \quad \text{(A-10)}$$

Now, let $(f_n)_{n\in\mathbb{N}}$ be a simple pointwise nondecreasing approximation of f from below. Then, by the monotone convergence theorem,

$$\int_S \mathrm{d}m(x) f(x) = \lim_{n\to\infty} \int_X \mathrm{d}m(x) f_n(x) \mathbb{1}_S(x).$$

Hence, by Definition A.5 and μ_{e_α}-integrability of f,

$$\int_X \mathrm{d}m(x) f_n(x) \mathbb{1}_S(x) = \lim_{\alpha\in I} \int_X \mathrm{d}\mu_{e_\alpha}(x) f_n(x)\mathbb{1}_S(x) \le \lim_{\alpha\in I} \int_S \mathrm{d}\mu_{e_\alpha}(x) f(x) \le C \lim_{\alpha\in I} \|e_\alpha\|_{\mathfrak{A}} \le C, \quad \text{(A-11)}$$

and taking the limit $n \to \infty$, we get the result. □

Proposition A.10 (equivalence of Definitions A.7 and A.8). *If a measurable function $f : X \to \mathbb{R}^+$ is $\mathfrak{m}$-integrable in the sense of Definition A.7, then it is $\mathfrak{m}$-integrable in the sense of Definition A.8. In addition, for any $S \in \Sigma$,*

$$\left\| \int_S \mathrm{d}\mathfrak{m}(x) f(x) \right\|_{\mathfrak{A}'} \le \int_S \mathrm{d}m(x) f(x). \quad \text{(A-12)}$$

Proof. We prove that

$$\left\{ \int_S \mathrm{d}\mathfrak{m}(x) f_n(x) \right\}_{n\in\mathbb{N}} \in \mathfrak{A}'_+$$

is a Cauchy sequence, where $(f_n)_{n\in\mathbb{N}}$ is a nondecreasing simple approximation of f. Observe that for any $n \ge m \in \mathbb{N}$, $f_n - f_m$ is a simple positive function, which can be written as

$$f_n - f_m = \sum_{j=1}^{N(n,m)} c_j^{(n,m)} \mathbb{1}_{S_j^{(n,m)}}. \quad \text{(A-13)}$$

Hence,

$$\left\| \int_S \mathrm{d}\mathfrak{m}(x)(f_n(x) - f_m(x)) \right\|_{\mathfrak{A}'} \le \sum_{j=1}^{N(n,m)} c_j^{(n,m)} m(S_j^{(n,m)} \cap S) = \int_S \mathrm{d}m(x)(f_n - f_m)(x) \xrightarrow[n,m\to\infty]{} 0, \quad \text{(A-14)}$$

where in the last limit we have used the dominated convergence theorem, since $f_n - f_m \le 2f$, and f is m-integrable by Lemma A.9. This proves both $\mathfrak{m}$-integrability of f in the sense of Definition A.8, and the bound (A-12). □

Therefore, the two definitions are indeed equivalent: Definition A.8 has the advantage of identifying constructively the integral as the limit of the integrals of simple approximations of the integrand, while Definition A.7 is useful to prove properties of the integral. The integral defined above is indeed linear in the integrand and monotonic.

Lemma A.11. *Let $f, g : X \to \mathbb{R}$ be two $\mathfrak{m}$-integrable functions. If for $\mathfrak{m}$-a.e. $x \in X$ we have that $g(x) \le f(x)$, then*

$$\int_X \mathrm{d}\mathfrak{m}(x)(f(x) - g(x)) \in \mathfrak{A}'_+. \quad \text{(A-15)}$$

Proof. The result follows from Definition A.7 and monotonicity of the usual integral. □

The dominated convergence theorem holds in a general form (see Theorems A.17 and A.18 below), which in particular implies that it applies to scalar functions.

A3. ***Integration of operator-valued functions.*** The integration of operator-valued functions is defined similarly to Definition A.8. Let us discuss first the integration of simple operator-valued functions and the approximation with simple functions in this context. An operator-valued function $g : X \to \mathfrak{B}$ is simple if there exist $N \in \mathbb{N}$, mutually disjoint measurable sets $S_1, \dots, S_N \in \Sigma$ and $c_1, \dots, c_N \in \mathfrak{B}$ such that for all $x \in X$,

$$g(x) = \sum_{j=1}^{N} c_j \mathbb{1}_{S_j}(x). \tag{A-16}$$

Let us recall that since $\mathfrak{A} \subset \mathfrak{B}$, for any $\omega \in \mathfrak{A}'$ and $B \in \mathfrak{B}$, we can define $\omega \circ B \in \mathfrak{A}'$ as

$$(\omega \circ B)(\,\cdot\,) := \omega(\,\cdot\, B) \quad \text{or} \quad (\omega \circ B)(\,\cdot\,) := \omega(B\,\cdot\,), \tag{A-17}$$

depending on which side $\mathfrak{A}$ is an ideal of $\mathfrak{B}$. If it is a two-sided ideal, both definitions are equivalent. Keeping this definition in mind, we can define the integral of simple functions as

$$\int_X \mathrm{d}\mathfrak{m}(x) g(x) = \sum_{j=1}^{N} \mathfrak{m}(S_j) \circ c_j \in \mathfrak{A}'. \tag{A-18}$$

Next, we recall hypotheses under which an operator-valued function admits a simple approximation.

Proposition A.12 (simple approximation [Cohn 2013, Proposition E.2]). *Let $f : X \to \mathfrak{B}$ be a measurable function. If $f(X)$ is separable, then f admits a simple approximation, i.e., there exists a sequence $\{f_n\}_{n\in\mathbb{N}}$ of simple functions such that for all $x \in X$ and $n \in \mathbb{N}$,*

$$\|f_n(x)\|_{\mathfrak{B}} \le \|f(x)\|_{\mathfrak{B}} \quad \textit{and} \quad \lim_{n\to\infty} \|f(x) - f_n(x)\|_{\mathfrak{B}} = 0. \tag{A-19}$$

Due to this result, in the following we only consider operator-valued functions with *separable range*, even if not stated explicitly.

Definition A.13 (integrability III). A measurable function with separable range $f : X \to \mathfrak{B}$ is $\mathfrak{m}$-integrable if and only if, for any $S \in \Sigma$, the sequence of simple integrals

$$\left\{ \int_X \mathrm{d}\mathfrak{m}(x) f_n(x) \mathbb{1}_S(x) \right\}_{n\in\mathbb{N}} \in \mathfrak{A}' \tag{A-20}$$

is Cauchy, where $\{f_n\}_{n\in\mathbb{N}}$ is any approximation of f in terms of simple functions. The integral is then defined as

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) = \lim_{n\to\infty} \int_X \mathrm{d}\mathfrak{m}(x) f_n(x) \mathbb{1}_S(x), \tag{A-21}$$

and it is independent of the chosen approximation.

Definition A.14 (absolute integrability). A measurable function with separable range $f : X \to \mathfrak{B}$ is $\mathfrak{m}$-absolutely integrable if and only if $\|f(\,\cdot\,)\|_{\mathfrak{B}}$ is m-integrable.

In fact, any $\mathfrak{m}$-absolutely integrable function is also $\mathfrak{m}$-integrable.

Proposition A.15 (integrability and absolute integrability). *Let $f : X \to \mathfrak{B}$ be an $\mathfrak{m}$-absolutely integrable function. Then f is also $\mathfrak{m}$-integrable and, for all $S \in \Sigma$,*

$$\left\| \int_S \mathrm{d}\mathfrak{m}(x) f(x) \right\|_{\mathfrak{A}'} \le \int_S \mathrm{d}m(x) \| f(x) \|_{\mathfrak{B}}. \tag{A-22}$$

Proof. The proof is completely analogous to that of Proposition A.10. We omit it for the sake of brevity. □

Corollary A.16 (integrability of bounded functions). *Any function $f : X \to \mathfrak{B}$ with separable range such that $\| f(\cdot) \|_{\mathfrak{B}}$ is m-a.e. uniformly bounded is $\mathfrak{m}$-integrable.*

We are now in a position to state two versions of the dominated convergence theorem for operator-valued functions. The second, that makes crucial use of absolute integrability, is the most convenient in our concrete applications. Note that both results easily apply to the special case of scalar functions discussed in the previous section.

Theorem A.17 (dominated convergence I [Bartle 1956, Theorem 6]). *Let $\{f_n\}_{n\in\mathbb{N}}$, $f_n : X \to \mathfrak{B}$ for all $n \in \mathbb{N}$, be a sequence of $\mathfrak{m}$-integrable operator-valued functions strongly converging $\mathfrak{m}$-a.e. to $f : X \to \mathfrak{B}$. If there exists an $\mathfrak{m}$-integrable operator-valued function g such that for all $n \in \mathbb{N}$ and $S \in \Sigma$*

$$\left\| \int_S \mathrm{d}\mathfrak{m}(x) f_n(x) \right\| \le \left\| \int_S \mathrm{d}\mathfrak{m}(x) g(x) \right\|, \tag{A-23}$$

then f is $\mathfrak{m}$-integrable and for any $S \in \Sigma$

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) = \lim_{n\to\infty} \int_S \mathrm{d}\mathfrak{m}(x) f_n(x). \tag{A-24}$$

Theorem A.18 (dominated convergence II). *Let $\{f_n\}_{n\in\mathbb{N}}$, $f_n : X \to \mathfrak{B}$ for all $n \in \mathbb{N}$, be a sequence of operator-valued functions strongly converging μ-a.e. to $f : X \to \mathfrak{B}$. If there exists an m-integrable function $G : X \to \mathbb{R}^+$ such that $\mathfrak{m}$-a.e.*

$$\| f_n(x) \|_{\mathfrak{B}} \le G(x), \tag{A-25}$$

then, for any $n \in \mathbb{N}$, f_n and f are $\mathfrak{m}$-absolutely integrable, and

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) = \lim_{n\to\infty} \int_S \mathrm{d}\mathfrak{m}(x) f_n(x). \tag{A-26}$$

Proof. By the dominated convergence theorem for scalar measures and functions applied to m and $\{\| f_n(\cdot) \|_{\mathfrak{B}}\}_{n\in\mathbb{N}}$, respectively, we get that $\| f_n(\cdot) \|_{\mathfrak{B}}$ and $\| f(\cdot) \|_{\mathfrak{B}}$ are both m-integrable and therefore, by Proposition A.15, it follows that f_n and f are also $\mathfrak{m}$-integrable. Now, for any $S \in \Sigma$, again by Proposition A.15,

$$\left\| \int_S \mathrm{d}\mathfrak{m}(x)(f - f_n)(x) \right\|_{\mathfrak{A}'} \le \int_S \mathrm{d}m(x) \| (f - f_n)(x) \|_{\mathfrak{B}}.$$

Therefore by the dominated convergence theorem for m applied to the sequence of scalar functions $\{\| (f - f_n)(x) \|_{\mathfrak{B}}\}_{n\in\mathbb{N}}$, it follows that in the strong topology of $\mathfrak{A}'$,

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) = \lim_{n\to\infty} \int_S \mathrm{d}\mathfrak{m}(x) f_n(x). \qquad \square$$

A4. ***Integration of functions with values in unbounded operators.*** Let us restrict attention, for this section, to the concrete case $\mathfrak{A} = \mathscr{B}(L^2(\mathbb{R}^{dN}))$. In the applications described above, it is sometimes necessary to integrate functions from some measurable space X to the unbounded operators on $L^2(\mathbb{R}^{dN})$ (albeit with a rather explicit form). It is possible to define the integration of such functions with respect to suitable generalized state-valued measures, as already outlined in Section 2B. Let us repeat here the argument for the sake of completeness.

Let $\mathcal{T} > 0$ be an operator on $L^2(\mathbb{R}^{dN})$, possibly unbounded. A generalized state-valued measure is in the domain of $\mathcal{T}$ if and only if there exists a generalized state-valued measure $\mathfrak{n}_{\mathcal{T}}$ such that for all $\mathcal{B} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$ and for any $S \in \Sigma$,

$$\mathfrak{n}_{\mathcal{T}}(S)[\mathcal{T}^{-1/2}\mathcal{B}\mathcal{T}^{-1/2}] = \mathfrak{n}(S)[\mathcal{B}].$$

Given a measure in the domain of $\mathcal{T}$, we can integrate functions singular "at most as $\mathcal{T}$". Let $\mathcal{F}$ be a function from X to the (closed and densely defined) operators on $L^2(\mathbb{R}^{dN})$. Then $\mathcal{F}$ is $\mathfrak{n}$-absolutely integrable, with $\mathfrak{n}$ in the domain of $\mathcal{T}$, if and only if for $\mathfrak{n}$-a.e. $x \in X$,

- $\mathcal{T}^{-1/2}\mathcal{F}(x)\mathcal{T}^{-1/2} \in \mathscr{B}(L^2(\mathbb{R}^{dN}))$;
- $\mathcal{T}^{-1/2}\mathcal{F}(x)\mathcal{T}^{-1/2}$ is $\mathfrak{n}_{\mathcal{T}}$-absolutely integrable.

Given an absolutely integrable function, we can define the integral as follows: for any $S \in \Sigma$,

$$\int_S d\mathfrak{n}(x)[\mathcal{F}(x)] = \int_S d\mathfrak{n}_{\mathcal{T}}(x)[\mathcal{T}^{-1/2}\mathcal{F}(x)\mathcal{T}^{-1/2}].$$

A5. ***Two-sided integration.*** If $\mathfrak{A}$ is a two-sided ideal of $\mathfrak{B}$, we can give a slight generalization of the operator-valued integration, to accommodate integration of one function to the left and one function to the right of the measure. We use the notations and definitions of Section A3. Let $g, h : X \to \mathfrak{B}$ be two simple functions,

$$g(x) = \sum_{j=1}^{N} c_j \mathbb{1}_{S_j}(x), \quad h(x) = \sum_{j=1}^{M} d_j \mathbb{1}_{T_j}(x).$$

In addition, for any $B, C \in \mathfrak{B}$ and for any $\omega \in \mathfrak{A}'$, let us define $B \circ \omega \circ C \in \mathfrak{A}'$ by

$$(B \circ \omega \circ C)(\,\cdot\,) := \omega(B \cdot C). \tag{A-27}$$

Hence, it is possible to define two-sided simple integration as

$$\int_X g(x) d\mathfrak{m}(x) h(x) = \sum_{j=1}^{N}\sum_{k=1}^{M} c_j \circ \mu(S_j \cap T_k) \circ d_k. \tag{A-28}$$

Moreover, if $f_1, f_2 : X \to \mathfrak{B}$ have separable range, it is straightforward to extend Definition A.13 to define the two-sided integral

$$\int_S f_1(x) d\mathfrak{m}(x) f_2(x) \in \mathfrak{A}'. \tag{A-29}$$

If the above integral exists, we say that the pair f_1, f_2 is $\mathfrak{m}$-two-sided-integrable (the order is relevant). This notion also preserves positivity: for all f such that f^*, f is $\mathfrak{m}$-two-sided-integrable, then

$$\int_S f^*(x)\mathrm{d}\mathfrak{m}(x)f(x) \in \mathfrak{A}'_+. \tag{A-30}$$

A pair of functions with separable range $f_1, f_2 : X \to \mathfrak{B}$ are $\mathfrak{m}$-two-sided-absolutely integrable if and only if $\|f_1(\cdot)\|_{\mathfrak{B}}\|f_2(\cdot)\|_{\mathfrak{B}}$ is m-integrable. The analogue of Proposition A.15 is the following.

Proposition A.19 (integrability and absolute integrability). *Let $f_1, f_2 : X \to \mathfrak{B}$ be $\mathfrak{m}$-two-sided-absolutely integrable. Then, f_1, f_2 and f_2, f_1 are both $\mathfrak{m}$-two-sided-integrable and, for all $S \in \Sigma$,*

$$\left\| \int_S f_1(x)\mathrm{d}\mathfrak{m}(x) f_2(x) \right\|_{\mathfrak{A}'} \le \int_S \mathrm{d}m(x) \|f_1(x)\|_{\mathfrak{B}} \|f_2(x)\|_{\mathfrak{B}}, \tag{A-31}$$

with analogous bound when f_1 and f_2 are exchanged on the left-hand side.

Finally, dominated convergence applies to two-sided integration too.

Theorem A.20 (dominated convergence III). *Let $\{f_n\}_{n\in\mathbb{N}}$ and $\{g_n\}_{n\in\mathbb{N}}$, $f_n, g_n : X \to \mathfrak{B}$ for all $n \in \mathbb{N}$, be two sequences of operator-valued functions strongly converging $\mathfrak{m}$-a.e. to $f, g : X \to \mathfrak{B}$, respectively. If there exists an m-square-integrable function $G : X \to \mathbb{R}^+$ such that $\mathfrak{m}$-a.e.*

$$\|f_n(x)\|_{\mathfrak{B}} \le G(x), \quad \|g_n(x)\|_{\mathfrak{B}} \le G(x), \tag{A-32}$$

then, for any $n \in \mathbb{N}$, f_n, g_n and f, g are $\mathfrak{m}$-two-sided-absolutely integrable, and

$$\int_S f(x)\mathrm{d}\mathfrak{m}(x)g(x) = \lim_{n\to\infty} \int_S f_n(x)\mathrm{d}\mathfrak{m}(x)g_n(x), \tag{A-33}$$

$$\int_S g(x)\mathrm{d}\mathfrak{m}(x)f(x) = \lim_{n\to\infty} \int_S g_n(x)\mathrm{d}\mathfrak{m}(x)f_n(x). \tag{A-34}$$

A6. *Radon–Nikodým property and push-forward.* If an operator-valued function does not have a separable range, it may fail to have an approximation with simple functions. It is possible to give an alternative definition of integration if $\mathfrak{A}'$ is a *separable* space, as it is the case for the trace class operators on a separable Hilbert space $\mathscr{L}^1(\mathscr{K})$, thanks to the following property.

Theorem A.21 (Radon–Nikodým property [Dunford and Pettis 1940, Theorem 2.1.0]). *If $\mathfrak{A}'$ is separable, then it has the **Radon–Nikodým property**: for every algebraic state-valued measure $\mathfrak{m}$, there exists a function $\varrho : X \to \mathfrak{A}'_+$, which is m-Bochner-integrable and such that, for all $S \in \Sigma$,*

$$\mathfrak{m}(S) = \int_S \mathrm{d}m(x)\varrho(x). \tag{A-35}$$

*The function ϱ is the **Radon–Nikodým derivative** of $\mathfrak{m}$ with respect to m, denoted by $\varrho = \mathrm{d}\mathfrak{m}/\mathrm{d}m$.*

Therefore, it is natural to give the following alternative definition of integrability. Recall that for any $\Gamma \in \mathfrak{A}'$ and $B \in \mathfrak{B}$ we define $(\Gamma \circ B)(\cdot) = \Gamma(B\,\cdot)$ if $\mathfrak{A}$ is a left ideal of $\mathfrak{B}$, and $(\Gamma \circ B)(\cdot) = \Gamma(\cdot\, B)$ if $\mathfrak{A}$ is a right ideal of $\mathfrak{B}$. If $\mathfrak{A}$ is a two-sided ideal, the notation ΓB denotes indifferently either of the two. In this case, for any $B, C \in \mathfrak{B}$, we can define $(B \circ \Gamma \circ C)(\cdot) = \Gamma(B \cdot C)$.

Definition A.22 (integrability IV). Suppose that $\mathfrak{A}'$ is separable, and let $f, g : X \to \mathfrak{B}$ be measurable functions (possibly with nonseparable range) and $\mathfrak{m}$ be an algebraic state-valued measure with Radon–Nikodým derivative $\varrho = \mathrm{d}\mathfrak{m}/\mathrm{d}m$. Then f is $\mathfrak{m}$-integrable if and only if $\varrho \circ f \in \mathfrak{A}'$ is m-Bochner-integrable and, for any $S \in \Sigma$,

$$\int_S \mathrm{d}\mathfrak{m}(x) f(x) := \int_S \mathrm{d}m(x)\varrho(x) \circ f(x) \in \mathfrak{A}'. \tag{A-36}$$

If in addition $\mathfrak{A}$ is a two-sided ideal of $\mathfrak{B}$, then f, g is $\mathfrak{m}$-two-sided-integrable if and only if $f\varrho g \in \mathfrak{A}'$ is m-Bochner-integrable and, for any $S \in \Sigma$,

$$\int_S f(x)\mathrm{d}\mathfrak{m}(x) g(x) := \int_S \mathrm{d}m(x) f(x) \circ \varrho(x) \circ g(x) \in \mathfrak{A}'. \tag{A-37}$$

It is straightforward to see that Definition A.22 is equivalent to Definition A.13 and the analogous one for the two-sided integral for any f, g with separable range, and therefore Definition A.22 extends Definition A.13 to any separable $\mathfrak{A}'$. In addition, since m-Bochner-integrability is equivalent to $\mathfrak{m}$-absolute integrability, it follows that, if $\mathfrak{A}'$ is separable, then $\mathfrak{m}$-integrability is equivalent to $\mathfrak{m}$-absolute-integrability. Hence, all the results of Sections A2, A3 and A5 extend, if $\mathfrak{A}'$ is separable, to functions with nonseparable range.

Suppose now that X is a topological vector space and Σ is the corresponding Borel σ-algebra. In this context, Bochner's theorem holds for algebraic state-valued measures [Falconi 2018b]: the Fourier transform

$$\widehat{\mathfrak{m}}(\xi) := \int_X \mathrm{d}\mathfrak{m}(x) e^{2i\xi(x)} \in \mathfrak{A}', \quad \text{with } \xi \in X', \tag{A-38}$$

identifies uniquely a measure. Therefore, the push-forward of an algebraic state-valued measure $\mathfrak{m}$ by means of a linear continuous map $\Phi : X \to Y$, where Y is again a topological vector space with the Borel σ-algebra, is conveniently defined using the Fourier transform, and this definition suffices for the purposes of this paper: more precisely, the push-forward measure $\Phi \sharp \mathfrak{m}$ is the measure on Y whose Fourier transform is defined by

$$(\widehat{\Phi \sharp \mathfrak{m}})(\eta) := \int_X \mathrm{d}\mathfrak{m}(x) e^{2i\eta(\Phi(x))} \in \mathfrak{A}', \quad \text{with } \eta \in Y'. \tag{A-39}$$

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MICHELE CORREGGI: michele.correggi@polimi.it
Dipartimento di Matematica, Politecnico di Milano, Milan, Italy

MARCO FALCONI: marco.falconi@polimi.it
Dipartimento di Matematica, Politecnico di Milano, Milan, Italy

MARCO OLIVIERI: olivieri.math@gmail.com
Fakultät für Mathematik, Karlsruhe Institut für Technologie, Karlsruhe, Germany
Current address: *Department of Mathematics, Aarhus Universitet, Aarhus, Denmark*

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