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CONVERGENCE OF STATES FOR POLARON MODELS IN THE CLASSICAL LIMIT

MARCO FALCONI, ALESSANDRO OLGIATI, AND NICOLAS ROUGERIE

ABSTRACT. We consider the quasi-classical limit of Nelson-type regularized polaron models describing a particle interacting with a quantized bosonic field. We break translation-invariance by adding an attractive external potential decaying at infinity, acting on the particle. In the strong coupling limit where the field behaves classically we prove that the model's energy quasi-minimizers strongly converge to ground states of the limiting Pekar-like non-linear model. This holds for arbitrarily small external attractive potentials, hence this binding is fully due to the interaction with the bosonic field. We use a new approach to the construction of quasi-classical measures to revisit energy convergence, and a localization method in a concentration-compactness type argument to obtain convergence of states.

CONTENTS

| | |
|---|----|
| 1. Introduction | 1 |
| 2. Main results | 3 |
| 2.1. Model | 3 |
| 2.2. Statements | 6 |
| 2.3. Organization of the paper | 7 |
| 3. Reduced densities, localization of states and localization of energies | 8 |
| 3.1. Reduced densities | 8 |
| 3.2. Localization of states | 10 |
| 3.3. Energy localization | 12 |
| 4. Quasi-classical measures | 16 |
| 4.1. Notation | 16 |
| 4.2. The theorem | 16 |
| 4.3. Proof of Theorem 4.3 | 19 |
| 5. Convergence of the energy | 22 |
| 5.1. Generalized Pekar energies | 23 |
| 5.2. Proof of Theorem 5.1 | 25 |
| 6. Convergence of states, proof of Theorem 2.3 | 26 |
| References | 29 |

1. INTRODUCTION

A quantum particle interacting with a quantized bosonic field (e.g. an electron interacting with the phonons of a crystal) may exhibit self-trapping: the particle is confined in a “hole” of its own making in the field. Usual linear models (Fröhlich’s polaron, Nelson model) are translation invariant

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and this phenomenon thus may not take the form of existence of actual bound states. One of the strongest mathematical evidence for the phenomenon is the existence of energy minimizers for the non-linear quasi-classical approximations of the models. In the case of the Fröhlich polaron [46, 56], the limiting model is Pekar's, for which the existence and uniqueness (up to translations) of ground states was proven in [40, 44]. Other related models also exhibit this phenomenon, some being studied e.g. in [6, 7, 25, 24, 38, 39, 48].

The validity of the quasi-classical approximation has been established in [15, 42, 45] in the strong-coupling limit at the level of the ground state energy. Quantum corrections are investigated in [8, 23, 20]. The corresponding dynamical problem is considered e.g. in [11, 22, 33, 32, 18, 27, 26]. If a trapping external potential (increasing to infinity at spatial infinity) is further added to the model, the convergence of ground energy states to quasi-classical minimizers is proved in [12].

Here we shall break the translation invariance by an arbitrarily small, decaying, external attractive potential, and prove that this is sufficient for self-trapping in the quasi-classical limit. For simplicity we consider Nelson-type models with regular particle-field interactions, where the definition of the Hamiltonian

$$H_\alpha^{(V)} := (-\Delta + V) \otimes \mathbb{1} + \alpha^{-2} \left(\mathbb{1} \otimes \int_{\mathbb{R}^d} T(k) \hat{c}^\dagger(k) \hat{c}(k) dk + \alpha \int_{\mathbb{R}^d} (e^{ik \cdot x} \hat{v}(k) \hat{c}^\dagger(k) + \text{h.c.}) dk \right) \quad (1.1)$$

as a self-adjoint operator is straightforward (the Lieb-Yamakazi method [43] or Gross transformation [56] are not needed). The above acts on

$$\mathfrak{H} := L^2(\mathbb{R}^d) \otimes \mathfrak{F}(L^2(\mathbb{R}^d)), \quad (1.2)$$

the tensor product of the particle and field Hilbert spaces, the latter being the bosonic Fock space constructed from the one-particle space $L^2(\mathbb{R}^d)$,

$$\mathfrak{F}(L^2(\mathbb{R}^d)) = \bigoplus_{n \geq 0} (L^2(\mathbb{R}^d))^{\otimes_{\text{sym}} n}.$$

The particle's coordinate is labeled by x , i.e. $e^{ik \cdot x}$ acts as multiplication on the particle's side. The standard bosonic operators $\hat{c}^\dagger(k), \hat{c}(k)$ create/annihilate a field excitation in the Fourier mode $k \in \mathbb{R}^d$, and satisfy usual canonical commutation relations (CCR).

The limit $\alpha \rightarrow \infty$ is a strong coupling one. A heuristic square completion in the second term of (1.1) indicates that the number of field excitations is of order α^2 in this limit. To obtain a well-defined limit we therefore multiply all terms involving the field degrees of freedom in (1.1) by α^{-2} . For the true Fröhlich polaron model, this is equivalent to a change of length/energy units [56].

One can see the strong coupling regime as a quasi-classical limit (i.e. a semi-classical limit for the field degrees of freedom only) by redefining creators/annihilators in the manner

$$\hat{a}^\dagger(k) := \alpha^{-1} \hat{c}^\dagger(k), \quad \hat{a}(k) := \alpha^{-1} \hat{c}(k) \quad (1.3)$$

so that

$$H_\alpha^{(V)} := (-\Delta + V) \otimes \mathbb{1} + \mathbb{1} \otimes \int_{\mathbb{R}^d} T(k) \hat{a}^\dagger(k) \hat{a}(k) + \int_{\mathbb{R}^d} (e^{ik \cdot x} \hat{v}(k) \hat{a}^\dagger(k) + \text{h.c.}) \quad (1.4)$$

and

$$[\hat{a}(k), \hat{a}^\dagger(k')] = \alpha^{-2} \delta_{k=k'}, \quad [\hat{a}(k), \hat{a}(k')] = 0, \quad [\hat{a}^\dagger(k), \hat{a}^\dagger(k')] = 0 \quad (1.5)$$

for all $k, k' \in \mathbb{R}^d$. The data of the problem are

- The field's dispersion relation $T : \mathbb{R}^d \mapsto \mathbb{R}^+$ for which we assume a gap at 0, to avoid infrared problems. In polaron models one typically takes $T \equiv 1$.
- The field-particle interaction potential $v \in L^2(\mathbb{R}^d)$. For the Fröhlich polaron one should consider a singular dipole-charge interaction, something we could include with extra effort.
- The external potential $V : \mathbb{R}^d \mapsto \mathbb{R}^-$. Our point is that it can be arbitrarily small (but negative), so that we impose $V(x) \xrightarrow{|x| \rightarrow \infty} 0$.

We give more precise definitions and assumptions below. Our main goal is to show that binding holds in the $\alpha \rightarrow \infty$ limit for arbitrary V decaying at infinity, thus generalizing results of [12] applying to trapping potentials. We opt to consider only the case $v \in L^2(\mathbb{R}^d)$ because the difficulties linked to singular v on the one hand, and to lack of trapping on the other hand are rather orthogonal.

Our analysis bears on sequences of approximate ground states for $H_\alpha^{(V)}$, whose energy reproduce the infimum of the spectrum up to small corrections in the limit $\alpha \rightarrow \infty$. Let a sequence $(\Psi_\alpha)_\alpha \in \mathfrak{H}$ be such that

$$\langle \Psi_\alpha | H_\alpha^{(V)} \Psi_\alpha \rangle_{\mathfrak{H}} \leq \inf \sigma(H_\alpha^{(V)}) + o_\alpha(1), \quad \|\Psi_\alpha\|_{\mathfrak{H}} = 1. \quad (1.6)$$

In particular we can take for each α a sequence $(\Psi_{n,\alpha})_n$ such that

$$\langle \Psi_{n,\alpha} | H_\alpha^{(V)} \Psi_{n,\alpha} \rangle_{\mathfrak{H}} \xrightarrow{n \rightarrow \infty} \inf \sigma(H_\alpha^{(V)})$$

and diagonally extract a subsequence $(\Psi_{n,\alpha(n)})_n$. A consequence of our main results below is that if

$$\gamma_\alpha := \text{Tr}_{\mathfrak{F}(L^2(\mathbb{R}^d))} (|\Psi_\alpha\rangle\langle\Psi_\alpha|) \quad (1.7)$$

is the particle's (reduced) density matrix then

$$\boxed{\gamma_\alpha \xrightarrow{\alpha \rightarrow \infty} \int |u\rangle\langle u| dP(u) \text{ strongly in trace-class norm}} \quad (1.8)$$

where P is a Borel probability measure on the set of minimizers of the quasi-classical Pekar functional obtained as

$$\mathcal{E}_{\text{Pek}}^{(V)}[u] := \min_{\varphi \in L^2(\mathbb{R}^d)} \langle u \otimes \xi(\varphi) | H_\alpha^{(V)} u \otimes \xi(\varphi) \rangle_{\mathfrak{H}}.$$

Here

$$\xi(\varphi) = e^{a^\dagger(\varphi) - a(\varphi)} 1 \oplus 0 \oplus 0 \oplus \dots \in \mathfrak{F}(L^2(\mathbb{R}^d))$$

is a coherent state of the field (the definition of $a(\varphi)$, $a^\dagger(\varphi)$ is recalled in (2.3) below). The above means that an arbitrarily small potential well is sufficient to trap/bind the particle in the quasi-classical limit.

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2. MAIN RESULTS

2.1. Model. The natural Hilbert space for a system composed by one particle in \mathbb{R}^d and a quantum bosonic field is

$$\mathfrak{H} = L^2_{\text{part}}(\mathbb{R}^d) \otimes \mathfrak{F}, \quad (2.1)$$

with the bosonic Fock space

$$\mathfrak{F} := \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)) = \bigoplus_{n=0}^{\infty} (L_{\text{field}}^2(\mathbb{R}^d))^{\otimes_{\text{sym}} n}. \quad (2.2)$$

In most of the sequel, the α dependence of the model will be encoded into the fact that the annihilation operator $a(f)$ acting on \mathfrak{F} as

$$(a(f)\Psi_n)(x_1, \dots, x_{n-1}) = \alpha^{-1} \sqrt{n} \int_{\mathbb{R}^d} \overline{f(x)} \Psi_n(x, x_1, \dots, x_{n-1}) dx, \quad \forall \Psi_n \in L_{\text{sym}}^2(\mathbb{R}^{dn}) \quad (2.3)$$

and its adjoint $a^\dagger(f)$ satisfy the rescaled Canonical Commutation Relations (CCR)

$$[a(f), a(g)] = [a^\dagger(f), a^\dagger(g)] = 0, \quad [a(f), a^\dagger(g)] = \frac{\langle f, g \rangle}{\alpha^2}, \quad \forall f, g \in L_{\text{field}}^2(\mathbb{R}^d). \quad (2.4)$$

We still denote by $a(f), a^\dagger(g)$ the operators on \mathfrak{H} which act as (2.4) on the factor \mathfrak{F} and as the identity on the factor $L_{\text{part}}^2(\mathbb{R}^d)$. We associate to these operators the operator-valued distributions a_x, a_x^\dagger defined by

$$a(f) = \int_{\mathbb{R}^d} \overline{f(x)} a_x dx, \quad a^\dagger(f) = \int_{\mathbb{R}^d} f(x) a_x^\dagger dx, \quad (2.5)$$

together with their Fourier transforms

$$\hat{a}_k = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{ik \cdot x} a_x dx, \quad \hat{a}_k^\dagger = \frac{1}{(2\pi)^{d/2}} \int_{\mathbb{R}^d} e^{-ik \cdot x} a_x^\dagger dx \quad (2.6)$$

and the number operator

$$\mathcal{N}_\alpha := \int_{\mathbb{R}^d} a_x^\dagger a_x dx = \int_{\mathbb{R}^d} \hat{a}_k^\dagger \hat{a}_k dk. \quad (2.7)$$

Our Hamiltonian acts on \mathfrak{H} as

$$\begin{aligned} H_\alpha^{(V)} &= (-\Delta_x + V(x)) \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{N}_\alpha + \int_{\mathbb{R}^d} \left(e^{ik \cdot x} \hat{v}(k) \hat{a}_k^\dagger + e^{-ik \cdot x} \overline{\hat{v}(k)} \hat{a}_k \right) dk \\ &= (-\Delta_x + V(x)) \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{N}_\alpha + \int_{\mathbb{R}^d} \left(v(x-y) a_y^\dagger + \overline{v(x-y)} a_y \right) dy \end{aligned} \quad (2.8)$$

We made the simplifying choice $T \equiv 1$ in (1.1), corresponding to the Fröhlich polaron. We can easily accomodate functions such as

$$T(k) = (|k|^2 + 1)^s, \quad 0 \leq s \leq 1$$

i.e. a kinetic energy operator for the field such as $(1 - \Delta)^s$. This requires only an extra use of an IMS-like localization formula (from [31, Appendix B] for $s \neq 0, 1$) in Lemma 3.6 below.

Here V is an external potential, v is a function which couples the field and particle modes, and \hat{v} is its Fourier transform.

Assumption 2.1 (The external potential).

We assume that $V \in L_{\text{part}}^\infty(\mathbb{R}^d)$ is a strictly negative function such that

$$\lim_{|x| \rightarrow \infty} V(x) = 0. \quad (2.9)$$

Assumption 2.2 (The interaction).

We assume that $v \in L^2(\mathbb{R}^d)$ is real-valued.

We define the ground state energy

$$E_\alpha^{(V)} = \inf \sigma(H_\alpha^{(V)}). \quad (2.10)$$

It is known [15, 42, 45] that, to leading order as $\alpha \rightarrow \infty$, $E_\alpha^{(V)}$ is close to the minimal energy obtained through product trial states of the form

$$\Psi = \psi \otimes \xi(u),$$

where $\psi \in L^2_{\text{part}}(\mathbb{R}^d)$ is a particle wave-function and $\xi(u) \in \mathfrak{F}$ is the field coherent state defined by

$$\xi(u) = e^{a^\dagger(u) - a(u)} \Omega \in \mathfrak{F} \quad (2.11)$$

for $u \in L^2_{\text{field}}(\mathbb{R}^d)$. Here

$$\Omega = 1 \oplus 0 \oplus 0 \oplus \dots \in \mathfrak{F}$$

is the vacuum vector.

The expectation of $H_\alpha^{(V)}$ in $\Psi = \psi \otimes \xi(u)$ reads

$$\begin{aligned} \langle \psi \otimes \xi(u), H_\alpha^{(V)} \psi \otimes \xi(u) \rangle &= \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 dx + \int_{\mathbb{R}^d} V(x) |\psi(x)|^2 dx \\ &+ \|u\|_2^2 + \int_{\mathbb{R}^d \times \mathbb{R}^d} \left(u(y) + \overline{u(y)} \right) v(x-y) |\psi(x)|^2 dx dy \end{aligned} \quad (2.12)$$

Minimizing the above expression with respect to u (which is tantamount to a square completion) yields¹

$$u = u_\psi := -|\psi|^2 * v \quad (2.13)$$

and thus the Pekar functional is

$$\begin{aligned} \mathcal{E}_{\text{Pek}}^{(V)}(\psi) &= \int_{\mathbb{R}^d} |\nabla \psi(x)|^2 dx + \int_{\mathbb{R}^d} V(x) |\psi(x)|^2 dx \\ &- \iiint_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} v(x-y) v(x-z) |\psi(y)|^2 |\psi(z)|^2 dx dy dz. \end{aligned} \quad (2.14)$$

Observe that

$$\iiint_{\mathbb{R}^d \times \mathbb{R}^d \times \mathbb{R}^d} v(x-y) v(x-z) |\psi(y)|^2 |\psi(z)|^2 dx dy dz = \iint_{\mathbb{R}^d \times \mathbb{R}^d} W(x-y) |\psi(x)|^2 |\psi(y)|^2 dx dy$$

with

$$W(x-y) = \iint_{\mathbb{R}^d \times \mathbb{R}^d} v(z-x) v(z-y) dz = \iint_{\mathbb{R}^d \times \mathbb{R}^d} v(z) v(z+x-y) dz = (v * v)(y-x) \quad (2.15)$$

so that the effective interaction term in (2.14) is always a non-positive/attractive pair interaction, in the sense that

$$\widehat{W}(k) = |\widehat{v}(k)|^2 \geq 0.$$

Also note that, since we assume $v \in L^2$ we have that $W \in L^\infty$ by Young's inequality.

¹For $T = (|k|^2 + 1)^s$ this is replaced by $u_\psi = -(1 - \Delta)^{-s} (|\psi|^2 * v)$.

2.2. Statements. We define the minimal Pekar energy at mass $m > 0$ in the manner

$$E_{\text{Pek}}^{(V)}(m) = \inf \left\{ \mathcal{E}_{\text{Pek}}^{(V)}(\psi) \mid \|\psi\|_2^2 = m \right\} = \mathcal{E}_{\text{Pek}}^{(V)}(\psi_{V,m}), \quad (2.16)$$

with the convention that $E_{\text{Pek}}^{(0)}(m)$ is the minimal translation-invariant Pekar energy corresponding to the choice $V = 0$. We denote

$$\mathcal{M}_{\text{Pek}}^{(V)}(m) = \left\{ \psi \in L^2(\mathbb{R}^d) \mid \|\psi\|_2^2 = m, \mathcal{E}_{\text{Pek}}^{(V)}(\psi) = E_{\text{Pek}}^{(V)}(m) \right\}. \quad (2.17)$$

That the above is not empty (i.e. that Pekar minimizers always exist) follows from the usual concentration-compactness method as in [39, 24, 48] for example, or by using rearrangement inequalities as in [40] if W is assumed radial.

It follows from the results/methods of [42, 12, 15] that

$$\lim_{\alpha \rightarrow \infty} E_{\alpha}^{(V)} = E_{\text{Pek}}^{(V)}(1). \quad (2.18)$$

We shall revisit a proof of (2.18) along the lines of [12] for completeness, providing in particular an alternative construction of the quasi-classical measures used as main tools.

In this paper we are particularly interested in the associated convergence of states, which is our main result:

Theorem 2.3 (Convergence of states in the quasi-classical limit).

Let $\Psi_{\alpha} \in \mathfrak{S}$ be a (family of) normalized vector(s) such that

$$\langle \Psi_{\alpha}, H_{\alpha}^{(V)} \Psi_{\alpha} \rangle \leq E_{\alpha}^{(V)} + o_{\alpha}(1). \quad (2.19)$$

Let k, ℓ be non-negative integers with $k + \ell \leq 2$. Modulo extraction of a subsequence in α , for every bounded $A \in \mathcal{B}(L_{\text{part}}^2(\mathbb{R}^d))$ and for every $f_1, \dots, f_k, g_1, \dots, g_{\ell} \in L_{\text{field}}^2(\mathbb{R}^d)$,

$$\begin{aligned} \sqrt{k! \ell!} \left\langle \Psi_{\alpha}, A \otimes a^{\dagger}(g_1) \dots a^{\dagger}(g_{\ell}) a(f_1) \dots a(f_k) \Psi_{\alpha} \right\rangle &\xrightarrow{\alpha \rightarrow \infty} \\ \int_{\psi \in \mathcal{M}_{\text{Pek}}^{(V)}(1)} \langle \psi, A \psi \rangle_{L^2} \prod_{j=1}^k \langle f_j, u_{\psi} \rangle \prod_{j=1}^{\ell} \langle u_{\psi}, g_j \rangle dP(\psi), \end{aligned} \quad (2.20)$$

where P is a probability measure over the set of Pekar minimizers $\mathcal{M}_{\text{Pek}}^{(V)}(1)$ at mass 1 and u_{ψ} is defined as in (2.13).

A few comments:

- (1) Picking $k = \ell = 0$ in (2.20) gives

$$\text{Tr} [\gamma_{\alpha} A] \xrightarrow{\alpha \rightarrow \infty} \int_{\psi \in \mathcal{M}_{\text{Pek}}^{(V)}(1)} \langle \psi, A \psi \rangle_{L^2} dP(\psi)$$

for any bounded operator A , where the particle reduced density matrix is defined as in (1.7).

Hence

$$\gamma_{\alpha} \xrightarrow{*} \int_{\psi \in \mathcal{M}_{\text{Pek}}^{(V)}(1)} |\psi\rangle \langle \psi| dP(\psi)$$

weakly-star in the trace-class. Since P is a probability, the right-hand side has trace 1. Hence the trace of γ_{α} converges. The latter equals the trace-class norm because $\gamma_{\alpha} \geq 0$. The convergence is thus strong in the trace-class (see [13] or [57, Addendum H]), as claimed in (1.8).

- (2) Taking $A = \mathbb{1}$, $k = \ell = 1$ in (2.20) and varying $f_1, g_1 \in L^2(\mathbb{R}^d)$ yields that the field reduced density matrix described by the integral kernel

$$\mathrm{Tr}_{L^2_{\mathrm{part}}(\mathbb{R}^d)} [|\Psi_\alpha\rangle\langle\Psi_\alpha|a_x^\dagger a_y]$$

converges weakly-* in the trace-class to the operator with kernel

$$\int_{\psi \in \mathcal{M}_{\mathrm{Pek}}^{(V)}(1)} \overline{u_\psi(x)} u_\psi(y) dP(\psi).$$

Taking $k = 1$ or $\ell = 1$, varying A, f_1, g_1 , gives a similar convergence for what we shall call the field-particle density matrix in Section 3.

- (3) The limitation $k + \ell \leq 2$ comes from the fact that, for general quasi-minimizing sequences, we only have a control via the energy on the expectation of the field excitation number

$$\mathcal{N} = \sum_{j \geq 1} \mathbb{1}_{L^2(\mathbb{R}^d)} \otimes a^\dagger(f_j) a(f_j),$$

with $(f_j)_j$ a orthonormal basis of $L^2_{\mathrm{field}}(\mathbb{R}^d)$. Under the strongest assumption that

$$\langle \Psi_\alpha | \mathcal{N}^\kappa \Psi_\alpha \rangle \leq C_\kappa$$

independently of α , we can allow for $k + \ell \leq 2\kappa$ in the main result. If Ψ_α is a true eigenstate of the Hamiltonian (assuming such exist), estimates of this form follow from the variational equation and so-called pull-through formulae [1, 49].

- (4) Again, since the external potential can be arbitrarily small, its only function is to break translation invariance. The binding/self-trapping only comes from the particle-field interaction. In particular, in space dimensions $d \geq 3$, the Cwikel-Lieb-Rosenblum inequality [41, Chapter 4 and references therein] ensures that if $\|V\|_{L^{d/2}(\mathbb{R}^d)}$ is small enough, the Schrödinger operator $-\Delta + V$ acting on the particle has no bound states.
- (5) Our proof does not require a purely negative external potential V , but only that

$$E_{\mathrm{Pek}}^{(V)}(1) < E_{\mathrm{Pek}}^{(0)}(1)$$

which is certainly the case for $V < 0$ by using a translation-invariant ground state as trial state for the functional with trapping potential.

2.3. Organization of the paper. In essence we combine the philosophies of [12] and [35, 37]: quasi-classical measures, and systematic combination thereof with localization methods. This allows a concentration-compactness-type analysis of the many-body problem in the quasi-classical limit reminiscent of what was performed in [35] for the Bose gas in the mean-field limit (see [51, 50, 52] for review).

We will start by defining reduced particle/field/field-particle density matrices in Section 3. An important tool is then to define states localized in a given region of space, such that “the reduced densities of the localized state are the localizations of the densities of the initial state” in the spirit of [34] and references therein.

With this we may split the energy into the contribution of the region localized close to the potential well, and the contribution of the complement. Using (2.18) for both terms separately and simple binding properties of the classical Pekar energies (essentially that the classical energy in the potential well is smaller), we conclude that it is energetically favorable to have all the mass concentrated close to the potential well, which leads to binding/strong convergence.

We find it useful to revisit the construction of quasi-classical measures in Section 4. This was performed in [9, 11, 10, 12] based on a Weyl quantization approach building on [3, 4]. We provide an alternative construction yielding slightly stronger results by using anti-Wick quantization as in [35, 37], combining with ideas from [19].

Using the simplified construction of the measures, we give a self-contained proof of (2.18) in Section 5 for completeness, and because some of the steps are re-used when finally completing the proof of Theorem 2.3 in Section 6.

3. REDUCED DENSITIES, LOCALIZATION OF STATES AND LOCALIZATION OF ENERGIES

3.1. Reduced densities.

Identifying states on $\mathfrak{H} = L^2_{\text{part}}(\mathbb{R}^d) \otimes \mathfrak{F}$ with \mathfrak{F} -valued functions. We recall that, by the Schmidt decomposition, any $\Psi \in \mathfrak{H}$ can be written as

$$\Psi = \sum_{j=1}^{\infty} c_j u_j \otimes v_j, \quad (3.1)$$

where $\{u_j\}_{j \in \mathbb{N}}$ is a suitable orthonormal set in $L^2_{\text{part}}(\mathbb{R}^d)$, $\{v_j\}_{j \in \mathbb{N}}$ is a suitable orthonormal set in \mathfrak{F} , and $c_j \geq 0$ for all j . By construction then $\|\Psi\|^2 = \sum_{j=1}^{\infty} c_j^2$.

We also recall that $\Psi \in \mathfrak{H}$ can be written canonically as an element of the space $L^2(\mathbb{R}^d, \mathfrak{F})$. If $\Psi = u \otimes v$, where $u \in L^2_{\text{part}}(\mathbb{R}^d)$ and $v \in \mathfrak{F}$, is a factorized state, then Ψ is identified with the function $\Psi(\cdot) : \mathbb{R}^d \rightarrow \mathfrak{F}$ whose action is

$$\Psi(x) = u(x)v. \quad (3.2)$$

This definition is then extended by linearity to the whole \mathfrak{H} .

The identification (3.2) between vectors induces a similar one for states on \mathfrak{H} . A pure (normal) state on \mathfrak{H} is a rank-one projection $\Gamma = |\Psi\rangle\langle\Psi|$, where $\Psi \in \mathfrak{H}$ has unit norm. By (3.1) there exists an orthonormal set $\{u_j\}_{j \in \mathbb{N}}$ of elements of $L^2_{\text{part}}(\mathbb{R}^d)$, an orthonormal set $\{v_j\}_{j \in \mathbb{N}}$ of elements of $L^2_{\text{field}}(\mathbb{R}^d)$, and coefficients $\{c_j\}_{j \in \mathbb{N}}$ such that

$$\Gamma = \sum_{j,k=1}^{\infty} c_j \bar{c}_k |u_j\rangle\langle u_k| \otimes |v_j\rangle\langle v_k|. \quad (3.3)$$

We naturally identify Γ with the rank-one projection on $L^2(\mathbb{R}^d, \mathfrak{F})$ whose integral kernel is

$$\Gamma(x, y) = \sum_{j,k=1}^{\infty} c_j \bar{c}_k u_j(x) \overline{u_k(y)} |v_j\rangle\langle v_k|. \quad (3.4)$$

The identification is then extended by linearity to mixed states. Since $\Gamma(x, y)$ is of the form $|V(y)\rangle\langle U(x)|$, it is a trace-class operator on \mathfrak{F} for almost every $(x, y) \in \mathbb{R}^d \times \mathbb{R}^d$. We also note that $\Gamma(x, x) \geq 0$ for almost every $x \in \mathbb{R}^d$.

Reduced density matrices. For generic states Γ on \mathfrak{H} we will define objects that monitor the state of the two subsystems (i.e., the particle and the bosonic field). Let us first recall the standard definitions of reduced density matrices in Fock space. Let $\Gamma_{\mathfrak{F}}$ be a state on \mathfrak{F} satisfying

$$\text{Tr}_{\mathfrak{F}} [\mathcal{N}^k \Gamma_{\mathfrak{F}}] < +\infty.$$

for some $k \in \mathbb{N}$. For $p, q \in \mathbb{N} \cup \{0\}$, the (p, q) -reduced density matrix associated to $\Gamma_{\mathfrak{F}}$ is the operator

$$\Gamma_{\mathfrak{F}}^{(p,q)} : (L_{\text{field}}^2(\mathbb{R}^d))^{\otimes_{\text{sym}} q} \rightarrow (L_{\text{field}}^2(\mathbb{R}^d))^{\otimes_{\text{sym}} p}$$

defined by the relation

$$\left\langle g_1 \otimes_{\text{sym}} \cdots \otimes_{\text{sym}} g_p, \Gamma_{\mathfrak{F}}^{(p,q)} f_1 \otimes_{\text{sym}} \cdots \otimes_{\text{sym}} f_q \right\rangle = \text{Tr}_{\mathfrak{F}} \left(\Gamma_{\mathfrak{F}} a^\dagger(f_1) \cdots a^\dagger(f_p) a(g_1) \cdots a(g_p) \right) \quad (3.5)$$

for $g_1, \dots, g_p, f_1, \dots, f_q \in L_{\text{field}}^2(\mathbb{R}^d)$. We will mostly use $\Gamma_{\mathfrak{F}}^{(1,1)}$, $\Gamma_{\mathfrak{F}}^{(1,0)}$, and $\Gamma_{\mathfrak{F}}^{(0,1)}$. For the latter two the above definition reduces to

$$\begin{aligned} \langle g, \Gamma_{\mathfrak{F}}^{(1,0)} \rangle &= \text{Tr}_{\mathfrak{F}} [\Gamma_{\mathfrak{F}} a(g)] \\ \langle (\Gamma_{\mathfrak{F}}^{(0,1)})^*, f \rangle &= \text{Tr}_{\mathfrak{F}} [\Gamma_{\mathfrak{F}} a^\dagger(f)] = \overline{\langle f, [\gamma]^{(1,0)} \rangle}. \end{aligned} \quad (3.6)$$

or, in terms of operator-valued distributions,

$$\Gamma_{\mathfrak{F}}^{(1,0)}(x) = \text{Tr}_{\mathfrak{F}} [\gamma a_x] = \overline{[\gamma]^{(0,1)}(x)}. \quad (3.7)$$

Moreover, for $\Gamma_{\mathfrak{F}}^{(1,1)}$ we have the relation

$$\text{Tr}_{L_{\text{field}}^2(\mathbb{R}^d)} \left(\Gamma_{\mathfrak{F}}^{(1,1)} \right) = \text{Tr}_{\mathfrak{F}} (\mathcal{N} \Gamma_{\mathfrak{F}}). \quad (3.8)$$

We next define reduced density matrices for states on the full Hilbert space \mathfrak{H} .

Definition 3.1 (Reduced density matrices for particle and field).

Let Γ be a positive trace-class operator with unit trace on \mathfrak{H} , with the further property

$$\text{Tr}_{\mathfrak{H}} [1 \otimes \mathcal{N} \Gamma] < +\infty.$$

We define the associated

- *particle reduced density matrix* as the unit-trace, positive, trace-class operator γ on $L_{\text{part}}^2(\mathbb{R}^d)$ defined through the partial trace

$$\gamma = \text{Tr}_{\mathfrak{F}} (\Gamma), \quad (3.9)$$

or, equivalently, as the operator with integral kernel

$$\gamma(x, y) = \text{Tr}_{\mathfrak{F}} (\Gamma(x, y)). \quad (3.10)$$

Notice that, as a consequence of (3.4) and its extension to mixed states, $\Gamma(x, y)$ is indeed trace-class for almost every $x, y \in \mathbb{R}^d$.

- *field one-body reduced density matrix* as the unit-trace, positive, trace-class operator $\Gamma^{(1,1)}$ on $L_{\text{field}}^2(\mathbb{R}^d)$ defined by

$$\Gamma^{(1,1)} = \left[\text{Tr}_{L_{\text{part}}^2(\mathbb{R}^d)} (\Gamma) \right]^{(1,1)} = \left[\int_{\mathbb{R}^d} \Gamma(x, x) dx \right]^{(1,1)}. \quad (3.11)$$

- *field-particle reduced density matrix* as the operator-valued linear map

$$\sigma : L_{\text{field}}^2(\mathbb{R}^d) \rightarrow \mathcal{B}(L_{\text{part}}^2(\mathbb{R}^d))$$

whose action on a generic $f \in L_{\text{field}}^2(\mathbb{R}^d)$ is defined by

$$\langle u, \sigma(f)v \rangle = \text{Tr} (|v\rangle\langle u| \otimes (a^\dagger(f) + a(f)) \Gamma), \quad \forall u, v \in L_{\text{part}}^2(\mathbb{R}^d). \quad (3.12)$$

◇

We have the following properties of the field-particle reduced density matrix:

Lemma 3.2 (Field-particle reduced density matrix).

The field-particle reduced density matrix defined above takes values in the trace-class:

$$\sigma : L_{\text{field}}^2(\mathbb{R}^d) \rightarrow \mathcal{L}^1(L_{\text{part}}^2(\mathbb{R}^d)).$$

Denote $(\sigma(f))(x, y)$ the integral kernel of $\sigma(f)$ and

$$\sigma(x, x; z) = \text{Tr}_{\mathfrak{F}} \left[\Gamma(x, x) (a_z^\dagger + a_z) \right]$$

as an operator-valued distribution satisfying

$$(\sigma(f))(x, x) = \int_{\mathbb{R}^d} f(z) \sigma(x, x; z) dz.$$

The distribution $\sigma(x, x; z)$ is in fact a function in $L_x^1(L_z^2(\mathbb{R}^d))$.

Proof. To see that $\sigma(f)$ is indeed trace-class we may define it as an operator via the requirement

$$\begin{aligned} \langle u, \sigma(f)v \rangle &= \langle u, \sigma_+(f)v \rangle - \langle u, \sigma_-(f)v \rangle \\ &:= \text{Tr}(|v\rangle\langle u| \otimes (a^\dagger(f) + a(f))_+ \Gamma) - \text{Tr}(|v\rangle\langle u| \otimes (a^\dagger(f) + a(f))_- \Gamma) \end{aligned}$$

with A_\pm the positive and negative parts of a self-adjoint operator. This way, if

$$\text{Tr} \left(\mathbf{1} \otimes \sqrt{\mathcal{N}} \Gamma \right) < \infty$$

then $\sigma(f)$ is the difference of two positive trace-class operators.

Thus for every $f \in L_{\text{field}}^2(\mathbb{R}^d)$, the integral kernel $(\sigma(f))(x, y)$ of $\sigma(f)$ is the function

$$(\sigma(f))(x, y) = \text{Tr}_{\mathfrak{F}} \left[\Gamma(x, y) (a^\dagger(f) + a(f)) \right].$$

Notice in particular that

$$\int_{\mathbb{R}^d} |(\sigma(f))(x, x)| dx < +\infty$$

as is the case for the kernel of a trace-class operator. That $\sigma(x, x; z)$ is in $L_x^1(L_z^2(\mathbb{R}^d))$ follows from

$$\begin{aligned} \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} |\sigma(x, x; z)|^2 dz \right)^{1/2} dx &\leq \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} \text{Tr}_{\mathfrak{F}}(\Gamma(x, x)) \text{Tr}_{\mathfrak{F}}(a_z^\dagger a_z \Gamma(x, x)) dz \right)^{1/2} dx \\ &\leq \text{Tr}_{\mathfrak{F}}(\mathbf{1} \otimes (\mathcal{N} + 1)\Gamma) \end{aligned} \quad (3.13)$$

□

3.2. Localization of states. An important ingredient in the proof of our main result is the possibility to localize a generic state Γ on \mathfrak{H} to a certain region of \mathbb{R}^d both for the particle's and for the quantized field's degrees of freedom. We here adapt to our coupled system the known construction for a single bosonic (or fermionic, for that matter) field [2, 14, 28, 29, 34].

Proposition 3.3 (Construction of localized states).

Let $0 \leq q \leq 1$ be a linear operator on $L^2(\mathbb{R}^d)$, and Γ be a positive trace-class operator on \mathfrak{H} . Let $\gamma, \Gamma^{(1,1)}, \sigma$ be the reduced density matrices associated to Γ according to Definition 3.1.

There exists a positive trace-class operator Γ_q on \mathfrak{H} whose reduced density matrices are

$$\gamma_q = q \gamma q \quad (3.14)$$

$$\Gamma_q^{(1,1)} = q \left[\text{Tr}_{L_{\text{part}}^2(\mathbb{R}^d)}(q \Gamma q) \right]^{(1,1)} q \quad (3.15)$$

and, for $f \in L_{\text{field}}^2(\mathbb{R}^d)$,

$$\sigma_q(f) = q \sigma(qf) q. \quad (3.16)$$

Moreover,

$$\text{Tr}_{\mathfrak{H}} \Gamma = \text{Tr}_{\mathfrak{H}} \Gamma_q + \text{Tr}_{\mathfrak{H}} \Gamma_{(1-q^2)^{1/2}}. \quad (3.17)$$

Proof. We follow and adapt the proof of [29, Section A.1.2]. Define the partial isometry

$$\mathcal{Q} : L_{\text{field}}^2(\mathbb{R}^d) \ni f \mapsto qf \oplus (1 - q^2)^{1/2} f \in L_{\text{field}}^2(\mathbb{R}^d) \oplus L_{\text{field}}^2(\mathbb{R}^d). \quad (3.18)$$

and its second quantization²

$$\begin{aligned} G(\mathcal{Q}) &: \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)) \rightarrow \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d) \oplus L_{\text{field}}^2(\mathbb{R}^d)) \\ (G(\mathcal{Q})\Psi)^{(n)} &= \mathcal{Q}^{\otimes n} \Psi^{(n)}. \end{aligned} \quad (3.19)$$

The latter operator satisfies

$$G(\mathcal{Q}) a^\dagger(f) = a^\dagger(qf \oplus (1 - q^2)^{1/2} f) G(\mathcal{Q}). \quad (3.20)$$

Recall now that there exists a canonical isomorphism

$$U : \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d) \oplus L_{\text{field}}^2(\mathbb{R}^d)) \rightarrow \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)) \otimes \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)), \quad (3.21)$$

and define the creation and annihilator operators on $\mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)) \otimes \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d))$ as

$$\begin{aligned} c^\dagger(f) &= a^\dagger(f) \otimes \mathbb{1}_{\mathfrak{F}} & c(f) &= a(f) \otimes \mathbb{1}_{\mathfrak{F}} \\ d^\dagger(f) &= \mathbb{1}_{\mathfrak{F}} \otimes a^\dagger(f) & d(f) &= \mathbb{1}_{\mathfrak{F}} \otimes a(f). \end{aligned} \quad (3.22)$$

We denote with the same symbols the extensions of these operators to $\mathfrak{H} = L_{\text{part}}^2(\mathbb{R}^d) \otimes \mathfrak{F}$ which act as the identity on $L_{\text{part}}^2(\mathbb{R}^d)$. The relation between U , the latter creation and annihilation operators, and those on $\mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d) \oplus L_{\text{field}}^2(\mathbb{R}^d))$ is

$$\begin{aligned} U a^\dagger(f \oplus g) &= (c^\dagger(f) + d^\dagger(g)) U \\ U a(f \oplus g) &= (c(f) + d(g)) U. \end{aligned} \quad (3.23)$$

Finally, define the operator

$$\mathcal{Y}(\mathcal{Q}) = \mathbb{1}_{L_{\text{part}}^2(\mathbb{R}^d)} \otimes (UG(\mathcal{Q})) : \mathfrak{H} \rightarrow L_{\text{part}}^2(\mathbb{R}^d) \otimes \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)) \otimes \mathfrak{F}(L_{\text{field}}^2(\mathbb{R}^d)). \quad (3.24)$$

²The reader should think of the more familiar notation $\Gamma(\mathcal{Q})$ for the second quantization of an operator on the base space. In our setting such a notation would clash with the way we are denoting states Γ on \mathfrak{H} .

By the relations above, $\mathcal{Y}(\mathcal{Q})$ satisfies the intertwining properties (see [14, Lemma 2.14 and 2.15])

$$\begin{aligned}\mathcal{Y}(\mathcal{Q}) a^\dagger(f) &= \left(c^\dagger(qf) + d^\dagger((1-q^2)^{1/2}f) \right) \mathcal{Y}(\mathcal{Q}) \\ \mathcal{Y}(\mathcal{Q}) a(f) &= \left(c(qf) + d((1-q^2)^{1/2}f) \right) \mathcal{Y}(\mathcal{Q}) \\ \mathcal{Y}(\mathcal{Q}) a(qf) &= c(f) \mathcal{Y}(\mathcal{Q}) & \mathcal{Y}(\mathcal{Q}) a((1-q^2)^{1/2}f) &= d(f) \mathcal{Y}(\mathcal{Q}) \\ a^\dagger(qf) \mathcal{Y}(\mathcal{Q})^* &= \mathcal{Y}(\mathcal{Q})^* c^\dagger(f) & a^\dagger((1-q^2)^{1/2}f) \mathcal{Y}(\mathcal{Q})^* &= \mathcal{Y}(\mathcal{Q})^* d^\dagger(f)\end{aligned}\tag{3.25}$$

Moreover, since $\mathcal{Q}^* \mathcal{Q} = \mathbb{1}_{L^2_{\text{field}}(\mathbb{R}^d)}$, it follows that $\mathcal{Y}(\mathcal{Q})^* \mathcal{Y}(\mathcal{Q}) = \mathbb{1}_{\mathfrak{H}}$.

Let now Γ be a positive trace class operator on \mathfrak{H} . We define the q -localization of Γ as the trace-class operator Γ_q on \mathfrak{H} whose action on a factorized bounded operator $A \otimes B \in \mathcal{B}(L^2_{\text{part}}(\mathbb{R}^d)) \otimes \mathcal{B}(\mathfrak{F})$ is

$$\text{Tr}_{\mathfrak{H}} [(A \otimes B) \Gamma_q] = \text{Tr}_{\mathfrak{H}} [\mathcal{Y}(\mathcal{Q})^* (qAq \otimes B \otimes \mathbb{1}_{\mathfrak{F}}) \mathcal{Y}(\mathcal{Q}) \Gamma],\tag{3.26}$$

and the extension to non-factorized operators follows by linearity. The fact that Γ_q is positive follows from the positivity of Γ . Moreover, the identity $\mathcal{Y}(\mathcal{Q})^* \mathcal{Y}(\mathcal{Q}) = \mathbb{1}_{\mathfrak{H}}$ implies that

$$\text{Tr}_{\mathfrak{H}} \Gamma_q = \text{Tr}_{\mathfrak{H}} [(q^2 \otimes \mathbb{1}_{\mathfrak{F}}) \Gamma].\tag{3.27}$$

Repeating the construction by switching the roles of q and $(1-q^2)^{1/2}$ we similarly find

$$\text{Tr}_{\mathfrak{H}} \Gamma_{(1-q^2)^{1/2}} = \text{Tr}_{\mathfrak{H}} [(1-q^2) \otimes \mathbb{1}_{\mathfrak{F}}] \Gamma.\tag{3.28}$$

The last two identities prove (3.17).

In order to show (3.14) we compute

$$\langle g, \gamma_q f \rangle = \text{Tr}_{\mathfrak{H}} (|f\rangle \langle g| \otimes \mathbb{1}_{\mathfrak{F}} \Gamma_q) = \text{Tr}_{\mathfrak{H}} (|qf\rangle \langle qg| \otimes \mathbb{1}_{\mathfrak{F}} \Gamma) = \langle f, q \gamma q g \rangle.\tag{3.29}$$

This is precisely (3.14). In order to show (3.15), in turn, we recall (3.11) and (3.5) to write

$$\langle g, \Gamma_q^{(1,1)} f \rangle = \left\langle g, \left[\text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} (\Gamma_q) \right]^{(1,1)} f \right\rangle = \text{Tr}_{\mathfrak{H}} \left[\left(\mathbb{1}_{L^2_{\text{part}}(\mathbb{R}^d)} \otimes a^\dagger(f) a(g) \right) \Gamma_q \right].\tag{3.30}$$

Eq. (3.15) is then deduced using the definition of Γ_q and the intertwining properties (3.25). Finally, in order to show (3.16) we write, for a generic $O \in \mathcal{B}(L^2_{\text{part}}(\mathbb{R}^d))$,

$$\text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} [O \sigma_q(f)] = \text{Tr}_{\mathfrak{H}} [(O \otimes a(f)) \Gamma_q]$$

Again, the definition of Γ_q and the intertwining properties allow to conclude. \square

3.3. Energy localization. We fix a smooth partition of unity $\chi^2 + \eta^2 = 1$ with $\chi(x) = 1$ if $|x| \leq 1$ and $\chi(x) = 0$ if $|x| \geq 2$, and define $\chi_R(x) = \chi(x/R)$ and $\eta_R(x) = \eta(x/R)$. We further assume that χ , and thus η , are monotone functions. We then have

Proposition 3.4 (Energy localization).

Let V, v be as in Assumptions 2.1 and 2.2, and let $H_\alpha^{(V)}$ be defined in (2.8). Consider a family $(\Psi_\alpha)_\alpha$ of normalized vectors $\Psi_\alpha \in \mathfrak{H}_\alpha$ and the associated states $\Gamma_\alpha = |\Psi_\alpha\rangle \langle \Psi_\alpha|$. Assume that

$$\text{Tr} [H_\alpha^{(V)} \Gamma_\alpha] \leq C$$

uniformly as $\alpha \rightarrow \infty$. Let $\gamma_\alpha, \Gamma_\alpha^{(1,1)}, \sigma_\alpha$ be the reduced density matrices associated to Γ_α according to Definition 3.1. Let $\Gamma_{\alpha, \chi_R}, \Gamma_{\alpha, \eta_R}$ be the localized states corresponding to the choices $\Gamma = \Gamma_\alpha$ and $q = \chi_R, \eta_R$ in Proposition 3.3. Then

$$\begin{aligned} & \liminf_{\alpha \rightarrow \infty} \text{Tr}_{\mathfrak{H}} \left(H_\alpha^{(V)} \Gamma_\alpha \right) \\ & \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left[\text{Tr}_{\mathfrak{H}} \left(H_\alpha^{(V)} \Gamma_{\alpha, \chi_R} \right) + \text{Tr}_{\mathfrak{H}} \left(H_\alpha^{(0)} \Gamma_{\alpha, \eta_R} \right) \right]. \end{aligned} \quad (3.31)$$

We split the proof into three lemmas, corresponding to the three terms in the energy.

Lemma 3.5 (Particle energy localization).

In the same assumptions of Proposition 3.4 we have

$$\begin{aligned} \liminf_{\alpha \rightarrow \infty} \text{Tr}_{\mathfrak{H}} \left((-\Delta + V) \otimes 1 \Gamma_\alpha \right) & \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left[\text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(\chi_R (-\Delta + V) \chi_R \gamma_\alpha \right) \right. \\ & \quad \left. + \text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\eta_R \Delta \eta_R \gamma_\alpha \right) \right]. \end{aligned} \quad (3.32)$$

Proof. Let us first focus on proving a lower bound on the term involving $-\Delta$. Using the IMS formula

$$-\Delta = -\chi_R \Delta \chi_R - \eta_R \Delta \eta_R - |\nabla \chi_R|^2 - |\nabla \eta_R|^2.$$

The two gradient terms are bounded functions which, by the definition of χ_R and η_R , satisfy

$$|\nabla \chi_R|^2 + |\nabla \eta_R|^2 \leq \frac{C}{R^2}.$$

This immediately implies, using also the definition of γ_α ,

$$\begin{aligned} \text{Tr}_{\mathfrak{H}} \left(-\Delta \otimes 1 \Gamma_\alpha \right) & = \text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\Delta \gamma_\alpha \right) \\ & \geq \text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\chi_R \Delta \chi_R \gamma_\alpha \right) + \text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\eta_R \Delta \eta_R \gamma_\alpha \right) - \frac{C}{R^2}. \end{aligned}$$

Passing to the \liminf for $\alpha \rightarrow \infty$ followed by $R \rightarrow \infty$, we conclude

$$\liminf_{\alpha \rightarrow \infty} \text{Tr}_{\mathfrak{H}} \left(-\Delta \otimes 1 \Gamma_\alpha \right) \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left[\text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\chi_R \Delta \chi_R \gamma_\alpha \right) + \text{Tr}_{L^2_{\text{part}}(\mathbb{R}^d)} \left(-\eta_R \Delta \eta_R \gamma_\alpha \right) \right].$$

For the V -term in (3.32) we proceed in a similar way, by writing

$$V = \chi_R^2 V + \eta_R^2 V.$$

Since V is a bounded function that decays at infinity, we have, as $R \rightarrow \infty$, $V \eta_R^2 \geq -o_R(1)$. Passing to the two \liminf 's concludes the proof. \square

We next localize the field energy. We could generalize this to more general field dispersion relations using appropriate IMS formulas, cf the discussion following (2.8).

Lemma 3.6 (Field energy localization).

In the same assumptions of Proposition 3.4 we have

$$\begin{aligned} & \liminf_{\alpha \rightarrow \infty} \text{Tr}_{\mathfrak{H}} \left(1 \otimes \mathcal{N} \Gamma_\alpha \right) \\ & \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left\{ \text{Tr}_{L^2_{\text{field}}(\mathbb{R}^d)} \left[\chi_R \left(\int_{\mathbb{R}^d} \chi_R^2(x) \Gamma_\alpha(x, x) dx \right)^{(1,1)} \chi_R \right] \right. \\ & \quad \left. + \text{Tr}_{L^2_{\text{field}}(\mathbb{R}^d)} \left[\eta_R \left(\int_{\mathbb{R}^d} \eta_R^2(x) \Gamma_\alpha(x, x) dx \right)^{(1,1)} \eta_R \right] \right\}. \end{aligned} \quad (3.33)$$

Proof. Recalling (3.11) we have

$$\mathrm{Tr}_{\mathfrak{F}}(1 \otimes \mathcal{N} \Gamma_\alpha) = \mathrm{Tr}_{L^2_{\mathrm{field}}(\mathbb{R}^d)} \left(\left[\int_{\mathbb{R}^d} \Gamma_\alpha(x, x) dx \right]^{(1,1)} \right).$$

Using the fact that $\chi_R^2 + \eta_R^2 = 1$ twice and discarding the two mixed terms for a lower bound (recall that $\Gamma(x, x) \geq 0$) leads to

$$\begin{aligned} \mathrm{Tr}_{\mathfrak{F}}(1 \otimes \mathcal{N} \Gamma_\alpha) &\geq \mathrm{Tr}_{L^2_{\mathrm{field}}(\mathbb{R}^d)} \left(\chi_R \left[\int_{\mathbb{R}^d} \chi_R^2(x) \Gamma_\alpha(x, x) dx \right]^{(1,1)} \chi_R \right) \\ &\quad + \mathrm{Tr}_{L^2_{\mathrm{field}}(\mathbb{R}^d)} \left(\eta_R \left[\int_{\mathbb{R}^d} \eta_R^2(x) \Gamma_\alpha(x, x) dx \right]^{(1,1)} \eta_R \right). \end{aligned}$$

□

Finally we deal with the particle-field interaction:

Lemma 3.7 (Interaction energy localization).

Under the same assumptions as in Proposition 3.4 we have

$$\begin{aligned} \liminf_{\alpha \rightarrow \infty} \mathrm{Tr}_{\mathfrak{F}} \left(\int_{\mathbb{R}^d} v(\cdot - z) (a_z^\dagger + a_z) \Gamma_\alpha \right) \\ \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left[\iint_{\mathbb{R}^{2d}} \chi_R^2(x) \chi_R(z) v(x - z) \sigma_\alpha(x, x; z) dx dz \right. \\ \left. + \iint_{\mathbb{R}^{2d}} \eta_R^2(x) \eta_R(z) v(x - z) \sigma_\alpha(x, x; z) dx dz \right] \end{aligned} \quad (3.34)$$

Proof. First, by definition of σ_α

$$\mathrm{Tr}_{\mathfrak{F}} \left(\int_{\mathbb{R}^d} v(\cdot - z) (a_z^\dagger + a_z) \Gamma_\alpha \right) = \iint_{\mathbb{R}^{2d}} v(x - z) \sigma_\alpha(x, x; z) dx dz.$$

Using $\chi_R^2 + \eta_R^2 = 1$ we have

$$\begin{aligned} \iint_{\mathbb{R}^{2d}} v(x - z) \sigma_\alpha(x, x; z) dx dz &= \iint_{\mathbb{R}^{2d}} \chi_R^2(x) \chi_R(z) v(x - z) \sigma_\alpha(x, x; z) dx dz \\ &\quad + \iint_{\mathbb{R}^{2d}} \eta_R^2(x) \eta_R(z) v(x - z) \sigma_\alpha(x, x; z) dx dz \\ &\quad + \mathcal{E}_{\mathrm{Int}}^{(1)} + \mathcal{E}_{\mathrm{Int}}^{(2)}, \end{aligned} \quad (3.35)$$

with

$$\begin{aligned} \mathcal{E}_{\mathrm{Int}}^{(1)} &= \iint_{\mathbb{R}^{2d}} \chi_R^2(x) (1 - \chi_R(z)) v(x - z) \sigma_\alpha(x, x; z) dx dz \\ \mathcal{E}_{\mathrm{Int}}^{(2)} &= \iint_{\mathbb{R}^{2d}} \eta_R^2(x) (1 - \eta_R(z)) v(x - z) \sigma_\alpha(x, x; z) dx dz. \end{aligned} \quad (3.36)$$

Let us show that these are negligible in the limit $\alpha \rightarrow \infty$ followed by $R \rightarrow \infty$. The two terms are treated similarly, starting with $\mathcal{E}_{\text{Int}}^{(1)}$. First, we have

$$1 - \chi_R = \frac{\eta_R^2}{1 + \chi_R} \leq \eta_R^2.$$

In addition, since

$$\eta_R^2 = \eta_{4R}^2 + \eta_R^2 - \eta_{4R}^2,$$

we have the bound

$$\begin{aligned} |\mathcal{E}_{\text{Int}}^{(1)}| &\leq \iint_{\mathbb{R}^{2d}} \chi_R^2(x) \eta_{4R}^2(z) |v(x-z)| |\sigma_\alpha(x, x; z)| dx dz \\ &\quad + \iint_{\mathbb{R}^{2d}} \chi_R^2(x) (\eta_R^2(z) - \eta_{4R}^2(z)) |v(x-z)| |\sigma_\alpha(x, x; z)| dx dz. \end{aligned} \quad (3.37)$$

To control the first term in the right hand side we notice that $\chi_R^2(x) \eta_{4R}^2(z) \leq \mathbb{1}_{\{|x-z| \geq R\}}$, and therefore, by Cauchy-Schwarz,

$$\begin{aligned} &\iint_{\mathbb{R}^{2d}} \chi_R^2(x) \eta_{4R}^2(z) |v(x-z)| |\sigma_\alpha(x, x; z)| dx dz \\ &\leq \int_{\mathbb{R}^d} \left(\int_{\{|z-x| \geq R\}} |v(x-z)|^2 dz \right)^{1/2} \left(\int_{\mathbb{R}^d} |\sigma_\alpha(x, x; z)|^2 dz \right)^{1/2} dx \\ &\leq o_R(1) \end{aligned}$$

uniformly in α . Here we have used the fact that $v \in L^2(\mathbb{R}^d)$, as well as (3.13) and the fact that the energy of Γ_α is uniformly bounded by assumption.

For the second term in the decomposition (3.37) of $\mathcal{E}_{\text{Int}}^{(1)}$ we argue using an adaptation of Lions' concentration-compactness argument, already used in [35, Lemma 4.8]. Let us define the function

$$Q_\alpha(R) = \iint_{\mathbb{R}^{2d}} |v(x-z)| \mathbb{1}_{|z| \geq R} |\sigma_\alpha(x, x; z)| dx dz.$$

Then (recall that $\eta_R^2 \geq \eta_{4R}^2$ since η is monotone)

$$\iint_{\mathbb{R}^d} \chi_R^2(x) (\eta_R^2(z) - \eta_{4R}^2(z)) |v(x-z)| |\sigma_\alpha(x, x; z)| dx dz \leq Q_\alpha(R) - Q_\alpha(8R).$$

Now, for fixed α , the function $R \mapsto Q_\alpha(R)$ is non-increasing on $[0, \infty)$, and

$$0 \leq Q_\alpha(R) \leq \|v\|_{L^2} \int_{\mathbb{R}^d} \left(\int_{\mathbb{R}^d} |\sigma_\alpha(x, x; z)|^2 dz \right)^{1/2} dx \leq C_1$$

uniformly in α and R thanks to (3.13) and the fact that the energy of Γ_α is uniformly bounded. Then, by Helly's selection principle, there exists a subsequence α_k and a decreasing function $Q : [0, \infty) \rightarrow [0, C_1]$ such that

$$\lim_{k \rightarrow \infty} Q_{\alpha_k}(R) = Q(R), \quad \forall R \in [0, \infty).$$

Since $\lim_{R \rightarrow \infty} Q(R)$ exists by monotonicity and is finite, we conclude

$$\lim_{R \rightarrow \infty} \lim_{k \rightarrow \infty} (Q_{\alpha_k}(R) - Q_{\alpha_k}(8R)) = \lim_{R \rightarrow \infty} (Q(R) - Q(8R)) = 0.$$

Since the limit is the same for every subsequence of the initial sequence, the whole term must converge to zero. We conclude that

$$\lim_{R \rightarrow \infty} \lim_{\alpha \rightarrow \infty} \mathcal{E}_{\text{Int}}^{(1)} = 0$$

and argue similarly to obtain $\mathcal{E}_{\text{Int}}^{(2)} \rightarrow 0$. \square

We now conclude the

Proof of Proposition 3.4. The result follows immediately from Lemma 3.5, 3.6, and 3.7 after recalling the expressions of the reduced density matrices of the localized states Γ_{α, χ_R} and Γ_{α, η_R} from Proposition 3.3. \square

4. QUASI-CLASSICAL MEASURES

We revisit the construction of quasi-classical measures from [17, 16, 11, 12], linking them with the approach of [37]. Slightly improved statements are obtained by using anti-Wick rather than Weyl quantization in the basic definition of the measures, but otherwise the spirit is extremely similar. Related statements and ideas may be found in [19].

4.1. Notation. For a complex separable Hilbert space \mathfrak{H} we denote $\mathcal{B}(\mathfrak{H})$ the set of bounded operators acting thereon, $\mathcal{B}(\mathfrak{H})^*$ its dual and $\mathcal{S}(\mathfrak{H})$ the state-space, i.e.

$$\mathcal{S}(\mathfrak{H}) := \{ \omega \in \mathcal{B}(\mathfrak{H})^*, \omega(B) \geq 0 \text{ for all } 0 \leq B \in \mathcal{B}(\mathfrak{H}), \omega(\mathbb{1}) = 1 \}. \quad (4.1)$$

These are ‘‘abstract states’’ by opposition to trace-class operators, i.e. normal states. One advantage in considering them is that a sequence of abstract states always has a weak- \star cluster point which is a state. A bit of care is needed in using the weak- \star topology on $\mathcal{B}(\mathfrak{H})^*$ because the pre-dual $\mathcal{B}(\mathfrak{H})$, is not, in infinite dimension, separable. The compactness of sequences of states thus takes the form that (by the Banach-Alaoglu Theorem) given a sequence $(\omega_n)_n \in \mathcal{S}(\mathfrak{H})^{\mathbb{N}}$ there is a $\omega \in \mathcal{S}(\mathfrak{H})$ such that ω_n converges to ω along a subnet. This means that for any $B \in \mathcal{B}(\mathfrak{H})$

$$\omega_{h(\alpha)}(B) \rightarrow \omega(B) \quad (4.2)$$

where $h : A \mapsto \mathbb{N}$ is a monotone cofinal function from some directed set A to the integers. It is important to be able to test against the identity operator in (4.2), to ensure that ω is a state. With an abuse of notation we denote this convergence by

$$\omega_n \xrightarrow[\text{net}]{\star} \omega \quad (4.3)$$

where an extraction is implied.

4.2. The theorem. Let $\mathfrak{h}, \mathfrak{H}$ be two separable complex Hilbert spaces. We are interested in states of the composite system with Hilbert space

$$\mathfrak{H}_{\text{tot}} := \mathfrak{h} \otimes \mathfrak{F}(\mathfrak{H})$$

where $\mathfrak{F}(\mathfrak{H})$ is the bosonic Fock space constructed from \mathfrak{H} . We denote by \mathcal{N} the number operator on $\mathfrak{F}(\mathfrak{H})$ and

$$\mathfrak{H}_n := \mathfrak{H}^{\otimes_s n}$$

the n -particles sector. For a state Γ on $\mathfrak{H}_{\text{tot}}$, $\langle O \rangle_{\Gamma}$ denotes the expectation value of O in Γ .

For facilitated comparison with [37] we here follow the convention that annihilation and creation operators are unscaled (contrarily to the convention in (1.3)), so that the CCR takes the form (2.4)

$$[c(f), c(g)] = [c^\dagger(f), c^\dagger(g)] = 0, \quad [c(f), c^\dagger(g)] = \langle f, g \rangle, \quad \forall f, g \in L_{\text{field}}^2(\mathbb{R}^d) \quad (4.4)$$

for the creation and annihilation operators (cf (2.3))

$$c^\dagger(f) = \alpha a^\dagger(f), \quad c(f) = \alpha a(f).$$

Definition 4.1 (Reduced density matrices).

Let $\Gamma \in \mathcal{S}(\mathfrak{H}_{\text{tot}})$ be a state over $\mathfrak{H}_{\text{tot}}$. We define reduced densities $\Gamma^{(k,\ell)}$ as maps from $\mathcal{B}(\mathfrak{h})$ to $\mathcal{B}(\mathfrak{H}_\ell, \mathfrak{H}_k)$ (the bounded operators from \mathfrak{H}_ℓ to \mathfrak{H}_k) by the formula

$$\langle f_1 \otimes_s \dots \otimes_s f_k | \Gamma^{(k,\ell)}(A) g_1 \otimes_s \dots \otimes_s g_\ell \rangle := \langle A \otimes c^\dagger(g_1) \dots c^\dagger(g_\ell) c(f_1) \dots c(f_k) \rangle_\Gamma \quad (4.5)$$

where $A \in \mathcal{B}(\mathfrak{h})$ and $f_1, \dots, f_k, g_1, \dots, g_\ell \in \mathfrak{H}$. The definition makes sense as soon as

$$\langle \mathcal{N}^{\frac{k+\ell}{2}} \rangle_\Gamma < \infty$$

where

$$\mathcal{N} = \sum_{j \geq 1} c^\dagger(f_j) c(f_j)$$

for any orthonormal basis $(f_j)_j$ of \mathfrak{H} . ◇

Definition 4.2 (Anti-Wick observables).

To any $u \in \mathfrak{H}$ we associate a *coherent state* on $\mathfrak{F}(\mathfrak{H})$

$$\xi(u) := e^{-\frac{|u|^2}{2}} \bigoplus_{j \geq 0} \frac{1}{\sqrt{j!}} u^{\otimes j} \in \mathfrak{F}(\mathfrak{H}). \quad (4.6)$$

For any sequence $\varepsilon \rightarrow 0$ and any finite-dimensional subspace V of \mathfrak{H} we define the *anti-Wick quantization* of a function $b \in C_b^0(V)$ at scale ε , by

$$b_\varepsilon^{\text{aW}} := (\varepsilon\pi)^{-\dim(V)} \int_V b(u) \left| \xi\left(\frac{u}{\sqrt{\varepsilon}}\right) \right\rangle \left\langle \xi\left(\frac{u}{\sqrt{\varepsilon}}\right) \right| du. \quad (4.7)$$

◇

We aim at proving the

Theorem 4.3 (Quantum de Finetti for composite systems).

Consider a sequence $\varepsilon \rightarrow 0$ of positive parameters, and associated sequence Γ_ε of states over $\mathfrak{H}_{\text{tot}}$ satisfying

$$\langle (\varepsilon \mathcal{N})^\kappa \rangle_{\Gamma_\varepsilon} < +\infty \quad (4.8)$$

uniformly in ε , for some $1 \leq \kappa$.

There exists a probability measure $\mu \in \mathcal{P}(\mathfrak{H})$ and a μ -measurable map

$$\omega : \begin{cases} \mathfrak{H} \rightarrow \mathcal{S}(\mathfrak{h}) \\ u \mapsto \omega_u \end{cases}$$

with values in the state-space of \mathfrak{h} such that,

- (1) Expectations of anti-Wick observables converge and define the measure: along a subnet, for all $A \in \mathcal{B}(\mathfrak{h})$, $V \subset \mathfrak{H}$ a finite-dimensional subspace and $b \in C_c^0(V)$ we have

$$\langle A \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon} \xrightarrow[\text{net}]{\star} \int_{\mathfrak{H}} \omega_u(A) b(u) d\mu(u) \quad (4.9)$$

(2) *Reduced density matrices converge: along a subsequence, for A a compact operator or the identity*³

$$\sqrt{k!\ell!\varepsilon^k\varepsilon^\ell}\Gamma_\varepsilon^{(k,\ell)}(A) \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} \omega_u(A) |u^{\otimes k}\rangle \langle u^{\otimes \ell}| d\mu(u) \quad (4.10)$$

weakly- \star in the trace-class for all k, ℓ satisfying $\frac{k+\ell}{2} \leq \kappa$. More precisely

$$\sqrt{k!\ell!\varepsilon^k\varepsilon^\ell} \langle A \otimes c^\dagger(g_1) \dots c^\dagger(g_\ell) c(f_1) \dots c(f_k) \rangle_{\Gamma_\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} \omega_u(A) \prod_{j=1}^k \langle f_j | u \rangle \prod_{j=1}^{\ell} \langle u | g_j \rangle d\mu(u)$$

for all $f_1, \dots, f_k, g_1, \dots, g_\ell \in \mathfrak{H}$.

We shall rely on a version of the above in the non-composite case (where $\mathfrak{h} \otimes \mathfrak{F}(\mathfrak{H})$ is replaced by $\mathfrak{F}(\mathfrak{H})$) from [37, Sections 4 and 6]. This is also contained in [3, 4] where the construction is rather based on Weyl observables/quantizations rather than anti-Wick as we use here.

Before proceeding to the proof, we state as corollary the convergence of observables akin to the interaction energy of our main model.

Corollary 4.4 (Quantum de Finetti and the particle-field density matrix).

Let $\mathfrak{h} = L^2(\mathbb{R}^d)$, $v \in L^2(\mathbb{R}^d, \mathbb{R})$. Under the assumptions above (for $\kappa = 1$), after extracting a subsequence

$$\sqrt{\varepsilon} \left\langle \int_{\mathbb{R}^d} v(\cdot - y) (c^\dagger(y) + c(y)) dy \right\rangle_{\Gamma_\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} \int_{\mathbb{R}^d} \omega_u(v(\cdot - y)) (u(y) + \overline{u(y)}) dy d\mu(u) \quad (4.11)$$

where $v(\cdot - y)$ is understood as a multiplication operator on \mathfrak{h} . In other words

$$\iint_{\mathbb{R}^2 \times \mathbb{R}^2} \sigma_\varepsilon(x, x; z) v(x - z) dx dz \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} \int_{\mathbb{R}^d} \omega_u(v(\cdot - z)) (u(z) + \overline{u(z)}) dz d\mu(u) \quad (4.12)$$

where $\sigma_\varepsilon(x, y; z)$ is the integral kernel of the particle-density matrix of Γ_ε , as defined in Section 3.1.

Proof. Equation (3.13) shows that $(x, z) : \mapsto \sigma_\varepsilon(x, z; z)$ is uniformly bounded as a sequence in $L_x^1(L_z^2(\mathbb{R}^d))$, which is a subset of the dual of the Banach space $C_x^{0,b}(L_z^2(\mathbb{R}^d))$ of bounded continuous functions with values in $L^2(\mathbb{R}^d)$ (see e.g. [30]). Hence, modulo extraction of a subsequence

$$\iint_{\mathbb{R}^2 \times \mathbb{R}^2} \sigma_\varepsilon(x, x; z) \phi(x, z) dx dz \xrightarrow{\varepsilon \rightarrow 0} \iint_{\mathbb{R}^2 \times \mathbb{R}^2} \sigma_0(x, x; z) \phi(x, z) dx dz$$

for any $\phi \in C_x^0(L^2(\mathbb{R}^d))$, with σ_0 a Radon measure over $L^2(\mathbb{R}^d)$ (with a slight abuse of notation in the right-hand side of the above). For $v \in L^2(\mathbb{R}^d)$, the map $(x, z) \mapsto v(x - z)$ is in $C_x^{0,b}(L_z^2(\mathbb{R}^d))$ since the statement

$$\lim_{x \rightarrow x_0} \int_{\mathbb{R}^d} |v(x - y) - v(x_0 - y)|^2 dy = 0$$

is equivalent to $v * v$ being continuous at x_0 , which is true for $v \in L^2(\mathbb{R}^d)$ by [21, Proposition 8.8].

Thus we may assume that the left-hand sides of (4.11)-(4.12) converge for any $v \in L^2(\mathbb{R}^d)$. We now identify the limit σ_0 with the help of Theorem 4.3. By density we may restrict to testing with a

³In fact, modulo a subsequence, we can test with A in any separable subspace of the bounded operators.

smooth compactly supported v if needed, so that the multiplication operator $v(\cdot - y)$ is bounded on \mathfrak{h} . Theorem 4.3 implies that, along a subsequence, for any such $v, x_0 \in \mathbb{R}^d$ and $f \in L^2(\mathbb{R}^d)$,

$$\sqrt{\varepsilon} \langle v(\cdot - x_0) \otimes (c^\dagger(f) + c(f)) \rangle_{\Gamma_\varepsilon} \rightarrow \int_{\mathfrak{H}} \omega_u(v(\cdot - x_0)) (\langle f|u \rangle + \langle u|f \rangle) d\mu(u). \quad (4.13)$$

Introduce now a tiling $(Q_n^\varepsilon)_{0 \leq n \leq N}$ of $[0, R_\varepsilon]^d$, say with squares of centers x_n and vanishing side-length when $\varepsilon \rightarrow 0$, where $R_\varepsilon \rightarrow \infty$. We claim that, as operators,

$$\sqrt{\varepsilon} \left| \int_{\mathbb{R}^d} v(\cdot - y) (c_y^\dagger + c_y) dy - \sum_n (c^\dagger(\mathbb{1}_{Q_n^\varepsilon}) + c(\mathbb{1}_{Q_n^\varepsilon})) v(\cdot - x_n) \right| \leq o_\varepsilon(1) (\mathcal{N} + 1). \quad (4.14)$$

Indeed the left-hand side (omitting the absolute value) is equal to

$$\sum_n \int_{\mathbb{R}^d} (v(\cdot - y) - v(\cdot - x_n)) (c_y^\dagger + c_y) \mathbb{1}_{Q_n^\varepsilon}(y) dy$$

so that a Cauchy-Schwarz inequality gives

$$\begin{aligned} & \sqrt{\varepsilon} \left| \int_{\mathbb{R}^d} v(\cdot - y) (c_y^\dagger + c_y) dy - \sum_n (c^\dagger(\mathbb{1}_{Q_n^\varepsilon}) + c(\mathbb{1}_{Q_n^\varepsilon})) v(\cdot - x_n) \right| \\ & \leq C\delta \sum_n \int_{\mathbb{R}^d} c_y^\dagger c_y \mathbb{1}_{Q_n^\varepsilon}(y) dy + C\delta^{-1} \sum_n \int_{\mathbb{R}^d} (v(\cdot - y) - v(\cdot - x_n))^2 \mathbb{1}_{Q_n^\varepsilon}(y) dy \\ & \leq C\delta\varepsilon\mathcal{N} + \frac{C}{\delta} o_\varepsilon(1) \end{aligned}$$

using that

$$\sum_n \mathbb{1}_{Q_n^\varepsilon} \equiv 1,$$

recognizing a Riemann sum and using that $v \in L^2(\mathbb{R}^d)$. Choosing $\delta = \delta_\varepsilon \rightarrow 0$ suitably slowly vindicates (4.14).

Next we obtain, after possibly a further extraction of subsequence

$$\sqrt{\varepsilon} \left\langle \int_{\mathbb{R}^d} v(\cdot - y) (c^\dagger(y) + c(y)) dy \right\rangle_{\Gamma_\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} \sum_n \int_{\mathfrak{H}} \int_{\mathbb{R}^d} \omega_u(v(\cdot - x_n)) (u(y) + \overline{u(y)}) \mathbb{1}_{Q_n^\varepsilon}(y) dy d\mu(u). \quad (4.15)$$

This follows from (4.14), for each term

$$(c^\dagger(\mathbb{1}_{Q_n^\varepsilon}) + c(\mathbb{1}_{Q_n^\varepsilon})) v(\cdot - x_n)$$

is amenable to the use of (4.13). With a suitable truncation of the sum in and a diagonal extraction we obtain convergence for each term and the sum along a common subsequence. Finally, the right-hand side of (4.15) equals that of (4.11) by another Riemann sum argument, recalling that we may work with a smooth compactly supported v . \square

4.3. Proof of Theorem 4.3. We recall the statement of [37, Theorem 4.2]:

Theorem 4.5 (Grand-canonical quantum de Finetti theorem).

Consider a sequence $\varepsilon \rightarrow 0$ of positive parameters, and associated sequence Γ_ε of states over $\mathfrak{F}(\mathfrak{H})$ satisfying

$$\langle (\varepsilon\mathcal{N})^k \rangle_{\Gamma_\varepsilon} < +\infty$$

uniformly in ε , for some $1 \leq \kappa$.

There exists a unique probability measure $\mu \in \mathcal{P}(\mathfrak{H})$ such that, modulo the extraction of a subsequence,

- (1) Expectations of anti-Wick observables converge and define the measure: for all $V \subset \mathfrak{H}$ a finite-dimensional subspace and $b \in C_c^0(V)$ we have

$$\langle b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon} \rightarrow \int_{\mathfrak{H}} b(u) d\mu(u) \quad (4.16)$$

- (2) Reduced density matrices converge

$$\sqrt{k! \ell! \varepsilon^k \varepsilon^\ell} \Gamma_\varepsilon^{(k, \ell)} \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} |u^{\otimes k} \rangle \langle u^{\otimes \ell}| d\mu(u) \quad (4.17)$$

weakly- \star in the trace-class for all k, ℓ satisfying $\frac{k+\ell}{2} \leq \kappa$. In particular

$$\sqrt{k! \ell! \varepsilon^k \varepsilon^\ell} \langle a^\dagger(g_1) \dots a^\dagger(g_\ell) a(f_1) \dots a(f_k) \rangle_{\Gamma_\varepsilon} \xrightarrow{\varepsilon \rightarrow 0} \int_{\mathfrak{H}} \prod_{j=1}^k \langle f_j | u \rangle \prod_{j=1}^{\ell} \langle u | g_j \rangle d\mu(u)$$

for all $f_1, \dots, f_k, g_1, \dots, g_\ell \in \mathfrak{H}$.

Only the case $k = \ell$ of (4.17) is worked out explicitly in [37]. The adaptation to $k \neq \ell$ is however straightforward, only the core calculations from e.g. [36, Lemma 4.2] have to be adapted mutatis mutandis.

Proof of Theorem 4.3.

Step 1. Let $C_c^0(\mathfrak{H})$ denote continuous functions with compact support over \mathfrak{H} and consider the algebra of observables

$$\mathcal{A} := \mathcal{B}(\mathfrak{h}) \otimes C_c^0(\mathfrak{H}).$$

Starting from $\Gamma_\varepsilon \in \mathcal{S}(\mathfrak{h} \otimes \mathfrak{F}(\mathfrak{H}))$ as in the theorem's statement we define a state $\tilde{\Gamma}_\varepsilon \in (\mathcal{B}(\mathfrak{h}) \otimes C_c^0(\mathfrak{H}))^*$ over \mathcal{A} by testing it against a dense subset of elements of \mathcal{A} . Namely, for any $A \in \mathcal{B}(\mathfrak{H})$, any finite-dimensional $V \subset \mathfrak{H}$ and $b \in C_c^0(V)$, we set

$$\tilde{\Gamma}_\varepsilon(A \otimes b) := \langle A \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon}.$$

That way $(\tilde{\Gamma}_\varepsilon)_\varepsilon$ is a bounded sequence of positive linear forms over \mathcal{A} (seen as a Banach space) and therefore it has a weak cluster point $\tilde{\Gamma}_0 \in \mathcal{A}^*$. Namely, along a subnet

$$\tilde{\Gamma}_\varepsilon(C) \xrightarrow[\text{net}]{\star} \tilde{\Gamma}_0(C) \text{ for all } C \in \mathcal{A}.$$

We now identify the cluster point.

For any positive operator $A \in \mathcal{B}(\mathfrak{H})$, we can define a (non-normalized) state Γ_ε^A over $\mathfrak{F}(\mathfrak{H})$ by setting

$$\langle B \rangle_{\Gamma_\varepsilon^A} = \langle A \otimes B \rangle_{\Gamma_\varepsilon}.$$

Applying⁴ Theorem 4.5 to Γ_ε^A we find that there must exist a positive Borel measure μ_A on \mathfrak{H} such that

$$\langle A \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon} \xrightarrow[\text{net}]{\star} \int_{\mathfrak{H}} b(u) d\mu_A(u).$$

⁴Strictly speaking, we go back to the proof of Item (i) in [37] to identify any cluster point, not only sequential limits. This is done mutatis mutandis using Skorokhod's lemma [58].

However, since (the operator norm is used below)

$$\langle A \otimes b_\varepsilon^{aW} \rangle_{\Gamma_\varepsilon} \leq \|A\| \langle \mathbb{1} \otimes b_\varepsilon^{aW} \rangle_{\Gamma_\varepsilon}$$

for any positive function b from a finite-dimensional subspace of \mathfrak{H} , we find that

$$\int_{\mathfrak{H}} b(u) d\mu_A(u) \leq \|A\| \int_{\mathfrak{H}} b(u) d\mu_{\mathbb{1}}(u).$$

Picking any $V \subset \mathfrak{H}$ this implies that (approximating the characteristic function of V by a sequence of continuous functions)

$$\mu_{\mathbb{1}}(V) = 0 \Rightarrow \mu_A(V) = 0$$

for any positive bounded operator $A \in \mathcal{B}(\mathfrak{h})$. By Radon-Nykodym's theorem, we deduce that for any positive bounded A , there exists a map $u \mapsto \omega_u(A) \in L^1(\mathfrak{H}, d\mu_{\mathbb{1}})$ such that

$$\int_{\mathfrak{H}} b(u) d\mu_A(u) = \int_{\mathfrak{H}} b(u) \omega_u(A) d\mu_{\mathbb{1}}(u).$$

Upon redefining $\omega_u(A)$ if necessary we can assume $\mu_{\mathbb{1}}$ is a probability. From the definition it also follows that $\omega_u(A)$ is $\mu_{\mathbb{1}}$ almost-surely a bounded linear function of A .

Next we can split a general bounded operator in the form

$$A = A_{r+} - A_{r-} + iA_{i+} - iA_{i-} \quad (4.18)$$

with four positive operators $A_{r+}, A_{r-}, A_{i+}, A_{i-}$. Applying the above to each term separately we find a $\mu := \mu_{\mathbb{1}} \in \mathcal{P}(\mathfrak{H})$ and $u \mapsto \omega_u(\cdot)$ a $L^1(\mathfrak{H}, d\mu)$ map from \mathfrak{H} to the state-space of \mathfrak{h} such that

$$\langle A \otimes b_\varepsilon^{aW} \rangle_{\Gamma_\varepsilon} \stackrel{\star}{\underset{\text{net}}{\rightrightarrows}} \int_{\mathfrak{H}} \omega_u(A) d\mu(u)$$

for any $A \in \mathcal{B}(\mathfrak{H})$ and any $b \in C_c^0(V)$ with V a finite-dimensional subspace of \mathfrak{H} . This is the first statement of the theorem.

Step 2. Under our assumptions, $\sqrt{k! \ell! \varepsilon^k \varepsilon^\ell} \Gamma_\varepsilon^{(k, \ell)}(A)$ is a bounded sequence of trace-class operators for any positive bounded A and $\frac{k+\ell}{2} \leq \kappa$. Hence we may extract a weak- \star convergent subsequence. If A varies in a separable subspace of the bounded operators (e.g. the span of compact operators and the identity, as in the theorem's statement), we can use a dense countable subset thereof to obtain convergence along a common subsequence for all A , modulo a diagonal extraction argument.

To obtain the second statement of the theorem we further extract a subnet along which Item (1) holds. There remains to apply (4.17) to each (non-normalized) state Γ_ε^A defined above, with A a positive operator, and use the splitting (4.18) to generalize to all operators in the statement. The measure in (4.17) being the same as that in (4.16), we identify the limit in (4.10) by using (4.9). \square

Under more restrictive assumptions we may ensure that $\omega_u(\cdot)$ is almost surely a normal state, i.e. can be represented by a density matrix:

Corollary 4.6 (Quantum de Finetti for composite localized states).

Suppose that, in addition to the assumptions of Theorem 4.3, the sequence Γ_ε satisfies as well the bound

$$\langle L \otimes \mathbb{1} \rangle_{\Gamma_\varepsilon} < +\infty,$$

uniformly in ε , for some positive operator L on \mathfrak{h} with compact resolvent. Then the μ -measurable map ω of Theorem 4.3 takes values in the set of normal states on \mathfrak{h} , i.e. in the set of positive, normalized, trace-class operators.

Proof. On the one hand, we know that by Theorem 4.3, there exists a measure μ and a state-valued map ω such that the expectation of anti-Wick observables converges. In addition, as illustrated in the proof of the theorem, such convergence identifies the couple (μ, ω) .

Now, let us define the family of states

$$\Gamma_\varepsilon^{(L)} := (L+1)^{1/2} \Gamma_\varepsilon (L+1)^{1/2}.$$

For $\Gamma_\varepsilon^{(L)}$ we proceed as in the proof of Theorem 4.3, substituting the algebra of observables \mathcal{A} with

$$\mathcal{K} := \mathcal{L}^\infty(\mathfrak{h}) \otimes C_c^0(\mathfrak{S}),$$

where $\mathcal{L}^\infty(\mathfrak{h})$ is the space of compact operators. Thanks to this modification, we can identify a limit measure $\mu^{(L)}$, and a $\mu^{(L)}$ -measurable map

$$\omega^{(L)} : \begin{cases} \mathfrak{S} \rightarrow \mathcal{L}_{+,1}^1(\mathfrak{h}) \\ u \mapsto \omega_u^{(L)} \end{cases}$$

where $\mathcal{L}_{+,1}^1(\mathfrak{h})$ is the set of normal states on \mathfrak{h} , dual to the set of compact operators. The drawback is that in this case $\mu^{(L)}$ could fail to be a probability measure. Let us remark that one could identify different limit measures along different subsubnets of the one used to obtain (μ, ω) from Γ_ε .

Now, let us fix $A \in \mathcal{B}(\mathfrak{h})$, $V \subset \mathfrak{S}$ finite dimensional, and $b \in C_c^0(V)$. On the one hand, by Theorem 4.3, along the subsubnet

$$\langle A \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon} \rightarrow \int_{\mathfrak{S}} \omega_u(A) b(u) d\mu(u),$$

and on the other hand,

$$\langle (L+1)^{-1/2} A (L+1)^{-1/2} \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon^{(L)}} \rightarrow \int_{\mathfrak{S}} \omega_u^{(L)}((L+1)^{-1/2} A (L+1)^{-1/2}) b(u) d\mu^{(L)}(u),$$

since $(L+1)^{-1/2} A (L+1)^{-1/2} \in \mathcal{L}^\infty(\mathfrak{h})$ for any $A \in \mathcal{B}(\mathfrak{h})$. However,

$$\langle A \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon} = \langle (L+1)^{-1/2} A (L+1)^{-1/2} \otimes b_\varepsilon^{\text{aW}} \rangle_{\Gamma_\varepsilon^{(L)}}$$

by definition of $\Gamma_\varepsilon^{(L)}$, and thus

$$\int_{\mathfrak{S}} \omega_u(A) b(u) d\mu(u) = \int_{\mathfrak{S}} \omega_u^{(L)}((L+1)^{-1/2} A (L+1)^{-1/2}) b(u) d\mu^{(L)}(u),$$

which implies $\mu = \mu^{(L)}$, and, μ -almost surely,

$$\omega_u(\cdot) = \omega_u^{(L)}((L+1)^{-1/2} \cdot (L+1)^{-1/2}).$$

The limit is the same along any subsubnet, and thus it holds on the original subnet as well. Therefore, it follows that $\omega_u \in \mathcal{L}_{+,1}^1(\mathfrak{h})$. \square

5. CONVERGENCE OF THE ENERGY

For completeness we now revisit the proof of

Theorem 5.1 (Energy convergence).

With the assumptions and notation of Section 2, we have that

$$E_{(\alpha)}^{(V)} \xrightarrow{\alpha \rightarrow \infty} E_{\text{Pek}}^{(V)}(1).$$

In particular this holds true with the external potential $V \equiv 0$.

Our proof is in the spirit of [12], but we use quasi-classical measures as constructed in the previous section, leading to mild simplifications. In view of Theorem 4.3, the natural limit energy takes general abstract states as arguments. We discuss this first in a subsection, and proves that this does not lower the energy as compared to what was defined in Section 2. We will complete the proof of Theorem 5.1 in a second subsection.

5.1. Generalized Pekar energies. Let

$$h := -\Delta + V$$

and W be as in (2.15), and identified with the multiplication operator by $W(x-y)$ on the two-particle space $L^2_{\text{part}} \otimes L^2_{\text{part}}$.

We start this discussion by generalizing Pekar's energy functional to take mixed states as arguments:

Lemma 5.2 (Mixed Pekar functional).

Any minimizer of

$$\gamma \mapsto \text{Tr} [h\gamma] + \text{Tr} [W(x-y)\gamma \otimes \gamma]$$

amongst positive trace-class operators of trace 1 must be rank one. Hence any minimizer is of the form $\gamma = |\psi\rangle\langle\psi|$ with ψ a minimizer for (2.16) with $m = 1$.

Similar arguments may be found e.g. in [55, Section 5] or [5, Section 2].

Proof. The existence of minimizers follows by a concentration-compactness argument similar to that leading to the existence for (2.16). We skip details and denote γ_0 a minimizer.

Consider a variation

$$\gamma = (1 - \varepsilon)\gamma_0 + \varepsilon\sigma$$

with $0 < \varepsilon < 1$ and σ a positive trace-class operator of trace 1. Evaluating the energy of γ and taking ε small enough we find that necessarily (keeping only the $O(\varepsilon)$ term in the expansion)

$$\text{Tr} \left[\gamma \left(h + W * \rho_{\gamma_0} \right) \right] \leq \text{Tr} \left[\sigma \left(h + W * \rho_{\gamma_0} \right) \right]$$

where $\rho_{\gamma_0}(x) = \gamma_0(x, x)$ is the density of γ_0 .

Hence γ_0 must also minimize the linearized

$$\gamma \mapsto \text{Tr} \left[\gamma \left(h + W * \rho_{\gamma_0} \right) \right],$$

which in particular shows that the Schrödinger operator $h + W * \rho_{\gamma_0}$ has at least a ground energy state. Then, γ must have its image in the ground energy space of $h + W * \rho_{\gamma_0}$, but the latter has dimension one by well-known arguments (see e.g. [52, Theorem 2.3] or [47, Section XIII.12]). \square

We now turn to a functional taking generalized states as arguments. For an abstract state ω on $L^2_{\text{part}}(\mathbb{R}^d)$ (a positive linear functional over bounded operators acting on $L^2_{\text{part}}(\mathbb{R}^d)$) let, in analogy with (2.14),

$$\mathcal{E}_{\text{Pek}}^{(V)}(\omega) := \omega(h) + \omega \otimes \omega(W(x-y)) = \omega \otimes \omega \left(\frac{h_x + h_y}{2} + W(x-y) \right)$$

and (Gen for generalized)

$$E_{\text{Gen}}^{(V)} := \inf \left\{ \mathcal{E}_{\text{Pek}}^{(V)}(\omega), \omega \in \mathcal{S}(L^2(\mathbb{R}^d)) \text{ as defined in (4.1)} \right\}. \quad (5.1)$$

Under our assumptions one easily proves that

$$H_2 := \frac{h_x + h_y}{2} + W(x - y) \geq -C \quad (5.2)$$

for some constant C , and hence the infimum above is well-defined. We have the

Lemma 5.3 (Generalized energy = Pekar energy).

With the previous definitions

$$E_{\text{Gen}}^{(V)} = E_{\text{Pek}}^{(V)}(1).$$

Proof. In view of Assumption 2.1, we may for this proof assume without loss that $h \geq 0$ as an operator.

Denote $\mathfrak{h} = L^2(\mathbb{R}^d)$ for brevity. We have [54, Chapter 4] that the dual of bounded operators $(\mathcal{B}(\mathfrak{h}))^*$ is the bidual of the trace-class $\mathcal{L}^1(\mathfrak{h})$. Hence, by Goldstine's theorem⁵, for any abstract state ω there exists a net of positive trace-class operators γ_n such that

$$\text{Tr} [\gamma_n B] \xrightarrow[\text{net}]{\star} \omega(B) \quad (5.3)$$

for any bounded operator B . The rest of the proof is then akin to that of [12, Proposition 2.8].

For a state ω with $\mathcal{E}_{\text{Gen}}^{(V)}(\omega) < \infty$ it follows from (5.2) that $\omega(h) < \infty$ and $\omega \otimes \omega(H_2) < \infty$. Hence

$$\omega^h(B) := \omega(h^{1/2} B h^{1/2})$$

defines a positive linear functional on $\mathcal{B}(\mathfrak{h})$ as well, to which we may apply the above, obtaining a net of trace-class operators γ_n^h such that

$$\text{Tr} [\gamma_n^h B] \xrightarrow[\text{net}]{\star} \omega^h(B). \quad (5.4)$$

Applying (5.3) directly to ω yields another net γ_n , but testing (5.4) with B of the form $h^{-1/2} \tilde{B} h^{-1/2}$ for a bounded \tilde{B} shows that one can take

$$\gamma_n = h^{-1/2} \gamma_n^h h^{-1/2}.$$

Similarly

$$\omega_2(B_2) := \omega \otimes \omega \left(\sqrt{H_2 + C} B_2 \sqrt{H_2 + C} \right)$$

defines a positive linear functional on bounded operators B_2 on $\mathfrak{h}^{\otimes 2}$, where C is a constant such that $H_2 + C \geq 0$. We deduce that ω_2 is the limit of a net of trace-class operators that we may identify to

$$(h^{-1/2} \gamma_n^h h^{-1/2}) \otimes (h^{-1/2} \gamma_n^h h^{-1/2})$$

as above. Using (5.4) and the fact that W is a bounded multiplication operator, we conclude that for any state ω with $\mathcal{E}_{\text{Gen}}^{(V)}(\omega) < \infty$, there exists a net (γ_n) of trace-class operators such that

$$\mathcal{E}_{\text{Gen}}^{(V)}(\gamma_n) \xrightarrow[\text{net}]{\star} \mathcal{E}_{\text{Gen}}^{(V)}(\omega).$$

This leads to

$$E_{\text{Gen}}^{(V)} \geq \inf \left\{ \mathcal{E}_{\text{Pek}}^{(V)}(\gamma), \gamma \in \mathcal{L}^1(\mathfrak{h}), \gamma \geq 0, \text{Tr } \gamma = 1 \right\}. \quad (5.5)$$

⁵If X is a Banach space, its unit ball is dense in that of the bidual X^{**} for the weak- \star topology, see e.g. [53, Exercise 1 on page 128].

The opposite inequality follows from the variational principle. The right-hand side of the above is the Pekar energy (2.14) generalized to a mixed state

$$\gamma = \sum_{j \geq 1} \lambda_j |u_j\rangle\langle u_j|$$

with $\lambda_j \geq 0$, $\sum_j \lambda_j = 1$ and an orthonormal basis $(u_j)_j$ of \mathfrak{h} . We hence conclude from Lemma 5.2 that

$$E_{\text{Gen}}^{(V)} = E_{\text{Pek}}^{(V)}(1)$$

as desired. \square

5.2. Proof of Theorem 5.1. Again, without loss of generality (i.e. adding a constant if needed), we assume that $h \geq 0$. We consider a sequence of quasi-minimizers as in (2.19). Under our assumptions, applying the Cauchy-Schwarz inequality to the interaction term immediately leads to the a priori bound

$$\langle \Psi_\alpha | (-\Delta + V) \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{N}_\alpha | \Psi_\alpha \rangle \leq C \quad (5.6)$$

independently of α . Here \mathcal{N}_α is the scaled particle number (2.7). We apply Theorem 4.3 with $\kappa = 1$, obtaining a probability measure μ over $L^2(\mathbb{R}^d)$ and a μ -measurable map ω_u from $L^2(\mathbb{R}^d)$ to the state-space of $L^2(\mathbb{R}^d)$. Combining with Corollary 4.4 we may pass to the limit in the field energy and the interaction term. As regards the particle energy we denote γ_α the particle reduced density matrix of $|\Psi_\alpha\rangle\langle\Psi_\alpha|$. Since $\text{Tr}(\gamma_\alpha h) < \infty$, we have that

$$\gamma_\alpha^h(B) := \text{Tr}(h^{1/2} \gamma_\alpha h^{1/2} B)$$

defines a bounded sequence of positive linear forms over bounded operators. Extracting a further weakly- \star convergent subnet and identifying the limit by testing with B of the form $h^{-1/2} \tilde{B} h^{-1/2}$ we deduce that

$$\text{Tr}(h \gamma_\alpha) \xrightarrow[\text{net}]{\star} \int \omega_u(h) d\mu(u).$$

All in all

$$\begin{aligned} \liminf_{\alpha \rightarrow \infty} E_{(\alpha)}^{(V)} &\geq \int_{L^2(\mathbb{R}^d)} \left(\omega_u(h) + \|u\|_{L^2}^2 + \int_{\mathbb{R}^d} \omega_u(v(\cdot - z)) \left(u(z) + \overline{u(z)} \right) dz \right) d\mu(u) \\ &\geq \inf \left\{ \omega(h) + \|u\|_{L^2}^2 + \int_{\mathbb{R}^d} \omega(v(\cdot - z)) \left(u(z) + \overline{u(z)} \right) dz, u \in L^2(\mathbb{R}^d), \omega \in S(L^2(\mathbb{R}^d)) \right\} \end{aligned}$$

since μ is a probability measure. Minimizing with respect to u at fixed ω in a similar manner as in (2.14) leads to a real-valued u such that

$$u(z) = -\omega(v(\cdot - z))$$

and an energy

$$\begin{aligned} \omega(h) - \|u\|_{L^2}^2 &= \omega(h) - \iint \omega(v(\cdot - y)) \omega(v(\cdot - z)) dy dz \\ &= \omega(h) - \iint \omega_{x_1} \otimes \omega_{x_2} (v(x_1 - y) v(x_2 - z)) dy dz \\ &= \mathcal{E}_{\text{Pek}}^{(V)}(\omega) \end{aligned}$$

where we inverted the integral over y, z and the expectation in $\omega \otimes \omega$ in the last step, recalling (2.15). We conclude that

$$\liminf_{\alpha \rightarrow \infty} E_{(\alpha)}^{(V)} \geq E_{\text{Gen}}^{(V)}.$$

There remains to use Lemma 5.3 and recall that the upper bound

$$E_{\text{Pek}}^{(V)}(1) \geq E_{(\alpha)}^{(V)}$$

follows from the trial state argument sketched in Section 2.

6. CONVERGENCE OF STATES, PROOF OF THEOREM 2.3

Since our main result Theorem 2.3 is stated modulo subsequence, we take the liberty of not indicating all extractions of subsequences/subnets in the arguments of this section.

We start from a sequence of states

$$\Gamma_\alpha = |\Psi_\alpha\rangle\langle\Psi_\alpha|$$

as in the statement of the theorem. As in the previous section we have that

$$\langle\Psi_\alpha|(-\Delta + V) \otimes \mathbb{1} + \mathbb{1} \otimes \mathcal{N}_\alpha|\Psi_\alpha\rangle \leq C \quad (6.1)$$

and we may apply Theorem 4.3 with $\kappa = 1$, obtaining a probability measure μ over $L^2(\mathbb{R}^d)$ and a state-valued map ω_u . Let γ_α be the particle density matrix of Γ_α , as in Section 3.1. We may extract a weak- \star convergent subsequence in the trace-class:

$$\text{Tr} [\gamma_\alpha K] \xrightarrow{\alpha \rightarrow \infty} \text{Tr} [\gamma_\infty K] \quad (6.2)$$

for any compact operator K over $L^2(\mathbb{R}^d)$. Identifying the limit using Theorem 4.3, it must be that

$$\gamma_\infty = \int \omega_u^{\text{nor}} d\mu(u) \quad (6.3)$$

with ω_u^{nor} the normal part of ω_u , i.e. the unique trace-class operator satisfying

$$\omega_u(K) = \text{Tr} [\omega_u^{\text{nor}} K] \text{ for any compact operator } K. \quad (6.4)$$

Arguing in a similar manner for the field density matrix

$$\gamma^f := \Gamma_\alpha^{(1,1)}$$

we find

$$\gamma^f \xrightarrow[\alpha \rightarrow \infty]{\star} \int |u\rangle\langle u| d\mu(u)$$

along a subsequence, instead of just a subnet as in Theorem 4.3. As regards the particle-field density matrix σ_α , we consider $\sigma_\alpha(x, x; z)$ as a $L_x^1 L_z^2$ function as in the proof of Corollary 4.4 and deduce

$$\iint_{\mathbb{R}^2 \times \mathbb{R}^2} \sigma_\alpha(x, x; z) v(x-z) dx dz \xrightarrow{\alpha \rightarrow \infty} \int_{\mathfrak{H}} \int_{\mathbb{R}^d} \omega_u(v(\cdot - z)) \left(u(z) + \overline{u(z)} \right) dz d\mu(u).$$

Now, we aim at turning the weak convergences from (6.2) and Theorem 4.3 into strong ones. For that we prove that no mass is lost in the limit:

Lemma 6.1 (No loss of mass).

Let γ_∞ be the weak- \star limit of the particle density matrix, introduced above. We have that

$$\mathrm{Tr} [\gamma_\infty] = 1$$

and hence

$$\gamma_\alpha \xrightarrow{\alpha \rightarrow \infty} \gamma_\infty$$

along a subsequence, strongly in trace-class norm.

Proof. That the first statement implies the second is classical [13, 57]. We thus focus on the mass of the limit density matrix.

Step 1. Let χ_R be a localization function as in Section 3.3. We claim that

$$\mathrm{Tr} [\chi_R \gamma_\alpha \chi_R] \xrightarrow{\alpha \rightarrow \infty} \mathrm{Tr} [\chi_R \gamma_\infty \chi_R]. \quad (6.5)$$

Indeed, let γ_α^k be the positive operator

$$\gamma_\alpha^k = (1 - \Delta)^{1/2} \gamma_\alpha (1 - \Delta)^{1/2}.$$

It follows from (6.1) that γ_α^k is uniformly bounded in trace-class norm. Thus, modulo a possible further extraction

$$\gamma_\alpha^k \xrightarrow{\alpha \rightarrow \infty} \gamma_\infty^k = (1 - \Delta)^{1/2} \gamma_\infty (1 - \Delta)^{1/2}$$

weakly-star in the trace-class, where we identified the limit by testing against $(1 - \Delta)^{-1/2} K (1 - \Delta)^{-1/2}$ for a compact operator K . Then

$$\begin{aligned} \mathrm{Tr} [\chi_R \gamma_\alpha \chi_R] &= \mathrm{Tr} [\chi_R (1 - \Delta)^{-1/2} \gamma_\alpha^k (1 - \Delta)^{-1/2} \chi_R] \\ &\xrightarrow{\alpha \rightarrow \infty} \mathrm{Tr} [\chi_R (1 - \Delta)^{-1/2} \gamma_\infty^k (1 - \Delta)^{-1/2} \chi_R] \\ &= \mathrm{Tr} [\chi_R \gamma_\infty \chi_R] \end{aligned}$$

because $\chi_R (1 - \Delta)^{-1/2}$ is compact. Indeed, since χ_R is smooth with compact support it is in any L^p space, while $(1 - \Delta)^{-1/2}$ acts in Fourier variables as the multiplier by $(1 + |k|^2)^{-1/2}$, which belongs to L^q for $q > d$. Hence, the Kato-Seiler-Simon inequality [57, Chapter 4] implies that $\chi_R (1 - \Delta)^{-1/2}$ is in the Schatten space \mathcal{L}^q for any $q > d$.

Step 2. We now prove that

$$\lim_{R \rightarrow \infty} \lim_{\alpha \rightarrow \infty} \mathrm{Tr} [\chi_R \gamma_\alpha \chi_R] = 1. \quad (6.6)$$

Let χ_R be as above and

$$\eta_R = \sqrt{1 - \chi_R^2}.$$

Then (3.31) implies

$$\liminf_{\alpha \rightarrow \infty} \mathrm{Tr}_{\mathfrak{H}} (H_\alpha^{(V)} \Gamma_\alpha) \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} (\mathrm{Tr}_{\mathfrak{H}} (H_\alpha^{(V)} \Gamma_{\alpha, \chi_R}) + \mathrm{Tr}_{\mathfrak{H}} (\Gamma_{\alpha, \eta_R}) E_\alpha^{(0)}).$$

with Γ_{α, χ_R} and Γ_{α, η_R} the χ_R - and η_R -localized states constructed from Γ_α .

Next, combining with the energy upper bound obtained as sketched in Section 2,

$$E_{\mathrm{Pek}}^{(V)}(1) \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} (\mathrm{Tr}_{\mathfrak{H}} (\Gamma_{\alpha, \chi_R}) E_\alpha^{(V)} + \mathrm{Tr}_{\mathfrak{H}} (\Gamma_{\alpha, \eta_R}) E_\alpha^{(0)}).$$

Inserting the energy convergence from Theorem 5.1 and using (3.17) leads to

$$E_{\text{Pek}}^{(V)}(1) \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left(E_{\text{Pek}}^{(V)}(1) \text{Tr}_{\mathfrak{H}}(\Gamma_{\alpha, \chi_R}) + E_{\text{Pek}}^{(0)}(1) (1 - \text{Tr}_{\mathfrak{H}}(\Gamma_{\alpha, \chi_R})) \right)$$

so that

$$0 \geq \liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \left(E_{\text{Pek}}^{(0)}(1) - E_{\text{Pek}}^{(0)}(1) \right) (1 - \text{Tr}_{\mathfrak{H}}(\Gamma_{\alpha, \chi_R})).$$

But

$$E_{\text{Pek}}^{(V)}(1) < E_{\text{Pek}}^{(0)}(1)$$

since $V < 0$, as follows by using a translation-invariant ground state as trial state for the functional with trapping potential. It must thus be that

$$\liminf_{R \rightarrow \infty} \liminf_{\alpha \rightarrow \infty} \text{Tr}_{\mathfrak{H}}(\Gamma_{\alpha, \chi_R}) = 1,$$

which implies (6.6), using (3.14).

Conclusion. Combining (6.5) with (6.6) leads to

$$\lim_{R \rightarrow \infty} \text{Tr} [\chi_R \gamma_\infty \chi_R] = 1$$

and the result follows. \square

Combining the lemma with (6.3) implies that

$$\text{Tr} [\omega_u^{\text{nor}}] = 1$$

for μ -almost every u , where the normal part is defined as in (6.4). Hence ω_u coincides μ -almost surely with its normal part, a positive trace-class operator. We denote the latter γ_u , which has trace 1.

We may now return to Theorem 4.3 and pass to the limit in the energy as in Section 5 to obtain

$$\begin{aligned} E_{\text{Pek}}^{(V)}(1) &\geq \liminf_{\alpha \rightarrow \infty} E_{(\alpha)}^{(V)} \geq \int_{L^2(\mathbb{R}^d)} \left(\text{Tr} [h \gamma_u] + \|u\|_{L^2}^2 + \int_{\mathbb{R}^d} \text{Tr} [\gamma_u(v(\cdot - z))] (u(z) + \overline{u(z)}) dz \right) d\mu(u) \\ &\geq \int_{L^2(\mathbb{R}^d)} \left(\text{Tr} \left[\left(h + W * \rho_{\gamma_u} \right) \gamma_u \right] \right) d\mu(u) \\ &\geq E_{\text{Pek}}^{(V)}(1). \end{aligned}$$

To go to the second line we have minimized with respect to u , obtaining

$$u(z) = -\text{Tr} [\gamma_u v(\cdot - z)] = -\int_{\mathbb{R}^d} \rho_{\gamma_u}(x) v(x - z) dx \quad (6.7)$$

with $\rho_{\gamma_u}(x) = \gamma_u(x, x)$ the density of γ_u . To go to the third line we used Lemma 5.2, i.e. that the Pekar functional for mixed states leads to the same minimization problem as the usual one. This fact and the previous chain of inequalities (there must be equality throughout) also imply that for μ -almost every u ,

$$\gamma_u = |\psi\rangle\langle\psi|$$

with ψ a minimizer of the Pekar energy functional (2.14) at mass 1. We also must have (6.7) and hence

$$u = u_\psi = -v * |\psi|^2$$

as in (2.13) for μ -almost every u . Theorem 2.3 follows upon defining

$$dP(\psi) := \int \mathbb{1}_{u=u_\psi} d\mu(u).$$

REFERENCES

- [1] AMMARI, Z. Asymptotic completeness for a renormalized nonrelativistic Hamiltonian in quantum field theory: the Nelson model. *Math. Phys. Anal. Geom.* 3, 3 (2000), 217–285.
- [2] AMMARI, Z. Scattering theory for a class of fermionic Pauli-Fierz models. *J. Funct. Anal.* 208, 2 (2004), 302–359.
- [3] AMMARI, Z., AND NIER, F. Mean field limit for bosons and infinite dimensional phase-space analysis. *Ann. Henri Poincaré* 9 (2008), 1503–1574.
- [4] AMMARI, Z., AND NIER, F. Mean field limit for bosons and propagation of Wigner measures. *J. Math. Phys.* 50, 4 (2009), 042107.
- [5] BAUMGARTNER, B., AND SEIRINGER, R. Atoms with bosonic "electrons" in strong magnetic fields. *Annales Henri Poincaré* 2 (2001), 41.
- [6] BRETEAUX, S., FAUPIN, J., AND PAYET, J. Quasi-classical Ground States. I. Linearly Coupled Pauli-Fierz Hamiltonians. arXiv:2207.06053, 2022.
- [7] BRETEAUX, S., FAUPIN, J., AND PAYET, J. Quasi-classical Ground States. II. Standard Model of Non-relativistic QED. arXiv:2210.03448, 2022.
- [8] BROOKS, M., AND SEIRINGER, R. The Fröhlich Polaron at Strong Coupling - Part I: The Quantum Correction to the Classical Energy. arXiv:2211.03353, 2022.
- [9] CORREGGI, M., AND FALCONI, M. Effective potentials generated by field interaction in the quasi-classical limit. *Ann. Henri Poincaré* 19 (2018), 189–235.
- [10] CORREGGI, M., FALCONI, M., AND OLIVIERI, M. Magnetic Schrödinger operators as the quasi-classical limit of Pauli-Fierz-type models. *J. Spectr. Theory* (2019).
- [11] CORREGGI, M., FALCONI, M., AND OLIVIERI, M. Quasi-classical dynamics. *Journal of the European Mathematical Society* (2021).
- [12] CORREGGI, M., FALCONI, M., AND OLIVIERI, M. Ground state properties in the quasi-classical regime. *Analysis and PDEs* (2023).
- [13] DELL'ANTONIO, G. On the limits of sequences of normal states. *Comm. Pure Appl. Math.* 20 (1967), 413.
- [14] DEREZIŃSKI, J., AND GÉRARD, C. Asymptotic completeness in quantum field theory. Massive Pauli-Fierz Hamiltonians. *Rev. Math. Phys.* 11, 4 (1999), 383–450.
- [15] DONSKER, M. D., AND VARADHAN, S. R. S. Asymptotics for the polaron. *Comm. Pure Appl. Math.* 36, 4 (1983), 505–528.
- [16] FALCONI, M. Concentration of cylindrical wigner measures. *Commun. Contemp. Math.* 20, 5 (2018), 1750055.
- [17] FALCONI, M. Cylindrical wigner measures. *Doc. Math.* 23 (2018), 1677–1756.
- [18] FALCONI, M., LEOPOLD, N., MITROUSKAS, D., AND PETRAT, S. Bogoliubov dynamics and higher-order corrections for the regularized Nelson model. arXiv:2110.00458, 2021.
- [19] FANNES, M., LEWIS, J. T., AND VERBEURE, A. Symmetric states of composite systems. *Lett. Math. Phys.* 15 (1988), 255–260.
- [20] FELICIANGELI, D., AND SEIRINGER, R. The strongly coupled polaron on the torus: Quantum corrections to the Pekar asymptotics. *Archive for Rational Mechanics and Analysis* 242 (2021), 1835–1906.
- [21] FOLLAND, G. B. *Real analysis*, 2d ed. ed. Pure and Applied Mathematics. John Wiley & Sons, 2010.
- [22] FRANK, R. L., AND GANG, Z. Derivation of an effective evolution equation for a strongly coupled polaron. *Analysis and PDEs* 10, 2 (2017), 379–422.
- [23] FRANK, R. L., AND SEIRINGER, R. Quantum corrections to the pekar asymptotics of a strongly coupled polaron. *Communications on Pure and Applied Mathematics* 74 (2021), 544–588.
- [24] FRÖHLICH, J., JONSSON, B. L. G., AND LENZMANN, E. Boson stars as solitary waves. *Comm. Math. Phys.* 274, 1 (2007), 1–30.
- [25] FRÖHLICH, J., JONSSON, B. L. G., AND LENZMANN, E. Effective dynamics for boson stars. *Nonlinearity* 20, 5 (2007), 1031–1075.
- [26] GRIESEMER, M. On the dynamics of polarons in the strong-coupling limit. *Reviews in Mathematical Physics* 29, 10 (2017), 405–424.
- [27] GRIESEMER, M., SCHMID, J., AND SCHNEIDER, G. On the dynamics of the mean-field polaron in the high-frequency limit. *Letters in Mathematical Physics* 107 (2017), 405–424.
- [28] HAINZL, C., LEWIN, M., AND SOLOVEJ, J. P. The thermodynamic limit of quantum Coulomb systems. Part I. General theory. *Advances in Math.* 221 (2009), 454–487.

- [29] HAINZL, C., LEWIN, M., AND SOLOVEJ, J. P. The thermodynamic limit of quantum Coulomb systems. Part II. Applications. *Advances in Math.* 221 (2009), 488–546.
- [30] HYTÖNEN, T., VAN NEERVEN, J., VERAAR, M., AND WEIS, L. *Analysis in Banach spaces I*, vol. 63 of *Ergebnisse der Mathematik und ihrer Grenzgebiete*. Springer, 2016.
- [31] LENZMANN, E., AND LEWIN, M. On singularity formation for the L^2 -critical Bose star equation. *Nonlinearity* 24, 12 (2011), 3515.
- [32] LEOPOLD, N., MITROUSKAS, D., AND SEIRINGER, R. Derivation of the Landau-Pekar equations in a many-body mean-field limit. arXiv:2001.03993, 2020.
- [33] LEOPOLD, N., RADEMACHER, S., SCHLEIN, B., AND SEIRINGER, R. The Landau-Pekar equations: Adiabatic theorem and accuracy. arXiv:1904.12532, 2019.
- [34] LEWIN, M. Geometric methods for nonlinear many-body quantum systems. *J. Funct. Anal.* 260 (2011), 3535–3595.
- [35] LEWIN, M., NAM, P., AND ROUGERIE, N. Derivation of Hartree’s theory for generic mean-field Bose systems. *Adv. Math.* 254 (March 2014), 570–621.
- [36] LEWIN, M., NAM, P., AND ROUGERIE, N. Remarks on the quantum de Finetti theorem for bosonic systems. *Appl. Math. Res. Express (AMRX) 2015* (2015), 48–63.
- [37] LEWIN, M., NAM, P., AND ROUGERIE, N. Derivation of nonlinear Gibbs measures from many-body quantum mechanics. *J. Éc. Polytech. Math.* 2, 1 (2016), 553–606.
- [38] LEWIN, M., AND ROUGERIE, N. Derivation of Pekar’s Polarons from a Microscopic Model of Quantum Crystals. *SIAM J. Math. Anal.* 45, 3 (2013), 1267–1301.
- [39] LEWIN, M., AND ROUGERIE, N. On the binding of polarons in a mean-field quantum crystal. *ESAIM Control Optim. Calc. Var.* 19, 3 (July 2013), 629–656.
- [40] LIEB, E. H. Existence and uniqueness of the minimizing solution of Choquard’s nonlinear equation. *Studies in Applied Mathematics* 57 (Oct. 1977), 93–105.
- [41] LIEB, E. H., AND SEIRINGER, R. *The Stability of Matter in Quantum Mechanics*. Cambridge Univ. Press, 2010.
- [42] LIEB, E. H., AND THOMAS, L. E. Exact ground state energy of the strong-coupling polaron. *Comm. Math. Phys.* 183, 3 (1997), 511–519.
- [43] LIEB, E. H., AND YAMAKAZI, K. Ground state energy and effective mass of the polaron. *Phys. Rev.* 111 (1958), 728–733.
- [44] LIONS, P.-L. The Choquard equation and related questions. *Nonlinear Anal.* 4, 6 (1980), 1063–1072.
- [45] MIYAO, T., AND SPOHN, H. The bipolaron in the strong coupling limit. *Annales Henri Poincaré* 8, 7 (2007), 1333–1370.
- [46] MØLLER, J. S. The polaron revisited. *Rev. Math. Phys.* 18, 5 (2006), 485–517.
- [47] REED, M., AND SIMON, B. *Methods of Modern Mathematical Physics. IV. Analysis of operators*. Academic Press, New York, 1978.
- [48] RICAUD, J. On uniqueness and non-degeneracy of anisotropic polarons. *Nonlinearity* 29 (2016), 1509–1536.
- [49] ROSEN, L. The $(\phi^{2n})_2$ quantum field theory: higher order estimates. *Comm. Pure Appl. Math.* 24 (1971), 417–457.
- [50] ROUGERIE, N. De Finetti theorems, mean-field limits and Bose-Einstein condensation. arXiv:1506.05263, 2014. LMU lecture notes.
- [51] ROUGERIE, N. *Théorèmes de De Finetti, limites de champ moyen et condensation de Bose-Einstein*. Les cours Peccot. Spartacus IDH, Paris, 2016. Cours Peccot, Collège de France : février-mars 2014.
- [52] ROUGERIE, N. Scaling limits of bosonic ground states, from many-body to nonlinear Schrödinger. *EMS Surveys in Mathematical Sciences* 7, 2 (2020), 253–408.
- [53] RUDIN, W. *Functional Analysis*, second ed. International Series in Pure and Applied Mathematics. McGraw-Hill Book Co., New York, 1991.
- [54] SCHATTEN, R. *Norm Ideals of Completely Continuous Operators*, vol. 2 of *Ergebnisse der Mathematik und ihrer Grenzgebiete*. Folge, 1960.
- [55] SEIRINGER, R. Gross-Pitaevskii theory of the rotating Bose gas. *Comm. Math. Phys.* 229, 3 (2002), 491–509.
- [56] SEIRINGER, R. The polaron at strong coupling. In *Proceedings of QMath 14* (2019).
- [57] SIMON, B. *Trace ideals and their applications*, vol. 35 of *London Mathematical Society Lecture Note Series*. Cambridge University Press, Cambridge, 1979.
- [58] SKOROKHOD, A. *Integration in Hilbert space*. Ergebnisse der Mathematik und ihrer Grenzgebiete. Springer-Verlag, 1974.

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