

Derivation of the Gross-Pitaevskii Theory for Interacting Fermions in a Trap

Andrea Calignano and Michele Correggi

Abstract We study a dilute gas of interacting fermions at temperature $T = 0$ and chemical potential $\mu \in \mathbb{R}$. The particles are trapped by an external potential, and they interact via a microscopic attractive two-body potential with a two-body bound state. We prove the emergence of the macroscopic Gross-Pitaevskii theory as first-order contribution to the BCS energy functional in the regime of vanishing micro-to-macro scale parameter.

1 Introduction

The low-temperature behavior of interacting fermions has been widely studied in the physics literature (see, e.g, the monographs [23, 25]), in order to understand phenomena as the occurrence of superconductivity in materials, i.e., a sudden drop of resistivity below a certain critical temperature. A microscopic model for such a phenomenon was proposed in the '50s in [4] by J. Bardeen, L. Cooper and R. Schrieffer, and it is nowadays very well known as the BCS theory: the presence of an attraction between the fermions may be responsible for the formation of (weakly) bound pairs (Cooper pairs) of fermions with opposite spin; such pairs behave in all respect as charged bosons and as such they undergo Bose-Einstein condensation below a certain critical temperature. The emergence of this collective behavior of Cooper pairs is the signature of the occurrence of superconductivity in the material, and it can be understood starting from the minimization of the free energy of the system given by the *BCS energy functional* depending on the two-particle reduced density matrix.

Few years before the appearance of the BCS description of superconductivity, a much more phenomenological macroscopic explanation was provided

Dipartimento di Matematica, Politecnico di Milano, P.zza Leonardo da Vinci, 32, 20133, Milano, Italy

in [17] by V.L. Ginzburg and L.D. Landau. In the GL theory the superconducting features of the sample are encoded in an order parameter ψ , i.e., a complex wave function minimizing a suitable energy functional, which is supposed to approximate the free energy of the system (see [2, 7, 8, 9, 22] and references therein for some recent mathematical results). The connection between the two models was heuristically investigated in [18], but only much more recently a rigorous derivation of GL theory from the BCS model was obtained in [14] (see also the related papers [11, 13, 15, 19, 21]): it is shown that, in a translational invariant system in presence of slowly varying external potentials and close to the critical temperature for the superconductivity transition, the leading order of the BCS ground state energy is given by the minimum of the GL functional, provided the attraction admits at least a bound state and in the limit of zero ratio between the microscopic scale of the interaction and the macroscopic size of the sample. The zero-temperature analogue of the same result for a fermionic system in a bounded domain was successively obtained in [16], while a similar question for the Bogolubov-Hartree-Fock functional, i.e., the BCS energy functional with the addition of direct and exchange terms, was studied in [5].

The setting we consider here is quite close to the one addressed in [16, 21], i.e., we study the zero-temperature behavior of a gas of interacting fermions, but, unlike the previous references, here we assume the presence of a *confining external potential*. The particles interact via a two-body attraction, which is strong enough to bind two particles together. Naively, one may think that the fermions at low temperature would arrange in bounded pairs, so forming a bosonic gas, which then undergoes BE condensation. However, as in [5, 16, 21], one observes that the possibility to form a two-body bound state is in fact enough to generate the superconductivity transition, even though the gas does not exactly arrange in two-particle bound pairs.

Let us describe the setting more precisely: we set the length scale of the trap to be 1, while the microscopic interaction varies on a scale $h \ll 1$. The parameter h thus describes the ratio between the micro- and macroscopic scales and we study the limit $h \rightarrow 0$ of the ground state energy of the BCS energy functional and of any corresponding minimizer. We do not fix the number of particles a priori, but we study the grand-canonical problem in presence of a chemical potential μ .

We stress that the physical setting we are considering is not the typical one of BCS theory in which the formation of Cooper pairs occurs on a scale much larger than the mean interparticle distance. On the contrary, here, the size of bounded pairs is of order h and it is therefore much smaller than the mean distance travelled by fermions, which, as we are going to see, is of order $h^{1/3}$ (the density of particles is of order h^{-1}). There is however a physical regime in which this setting becomes meaningful, namely the BEC/BCS crossover region (see [21]), where for certain values of the two-particle scattering length, the picture is very close to the one considered here. Note also that, as a gas made of almost bosonic pairs, the system is dilute (see also next Remark 1

and the analogous discussions in [12, 24]), because the density times the microscopic volume where the interaction acts non-trivially is of order $h^{-1} \cdot h^3 = h^2 \ll 1$.

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1.1 BCS theory of superconductivity

In the BCS model all the information about the state of the system is encoded in two variables: the reduced one-particle density matrix γ and the pairing density matrix α . Hence, the system is fully described by an operator

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ \bar{\alpha} & 1 - \bar{\gamma} \end{pmatrix}, \quad 0 \leq \Gamma \leq 1, \quad (1)$$

acting on $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. The bar denotes complex conjugation, i.e., the integral kernels of the operators $\bar{\gamma}, \bar{\alpha}$ are $\overline{\gamma(x, y)}$ and $\overline{\alpha(x, y)}$, respectively. For a given BCS state Γ , the BCS functional at $T = 0$ in macroscopic units is given by

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] := \text{Tr } \mathfrak{h} \gamma + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha(x, y)|^2, \quad (2)$$

where the one-body operator $\mathfrak{h} = -h^2 \Delta + h^2 W - \mu$ describes the energy of non-interacting electrons at chemical potential $\mu < 0$. The BCS ground state energy is

$$E_\mu^{\text{BCS}} := \inf_{0 \leq \Gamma \leq 1} \mathcal{E}_\mu^{\text{BCS}}[\Gamma]. \quad (3)$$

Assumption 1 (Existence of a ground state) *We assume that V is real, radially symmetric, locally integrable and bounded from below. Moreover, the two-particle operator $-\Delta + V$ is assumed to admit a normalized ground state $\alpha_0 \in L^2(\mathbb{R}^6)$ with corresponding energy $-E_0$, $E_0 > 0$, which in particular implies that the negative part of V is non-zero.*

Assumption 2 (Spectral gap) *Let α_0 be the ground state as in Assumption 1 above. We assume that $\exists g > 0$ and $0 < \varepsilon < 1$, such that*

$$P_{\alpha_0}^\perp [-(1 - \varepsilon)\Delta + V + E_0] P_{\alpha_0}^\perp \geq g P_{\alpha_0}^\perp \quad (4)$$

where $P_{\alpha_0}^\perp$ stands for the projector onto the orthogonal complement of α_0 .

Assumption 3 (Trapping potential) *We also assume that $W \in C^1(\mathbb{R}^3)$ is positive and there exist $0 < \beta, c_1, c_2 < +\infty$ such that*

$$\begin{cases} c_1|x|^\beta \leq W(x) \leq c_2|x|^\beta, \\ |\nabla W(x)| \leq c_2\beta|x|^{\beta-1}, \end{cases} \quad \text{for } |x| \geq 1. \quad (5)$$

We stress that for the class of attractive potentials in Assumption 1, one can deduce by standard Agmon estimates (see, e.g., [1]) the exponential decay of the bound state wave function α_0 : there exists $b > 0$ such that

$$\int_{\mathbb{R}^3} dx |\alpha_0(x)|^2 e^{2bx} < +\infty. \quad (6)$$

Note also that Assumption 3 allows to Taylor expand

$$W(\eta + \xi/2) = W(\eta) + \frac{\xi}{2} \cdot \nabla W(\zeta), \quad (7)$$

with the variable ζ belonging to $(\eta, \eta + \xi/2)$. A special case of a potential satisfying Assumption 3 is obviously given by the harmonic potential. In this case, the two-body Hamiltonian perfectly decouples in relative and centre-of-mass coordinates, which allows to get rid of several error terms in the discussion below.

The condition $0 \leq \Gamma \leq 1$, which is often called admissibility of Γ , implies that the operator γ is hermitian, i.e. $\gamma(x, y) = \overline{\gamma(y, x)}$ and that α is such that $\overline{\alpha} = \alpha^\dagger$. Furthermore, the operators $\gamma, \alpha : L^2(\mathbb{R}^3) \rightarrow L^2(\mathbb{R}^3)$ have a specific physical meaning (see, e.g., [3] for a formal derivation): given a many-body fermionic state Ψ , we have

$$\gamma(x, y) = \langle a_x^\dagger a_y \rangle_\Psi, \quad \alpha(x, y) = \langle a_x a_y \rangle_\Psi \quad (8)$$

i.e., they represent the one-particle density matrix of the system and the wave function of a Cooper pair, respectively. Here a_x^\dagger, a_x are the fermionic creation and annihilation operators. In fact, in absence of any pairing between the fermions, the system is in the so-called *normal state*, which is characterized by a trivial off-diagonal component, i.e., $\alpha \equiv 0$. The emergence of superconductivity is then associated to a non-trivial α .

1.2 Gross-Pitaevskii theory

For any $D \in \mathbb{R}$, the Gross-Pitaevskii (GP) energy functional is defined as

$$\mathcal{E}_D^{\text{GP}}(\psi) := \int_{\mathbb{R}^3} d\eta \left\{ \frac{1}{4} |\nabla \psi|^2 + (W(\eta) - D) |\psi|^2 + g_{\text{BCS}} |\psi|^4 \right\}, \quad (9)$$

where the coefficient $g_{\text{BCS}} > 0$ represents the interaction strength among different pairs, and whose expression in terms of the microscopic quantities is provided in Theorem 1. The GP energy can be proven to be bounded from below for any positive g_{BCS} (see Corollary 1). We denote then the GP ground

state energy by

$$E_D^{\text{GP}} := \inf_{\psi \in \mathcal{D}^{\text{GP}}} \mathcal{E}_D^{\text{GP}}(\psi), \quad (10)$$

where $\mathcal{D}^{\text{GP}} = \{\psi \in H^1(\mathbb{R}^3) | W|\psi|^2 \in L^1(\mathbb{R}^3)\}$ is the natural minimization domain for (9). We denote by ψ_* the corresponding minimizer, which can be shown to be unique up to choice of the phase by strict convexity of the functional in $|\psi|^2$.

We point out here that, mathematically speaking, the GP functional introduced above may as well be named *Ginzburg-Landau* functional, although the energy does not look exactly as the usual GL energy, which in a homogeneous sample would read

$$\mathcal{E}^{\text{GL}}[\phi] = \int_{\mathbb{R}^3} d\eta \left\{ \frac{1}{4} |\nabla \phi|^2 + \tilde{g}_{\text{BCS}} (1 - |\phi|^2)^2 \right\}. \quad (11)$$

However, it is possible (see below and the discussion in [10, Sect. 1]) to reduce the minimization of (9) to the one of a functional very close to (11) (in fact, its inhomogeneous counterpart).

Notice that the GP wave function ψ is not normalized in L^2 since we are performing the energy minimization in the grand canonical setting, and therefore we may think that $\|\psi\|_2$ is determined by the value of the chemical potential μ . Let us denote by N such a quantity, i.e., $N := \|\psi_*\|_2^2$, and let f_0 be the positive minimizer of the GP energy

$$\tilde{\mathcal{E}}^{\text{GP}}[f] = \int_{\mathbb{R}^3} d\eta \left\{ \frac{1}{4} |\nabla f|^2 + W(\eta)|f|^2 + g_{\text{BCS}} N |f|^4 \right\},$$

with L^2 norm set equal to 1. Such a minimizer satisfies the variational equation

$$-\frac{1}{4} \Delta f_0 + W f_0 + 2g_{\text{BCS}} N f_0^3 = \mu_0 f_0,$$

for a chemical potential $\mu_0 = \tilde{E}^{\text{GP}} + gN \|f_0\|_4^4$, where we have set $\tilde{E}^{\text{GP}} := \inf_{\|\psi\|_2=1} \tilde{\mathcal{E}}^{\text{GP}}[\psi]$. With the splitting $\psi_* =: \sqrt{N} f_0 \phi_*$ and exploiting the variational equation for f_0 , one gets

$$E_D^{\text{GP}} = N \left\{ \tilde{E}^{\text{GP}} - D + \tilde{\mathcal{E}}^{\text{GL}}[\phi_*] \right\},$$

where the last term is a weighted Ginzburg-Landau functional explicitly given by

$$\tilde{\mathcal{E}}^{\text{GL}}[\phi] = \int_{\mathbb{R}^3} d\eta f_0^2 \left\{ \frac{1}{4} |\nabla \phi|^2 + \tilde{g}_{\text{BCS}} N f_0^2 (1 - |\phi|^2)^2 \right\}, \quad (12)$$

and ϕ_* its minimizer.

This makes apparent the connection between the GP and GL functionals, so that, from this point of view, both names are mathematically equivalent to identify (9). There is however a strong physical motivation (see also [21]) for

the choice we made, namely the fact that the physical regime we are investigating is a BEC one: as described in § 1, the mechanism behind the emergence of a collective behavior in the low-temperature Fermi gas considered here is not the usual BCS pairing phenomenon, but rather a condensation of fermionic pairs playing the role of bosonic molecules. The pairs have indeed a size of order $h \ll 1$ which is much smaller than the typical distance between the fermionic particles of order of the trap length scale $O(1)$.

2 Main Results

This section contains our main results about the semiclassical expansion of the BCS energy.

Theorem 1 (BCS energy). *Let $\mu = -E_0 + Dh^2$, for some $D \in \mathbb{R}$ and let Assumptions 1 to 3 be satisfied. Then,*

$$E_\mu^{\text{BCS}} = hE_D^{\text{GP}} + O(h^2), \quad (13)$$

as $h \rightarrow 0$, where

$$g_{\text{BCS}} := (2\pi)^3 \int_{\mathbb{R}^3} dp (p^2 + E_0) |\hat{\alpha}_0(p)|^4. \quad (14)$$

Moreover, for any approximate ground state Γ of the BCS functional, i.e., such that

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq E_\mu^{\text{BCS}} + \varepsilon h, \quad 0 < \varepsilon < +\infty, \quad (15)$$

its off-diagonal element α can be decomposed as

$$\alpha(x, y) = h^{-2} \psi \left(\frac{x+y}{2} \right) \alpha_0 \left(\frac{x-y}{h} \right) + r(x, y), \quad (16)$$

where $\psi \in \mathcal{D}^{\text{GP}}$ satisfies $\mathcal{E}_D^{\text{GP}}(\psi) \leq E_D^{\text{GP}} + \varepsilon + o(1)$, α_0 is the ground state of the two-particle operator and the correction r is small in the following sense:

$$\|r\|_{L^2}^2 = O(h), \quad \|\nabla r\|_{L^2}^2 + \|W|r|^2\|_{L^1} = O(h^{-1}). \quad (17)$$

Remark 1 (Diluteness). The expansion (16) together with the heuristics $\gamma \simeq \alpha \bar{\alpha}$ (see § 3.4) suggests that the density of the gas in our setting is proportional¹ to $h^{-1} |\psi|^2$, i.e., the total number of particles is of order h^{-1} . This vindicates the statement about the diluteness of the system since the range of the two-body interaction is $\propto h$ and therefore the diluteness parameter $h^{-1}h^3 = h^2 \ll 1$ is small.

¹ In fact, it may be possible to prove a weak version of such a statement as in [16, Proposition 1.11] using the Griffith's argument, i.e., variation w.r.t. to the external potential. However, we omit this discussion here for the sake of brevity.

Remark 2 (Properties of α_0). Note that by the estimate (6), $\alpha_0 \in L^1 \cup H^1(\mathbb{R}^3)$, which guarantees that $\hat{\alpha}_0 \in L^\infty(\mathbb{R}^3)$, so that $\hat{\alpha}_0 \in L^p(\mathbb{R}^3)$ for any $p \geq 2$ and g_{BCS} is a finite quantity.

Whether the system is superconducting in the asymptotic regime $h \rightarrow 0$ thus depends on the fact that the GP wave function ψ is non-trivial. For the GP minimizer this depends on the value of the coefficient D , which in turn is determined by the chemical potential μ . In fact, one can infer [16, 21] from the properties of the function

$$\mu \mapsto E_\mu^{\text{BCS}}, \quad (18)$$

which is continuous, concave, and monotone decreasing, that there exists a unique critical value $\mu_c(h)$ such that below μ_c superconductivity is present and above it the system is in the normal state. The exact definition of $\mu_c(h)$ is the following:

$$\mu_c(h) := \inf \{ \mu < 0 \mid E_\mu^{\text{BCS}} < 0 \}, \quad (19)$$

i.e., it marks the threshold of the transition from a zero ground state energy (normal state) to a strictly negative one.

Theorem 2 (Critical chemical potential). *Under the assumptions of Theorem 1, the critical chemical potential at which the superconductivity phase transition takes place is*

$$\mu_c(h) = -E_0 + E_W h^2 + o(h^2), \quad (20)$$

as $h \rightarrow 0$, where E_W is the ground state energy of the one-particle operator $-\frac{1}{4}\Delta + W$.

3 Proofs

The key ingredient to prove Theorem 1 and Theorem 2 is given by the following Proposition 1, which provides the link between the BCS and GL functionals.

Proposition 1 (BCS and GP functionals). *Let $\mu = -E_0 + Dh^2$, $D \in \mathbb{R}$. Then,*

(a) *Upper bound: for any $\psi \in \mathcal{D}^{\text{GP}}$ there exists an admissible state Γ_ψ such that*

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma_\psi] \leq h\mathcal{E}_D^{\text{GP}}(\psi) + Ch^2 \left[1 + (\max\{\mathcal{E}_D^{\text{GP}}(\psi), 0\})^2 \right]. \quad (21)$$

(b) *Lower bound: let Γ be an admissible BCS state such that $\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq C_\Gamma h$. Then, there exists $\psi \in \mathcal{D}^{\text{GP}}(\mathbb{R}^3)$ such that*

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \geq h\mathcal{E}_D^{\text{GP}}(\psi) - Ch^2. \quad (22)$$

Furthermore, there exists a function r such that the following decomposition holds:

$$\alpha(x, y) = h^{-2}\psi\left(\frac{x+y}{2}\right)\alpha_0\left(\frac{x-y}{h}\right) + r(x, y). \quad (23)$$

where the remainder r satisfies the bounds

$$\|r\|_{L^2}^2 \leq Ch, \quad \langle r | -\Delta + W | r \rangle_{L^2} \leq Ch^{-1}. \quad (24)$$

Let us then assume that Proposition 1 holds and prove Theorem 1 and Theorem 2. The proof of Proposition 1 will be given in next § 3.3 and § 3.4 by separately addressing points (a) and (b) of the statement.

Proof (Theorem 1). To prove the upper bound, we use the admissible trial state Γ_{ψ_*} , where we recall that ψ_* stands for the minimizer of the GP functional. We then obtain by (21)

$$E_\mu^{\text{BCS}} \leq \mathcal{E}_\mu^{\text{BCS}}[\Gamma_{\psi_*}] = h\mathcal{E}_D^{\text{GP}}(\psi_*) + O(h^2) = hE_D^{\text{GP}} + O(h^2), \quad (25)$$

since $\mathcal{E}_D^{\text{GP}}(\psi_*) = E_D^{\text{GP}} \leq 0$. In addition to proving a sharp upper bound for the ground state energy, the estimate above also yields the a priori bound $\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq Ch$ for any approximate minimizer Γ of the BCS energy. Hence, the minimizer satisfies (22), so that we can deduce the estimate from below matching the upper bound, along with the decomposition of α as in (23).

Proof (Theorem 2). We start from the trivial observation that

$$E_D^{\text{GP}} < 0, \quad \iff \quad D > E_W, \quad (26)$$

where we recall that E_W is the ground state energy of $-\frac{1}{4}\Delta + W$: indeed, if $D > E_W$, it suffices to use $\lambda\psi_W$, $\lambda > 0$, as a trial state for the GP energy, where ψ_W is the normalized ground state of $-\frac{1}{4}\Delta + W$, to get

$$E_D^{\text{GP}} = \lambda(E_W - D) + g_{\text{BCS}}\lambda^2\|\psi_W\|_{L^4}^4 < 0, \quad (27)$$

for λ small enough. On the other hand, if $D \leq E_W$, the functional is trivially positive, since

$$\mathcal{E}_D^{\text{GP}}(\psi) \geq (E_W - D)\|\psi\|_{L^2}^2. \quad (28)$$

Note also that ψ_* is non-trivial if and only if $E_D^{\text{GP}} < 0$.

Next, we prove the upper bound $\mu_c(h) \leq -E_0 + E_W h^2 + o(h^2)$ by showing that, if $\mu = -E_0 + Dh^2$, $D > E_W$, then there exists an admissible BCS state such that

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] < 0. \quad (29)$$

By Proposition 1, for any $\psi \in \mathcal{D}^{\text{GP}}$, there exists Γ_ψ admissible such that

$$h^{-1}\mathcal{E}_\mu^{\text{BCS}}[\Gamma_\psi] = \mathcal{E}_D^{\text{GP}}(\psi) + O(h). \quad (30)$$

This in particular holds true for $\psi = \psi_*$, so that

$$E_\mu^{\text{BCS}} \leq E_D^{\text{GP}} h + O(h^2) < 0, \quad (31)$$

if $D > E_W$.

Conversely, we now show that, if $E_\mu^{\text{BCS}} = 0$ for a certain $\mu = -E_0 + Dh^2$, then $D \leq E_W$, so completing the proof. By Theorem 1, indeed, if $E_\mu^{\text{BCS}} = 0$, then $E_D^{\text{GP}} = O(h)$ but the GP functional is independent of h and therefore $E_D^{\text{GP}} = 0$, which in turn implies that $D \leq E_W$ by (26).

3.1 GP functional

We discuss some useful properties of the GP functional (9) and its minimization. We recall that we denote by E^{GP} the infimum of (9) and by ψ_* any associated minimizer.

Proposition 2 (A priori bounds on ψ). *There exists $C < +\infty$, depending on $g_{\text{BCS}} > 0$, such that*

$$\|\nabla\psi\|_{L^2}^2 + \langle \psi | W | \psi \rangle + \|\psi\|_{L^4}^4 + \|\psi\|_{L^2}^2 \leq C [1 + \max\{\mathcal{E}_D^{\text{GP}}(\psi), 0\}] \quad (32)$$

for all $\psi \in \mathcal{D}^{\text{GP}}$.

Proof. We may assume that $D \geq 0$ otherwise the result is trivially obtained with $C = \max\{|D|^{-1}, g_{\text{BCS}}^{-1}, 4\}$. The starting point is the inequality

$$\begin{aligned} \langle \psi | -\frac{1}{4}\Delta + W | \psi \rangle + g_{\text{BCS}} \|\psi\|_{L^4}^4 &\leq D \|\psi\|_{L^2}^2 + \mathcal{E}_D^{\text{GP}}(\psi) \\ &\leq D \|\psi\|_2^2 + \max\{\mathcal{E}_D^{\text{GP}}(\psi), 0\}, \end{aligned} \quad (33)$$

which allows to bound from above both the quantities on the l.h.s. in terms of the L^2 norm and the GP energy of ψ . Next, we estimate for R large enough

$$\begin{aligned} \|\psi\|_{L^2}^2 &\leq \int_{|x| \leq R} dx |\psi|^2 + R^{-\beta} \int_{|x| > R} dx |x|^\beta |\psi|^2 \\ &\leq \sqrt{\frac{4\pi}{3}} R^{3/2} \|\psi\|_{L^4}^2 + CR^{-\beta} \langle \psi | W | \psi \rangle \\ &\leq C \left[R^{3/2} g_{\text{BCS}}^{-1} (D \|\psi\|_{L^2} + \sqrt{E}) + R^{-\beta} (\sqrt{D} \|\psi\|_{L^2}^2 + E) \right] \end{aligned}$$

where we have set $E := \max\{\mathcal{E}_D^{\text{GP}}(\psi), 0\}$ for short. Hence, for $R > (CD)^{1/\beta}$, we get

$$(1 - \frac{CD}{R^\beta}) \|\psi\|_{L^2}^2 - CR^{3/2} D \|\psi\|_{L^2} \leq C (R^{3/2} g_{\text{BCS}}^{-1} \sqrt{E} + R^{-\beta} E),$$

which implies

$$\|\psi\|_{L^2}^2 \leq \frac{C}{\left(1 - \frac{CD}{R^\beta}\right)^2} \left[\left(1 - \frac{CD}{R^\beta}\right) \left(R^{3/2} g_{\text{BCS}}^{-1} \sqrt{E} + R^{-\beta} E\right) + C^2 R^3 D^2 \right] \quad (34)$$

and thus the result.

Corollary 1 (Boundedness from below of $\mathcal{E}_D^{\text{GP}}(\psi)$). *For any $g_{\text{BCS}} > 0$, there exists a finite constant $C < +\infty$ such that*

$$E_D^{\text{GP}} \geq -C. \quad (35)$$

Proof. Again, $E_D^{\text{GP}} = 0$, if $D \leq 0$, and there is nothing to prove, so let us assume that $D > 0$. In this case it suffices to observe that $E_D^{\text{GP}} \leq 0$, which can be obtained by simply testing the GP energy on the trivial wave function $\psi \equiv 0$. Hence, Proposition 2 implies that $\exists C < +\infty$ such that $\|\psi\|_{L^2}^2 \leq C$ for any ψ with non-positive energy, which in turn yields the lower bound $E_D^{\text{GP}} \geq -C|D|$ and thus the result.

The existence of a minimizer ψ_* which is also unique up to gauge transformation can be deduced by standard methods in variational calculus, and any such a minimizer solves the variational equation

$$-\frac{1}{4}\Delta\psi_* + (W - D)\psi_* + 2g_{\text{BCS}}|\psi_*|^2\psi_* = 0. \quad (36)$$

Under Assumption 3, one can also show that $\psi_* \in C^3 \cap L^\infty(\mathbb{R}^3)$ and it can be chosen strictly positive.

3.2 Semiclassical estimates

Before attacking the proof of Proposition 1, it is useful to state some technical but standard semiclassical bounds to be used in the rest of the paper.

Proposition 3 (Semiclassical estimates). *Let $\mu = -E_0 + h^2 D$, $D \in \mathbb{R}$ and let*

$$\alpha_\psi(x, y) := h^{-2} \psi\left(\frac{x+y}{2}\right) \alpha_0\left(\frac{x-y}{h}\right), \quad (37)$$

for any $\psi \in \mathcal{D}^{\text{GP}}$. Then, the following estimates hold as $h \rightarrow 0$:

$$\left| \text{Tr } \mathfrak{h} \alpha_\psi \overline{\alpha_\psi} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha_\psi(x, y)|^2 - h \langle \psi | -\frac{1}{4}\Delta + W - D | \psi \rangle_{L^2(\mathbb{R}^3)} \right| \leq A_0 h^2, \quad (38)$$

where

$$A_0 = C \left(\|W|\psi|^2\|_{L^1} + \|\psi\|_{L^2}^2 \right); \quad (39)$$

$$\begin{aligned} & \left| \text{Tr } \mathfrak{h} \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} - h g_{\text{BCS}} \|\psi\|_{L^4}^4 \right| \\ & \leq Ch^2 \left[\|\nabla \psi\|_{L^2}^4 + \|W|\psi|^2\|_{L^1}^2 + \|\psi\|_{L^2}^4 + A_0 h \right]. \end{aligned} \quad (40)$$

Before discussing the proof of the above Proposition, it is convenient to state a technical result about the reduced density α_ψ which is going to be used several times. In the following we will often use the center-of-mass coordinates

$$\eta := \frac{1}{2}(x + y), \quad \xi := x - y, \quad (41)$$

and use the notation

$$\tilde{\alpha}_\psi(\eta, \xi) := \alpha_\psi(x, y). \quad (42)$$

Lemma 1. *Let α_ψ be as (37). Then, for any $n \in \mathbb{N}$ even,*

$$\|\alpha_\psi\|_{\mathfrak{S}^n}^n \leq Ch^{n-3} \|\psi\|_{L^n}^n \|\hat{\alpha}_0\|_{L^n}^n, \quad (43)$$

$$\|\nabla_\xi \tilde{\alpha}_\psi\|_{\mathfrak{S}^n}^n \leq h^{-3} \|\psi\|_{L^n}^n \|\cdot\| \hat{\alpha}_0\|_{L^n}^n, \quad (44)$$

where $\|\cdot\|_{\mathfrak{S}^n}$ stands for the Schatten norm of order $n \in \mathbb{N}$.

Proof. See [5, Lemma 1]. The extension to any $n \in \mathbb{N}$ is obtained by simply observing that, thanks to the monotonicity of Schatten norms, $\|\alpha_\psi\|_{\mathfrak{S}^\infty} \leq \|\alpha_\psi\|_{\mathfrak{S}^n}$ for any $n \in \mathbb{N}$, which allows to use (43) and (44) repeatedly to extend the result to all natural numbers.

We are now in position to present the proof of Proposition 3.

Proof (Proposition 3). Using the change to center-of-mass and relative coordinates, one gets

$$\begin{aligned} & \text{Tr } \mathfrak{h} \alpha_\psi \overline{\alpha_\psi} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha_\psi(x, y)|^2 \\ & = \langle \tilde{\alpha}_\psi | -\frac{1}{4}h^2 \Delta_\eta + h^2 W(\eta + \xi/2) - h^2 D | \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)} \\ & \quad + \langle \tilde{\alpha}_\psi | -h^2 \Delta_\xi + V(\xi/h) + E_0 | \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)} \\ & = \langle \tilde{\alpha}_\psi | -\frac{1}{4}h^2 \Delta_\eta + h^2 W(\eta + \xi/2) - h^2 D | \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)}. \end{aligned} \quad (45)$$

where we used that α_0 is the normalized zero energy eigenvector of the operator $-\Delta + V + E_0$. The result then follows from next Lemma 2.

In order to prove the second estimate, we use the cyclicity of the trace and the symmetry of the Laplacian, to get

$$\begin{aligned} \text{Tr } \Delta \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} & = \langle \alpha_\psi \overline{\alpha_\psi} \alpha_\psi | \frac{1}{2}(\Delta_x + \Delta_y) \alpha_\psi \rangle_{L^2(\mathbb{R}^6)} \\ & = \langle \tilde{\omega}_\psi | \frac{1}{4} \Delta_\eta \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)} + \langle \tilde{\omega}_\psi | \Delta_\xi \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)}, \end{aligned} \quad (46)$$

where we have set for short $\tilde{\omega}_\psi(\eta, \xi) := (\alpha_\psi \overline{\alpha_\psi} \alpha_\psi)(x, y)$. Introducing the coordinates

$$X = \frac{1}{4}(x_1 + x_2 + x_3 + x_4), \quad \xi_k = x_{k+1} - x_k, \quad k = 1, 2, 3, \quad (47)$$

and rescaling the relative ones, we obtain

$$\begin{aligned} \text{Tr}(-h^2\Delta + E_0) \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} &= h \int_{\mathbb{R}^{12}} dX d\xi_1 d\xi_2 d\xi_3 \psi(X - hs) \overline{\psi(X - ht)} \times \\ &\quad \psi(X + hs) \overline{\psi(X + ht)} [(-\Delta + E_0) \alpha_0(\xi_1) \overline{\alpha_0(\xi_2)} \alpha_0(\xi_3) \overline{\alpha_0(\xi_*)}] \\ &\quad - \frac{1}{4} h^2 \langle \tilde{\omega}_\psi | \Delta_\eta \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)}, \end{aligned} \quad (48)$$

where $\xi_* := -\xi_1 - \xi_2 - \xi_3$ and s, t are functions of ξ_1, ξ_2, ξ_3 , i.e.,

$$s := \frac{1}{4}(\xi_1 + 2\xi_2 + \xi_3), \quad t := \frac{1}{4}(\xi_3 - \xi_1). \quad (49)$$

From this expression we are going to extract the quartic term needed to reconstruct the GP functional times h plus higher order contributions. The fundamental theorem of calculus allows to rewrite the first term on the r.h.s. of (48) as

$$\begin{aligned} h \|\psi\|_{L^4}^4 \int_{\mathbb{R}^9} d\xi_1 d\xi_2 d\xi_3 [(-\Delta + E_0) \alpha_0(\xi_1) \overline{\alpha_0(\xi_2)} \alpha_0(\xi_3) \overline{\alpha_0(\xi_*)}] \\ + h \int_{\mathbb{R}^{12}} dX d\xi_1 d\xi_2 d\xi_3 \int_0^1 d\tau \frac{d}{d\tau} \left(\psi(X - \tau hs) \overline{\psi(X - \tau ht)} \times \right. \\ \left. \times \psi(X + \tau hs) \overline{\psi(X + \tau ht)} \right) [(-\Delta + E_0) \alpha_0(\xi_1) \overline{\alpha_0(\xi_2)} \alpha_0(\xi_3) \overline{\alpha_0(\xi_*)}] \\ =: h g_{\text{BCS}} \|\psi\|_{L^4}^4 + h^2 I_1, \end{aligned} \quad (50)$$

thanks to the explicit computation

$$\begin{aligned} \int_{\mathbb{R}^9} d\xi_1 d\xi_2 d\xi_3 [(-\Delta + E_0) \alpha_0(\xi_1) \overline{\alpha_0(\xi_2)} \alpha_0(\xi_3) \overline{\alpha_0(\xi_*)}] \\ = (2\pi)^3 \int_{\mathbb{R}^3} dp (p^2 + E_0) |\hat{\alpha}_0(p)|^4. \end{aligned}$$

Hence, (48) yields

$$\text{Tr}(-h^2\Delta + E_0) \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} = h g_{\text{BCS}} \|\psi\|_{L^4}^4 + h^2 (I_1 + I_2), \quad (51)$$

where

$$I_2 := -\frac{1}{4} \langle \alpha_\psi \overline{\alpha_\psi} \alpha_\psi | \Delta_\eta \alpha_\psi \rangle_{L^2(\mathbb{R}^6)}. \quad (52)$$

The estimate on the term containing the external potential immediately follows from Lemma 2 using Hölder inequality with exponents $\frac{1}{2}, \frac{1}{3}$ and $\frac{1}{6}$:

$$\begin{aligned}
|\mathrm{Tr} W \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi}| &\leq \mathrm{Tr} \left| W^{1/2} \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} W^{1/2} \right| \\
&\leq \left\| W^{1/2} \alpha_\psi \right\|_{\mathfrak{S}^2} \left\| W^{1/2} \alpha_\psi \right\|_{\mathfrak{S}^6} \left\| \overline{\alpha_\psi} \alpha_\psi \right\|_{\mathfrak{S}^3} \leq \left\| W^{1/2} \alpha_\psi \right\|_{\mathfrak{S}^2}^2 \left\| \alpha_\psi \right\|_{\mathfrak{S}^6}^2 \\
&\leq Ch \|\psi\|_{L^6}^2 \|\hat{\alpha}_0\|_{L^6}^2 \left\| W^{1/2} \alpha_\psi \right\|_{L^2}^2 \leq C \|\psi\|_{L^6}^2 \left[\|W|\psi|^2\|_{L^1} + hA_0 \right], \quad (53)
\end{aligned}$$

by the monotonicity of Schatten norms and Lemma 1. The replacement of $\|\psi\|_{L^6}^2$ with $\|\nabla\psi\|_{L^2}^2 + \|\psi\|_{L^2}^2$ can be done via Sobolev inequality.

Lemma 2. *Let α_ψ be as (37) and A_0 as in (39), then*

$$\left| \langle \alpha_\psi | W | \alpha_\psi \rangle_{L^2(\mathbb{R}^6)} - h^{-1} \int_{\mathbb{R}^3} d\eta W(\eta) |\psi|^2 \right| \leq A_0. \quad (54)$$

Proof. Using center-of-mass and relative coordinates as before, we get by the Taylor expansion (7)

$$\begin{aligned}
\frac{1}{2} \langle \alpha_\psi | W(x) + W(y) | \alpha_\psi \rangle_{L^2(\mathbb{R}^6)} &= \frac{1}{2} \langle \tilde{\alpha}_\psi | W(\eta + \xi/2) | \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)} \\
&\quad + \frac{1}{2} \langle \tilde{\alpha}_\psi | W(\eta - \xi/2) | \tilde{\alpha}_\psi \rangle_{L^2(\mathbb{R}^6)} \\
&= h^{-1} \int_{\mathbb{R}^3} d\eta W(\eta) |\psi(\eta)|^2 + \frac{1}{2} h^{-4} \int_{\mathbb{R}^6} d\eta d\xi \xi \cdot \nabla W(\zeta) |\psi(\eta)|^2 |\alpha_0(\xi/h)|^2,
\end{aligned}$$

where we recall that $\tilde{\alpha}_\psi(\eta, \xi) = \alpha_\psi(x, y)$. Hence, we have only to estimate the last term on the r.h.s. of the expression above: by Assumption 3 on W , we deduce that, since $\zeta \in (\eta, \eta + \xi/2)$,

$$\begin{aligned}
\frac{1}{2} h^{-4} \int_{\mathbb{R}^6} d\eta d\xi \xi \cdot \nabla W(\zeta) |\psi(\eta)|^2 |\alpha_0(\xi/h)|^2 \\
\leq C \int_{\mathbb{R}^6} d\eta d\xi |\xi| \left(h^{\beta-1} |\xi|^{\beta-1} + |\eta|^{\beta-1} + 1 \right) |\psi(\eta)|^2 |\alpha_0(\xi)|^2 \quad (55)
\end{aligned}$$

which immediately implies the result, via the trivial bounds $|x|^{\beta-1} \leq W(x)+1$ (again by Assumption 3) and

$$\left\| |\cdot|^{\beta/2} \alpha_0 \right\|_{L^2}^2 \leq C, \quad \left\| |\cdot|^{1/2} \alpha_0 \right\|_{L^2}^2 \leq C, \quad (56)$$

which follows from (6).

Lemma 3. *Let I_1, I_2 as in (50) and (52). Then, as $h \rightarrow 0, \exists C < +\infty$ such that*

$$|I_1| + |I_2| \leq C \|\nabla \psi\|_{L^2}^4. \quad (57)$$

Proof. By [5, Proof of Lemma 1], there exist two finite constants C_1, C_2 such that

$$\begin{aligned} |I_1| &\leq C_1 \|\nabla \psi\|_{L^2}^4 \|\cdot\| \alpha_0 \|_{L^2} \|\alpha_0\|_{L^2} \|\alpha_0\|_{L^1} \|V \alpha_0\|_{L^1}, \\ |I_2| &\leq C_2 \|\nabla \psi\|_{L^2}^4. \end{aligned}$$

The result then follows from the properties of α_0 (see Remark 2).

3.3 Energy upper bound

The result is obtained by testing the BCS energy functional on a suitable trial state. We define an admissible state Γ_ψ , with off-diagonal element given by α_ψ as in (37) and $\psi \in \mathcal{D}^{\text{GP}}$, and upper left entry

$$\gamma_\psi := \alpha_\psi \overline{\alpha_\psi} + (1 + \lambda h) \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi}, \quad (58)$$

for some $\lambda \in \mathbb{R}^+$.

Remark 3 (Admissibility). The admissibility requirement makes the correction of order λh necessary. In fact, any correction of order h^β , $0 < \beta \leq 1$, would work, if λ is chosen appropriately, but $\beta = 1$ gives the best error bound in our estimates. Indeed, the state is admissible if and only if $\gamma - \gamma^2 - \alpha \overline{\alpha} \geq 0$ (see, e.g., [5, Eq. (4.8)]), which, assuming that the quartic correction is proportional to λh^β , yields the condition

$$\lambda h^\beta - (1 + \lambda h^\beta)^2 (\alpha_\psi \overline{\alpha_\psi})^2 - 2(1 + \lambda h^\beta) \alpha_\psi \overline{\alpha_\psi} \geq 0. \quad (59)$$

Since $\|\alpha_\psi\|_\infty \leq \|\alpha_\psi\|_6 \leq Ch^{1/2}$, this bound implies that we may choose $0 < \beta < 1$, and the latter condition would be satisfied for any value of λ . For $\beta = 1$, on the other hand, one is forced to take the parameter λ large enough, but the inequality may still hold.

We now apply Proposition 3 to get

$$\begin{aligned} \mathcal{E}_\mu^{\text{BCS}}[\Gamma_\psi] &= \text{Tr } \mathfrak{h} \gamma_\psi + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha_\psi(x, y)|^2 \\ &= \text{Tr } \mathfrak{h} \alpha_\psi \overline{\alpha_\psi} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha_\psi(x, y)|^2 + (1 + \lambda h) \text{Tr } \mathfrak{h} \alpha_\psi \overline{\alpha_\psi} \alpha_\psi \overline{\alpha_\psi} \\ &\leq h \int_{\mathbb{R}^3} d\eta \left\{ \frac{1}{4} |\nabla \psi|^2 + (W - D) |\psi|^2 + g_{\text{BCS}} |\psi|^4 \right\} \\ &\quad + Ch^2 \left[\|\nabla \psi\|_{L^2}^4 + \|W |\psi|^2\|_{L^1}^2 + \|\psi\|_{L^2}^4 + 1 \right] \quad (60) \end{aligned}$$

as $h \rightarrow 0$. The upper bound (21) is thus a straightforward consequence of (32).

3.4 Energy lower bound

We consider any admissible BCS state Γ satisfying $\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq C_\Gamma h$, whose existence is ensured by the analysis in the previous § 3.3. The integral kernel of α , the upper-right entry of Γ , can be decomposed as

$$\alpha(x, y) = \alpha_\psi(x, y) + r(x, y) = h^{-2} \psi\left(\frac{x+y}{2}\right) \alpha_0\left(\frac{x-y}{h}\right) + r(x, y). \quad (61)$$

where r is chosen to be orthogonal to α_0 :

$$\langle \alpha_0(\cdot/h) | \tilde{r} \rangle_{L^2_\xi(\mathbb{R}^3)} = 0, \quad (62)$$

where $\tilde{r}(\eta, \xi) := r(x, y)$ and the coordinates η, ξ are defined in (41). With such a choice, the order parameter ψ is naturally defined in terms of α as (recall the notation $\tilde{\alpha}(\eta, \xi) := \alpha(x, y)$)

$$\psi(\eta) := h^{-1} \langle \alpha_0(\cdot/h) | \tilde{\alpha} \rangle_{L^2_\xi(\mathbb{R}^3)} = h^{-1} \int_{\mathbb{R}^3} d\xi \alpha_0(\xi/h) \tilde{\alpha}(\eta, \xi), \quad (63)$$

Note also that, because of the orthogonality of r to α_0 , one immediately gets

$$\|\alpha\|_{L^2(\mathbb{R}^6)}^2 = \|\alpha_\psi\|_{L^2(\mathbb{R}^6)}^2 + \|r\|_{L^2(\mathbb{R}^6)}^2 = h^{-1} \|\psi\|_{L^2}^2 + \|r\|_{L^2}^2. \quad (64)$$

The physical meaning of such a decomposition is apparent: α represents the wave function of a pair of particles and it almost factorizes in the coordinates of the center-of-mass reference frame. More precisely, α_0 describes the wave function in the relative coordinate living on the microscopic scale h , while ψ is the wave function in the in center-of-mass coordinate and varies on the macroscopic scale.

We start with a preliminary lower bound on the BCS energy functional in terms of the off diagonal entry α of Γ . Indeed, for any admissible Γ , it can be seen that one can bound $\mathcal{E}_\mu^{\text{BCS}}[\Gamma]$ from below in terms of a functional of α alone.

Lemma 4. *Let $\mu = -E_0 + h^2 D$, $D \in \mathbb{R}$. For any admissible Γ and for h small enough,*

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \geq \text{Tr } \mathfrak{h} \alpha \bar{\alpha} + \text{Tr } \mathfrak{h} \alpha \bar{\alpha} \alpha \bar{\alpha} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha(x, y)|^2. \quad (65)$$

Proof. The proof is given, e.g., in [16, Proposition 6.2]. We spell it in details here for the sake of completeness. The admissibility of Γ , i.e., the condition $0 \leq \Gamma \leq 1$, is equivalent to

$$\gamma - \gamma^2 - \alpha \bar{\alpha} \geq 0. \quad (66)$$

Since for h small enough \mathfrak{h} is positive, as it follows from the trivial bound

$$\mathfrak{h} \geq E_0 - Dh^2 > 0, \quad (67)$$

we can use the monotonicity of the trace and apply the above inequality to get the result, since (66) implies that $\gamma \geq \alpha\bar{\alpha} + \alpha\bar{\alpha}\alpha\bar{\alpha}$ (see [16, Eq. (6.2)]).

The next lower bound give more information on the decomposition (61).

Lemma 5. *Let $\mu = -E_0 + h^2D$, $D \in \mathbb{R}$, and let Γ an admissible BCS state with upper-right entry α as in (61). Then, there exists a finite constant C such that (recall (39)), as $h \rightarrow 0$,*

$$\begin{aligned} \text{Tr } \mathfrak{h} \alpha\bar{\alpha} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha(x, y)|^2 &\geq h \langle \psi | -\frac{1}{4}\Delta + W - D | \psi \rangle_{L^2(\mathbb{R}^3)} \\ &+ \frac{1}{2}g \|r\|_{L^2(\mathbb{R}^6)}^2 + h^2 \left[\langle \tilde{r} | -\frac{1}{4}\Delta_\eta - \varepsilon\Delta_\xi + \frac{1}{2}W - D | \tilde{r} \rangle_{L^2(\mathbb{R}^6)} - A_0 \right]. \end{aligned} \quad (68)$$

Proof. Plugging in the operator bound (67), we can immediately get rid of the second term in (65) to obtain

$$\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \geq \text{Tr } \mathfrak{h} \alpha\bar{\alpha} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha(x, y)|^2 + (E_0 - h^2D) \|\alpha\|_{\mathfrak{S}^4}^4,$$

and the last term can be dropped since it is positive. Next, we estimate the first term, which reads

$$\begin{aligned} \text{Tr } \mathfrak{h} \alpha\bar{\alpha} + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha(x, y)|^2 \\ = \int_{\mathbb{R}^6} d\eta d\xi \bar{\alpha}(\eta, \xi) \left(-\frac{1}{4}h^2\Delta_\eta - h^2\Delta_\xi + h^2W(\eta + \xi/2) + \right. \\ \left. V(\xi/h) - \mu \right) \tilde{\alpha}(\eta, \xi). \end{aligned}$$

By plugging in the decomposition (61), we get

$$\begin{aligned} \text{Tr } \mathfrak{h} \alpha\bar{\alpha} &= \langle \alpha_\psi | \mathfrak{h} | \alpha_\psi \rangle + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |\alpha_\psi(x, y)|^2 \\ &+ \langle r | \mathfrak{h} | r \rangle + \int_{\mathbb{R}^6} dx dy V\left(\frac{x-y}{h}\right) |r(x, y)|^2 + 2h^2 \Re \langle \alpha_\psi | W r \rangle, \end{aligned} \quad (69)$$

since the potential W is the only operator which does not factorize in the decomposition $L^2(\mathbb{R}^6) = L_\eta^2(\mathbb{R}^3) \otimes L_\xi^2(\mathbb{R}^3)$. The sum of the first two terms has already been estimated in Proposition 3, so that it just remains to consider the quadratic expression on r and the mixed term.

The mixed term can be controlled by exploiting the Taylor expansion (7) and the orthogonality (62), obtaining

$$\begin{aligned}
2h^2 |\Re \langle \alpha_\psi | W r \rangle| &= 2 \left| \int_{\mathbb{R}^6} d\eta d\xi \xi \cdot \nabla W(\zeta) \bar{\psi}(\eta) \alpha_0(\xi/h) \tilde{r}(\eta, \xi) \right| \\
&\leq C \int_{\mathbb{R}^6} d\eta d\xi |\xi| \left(|\xi|^{\beta-1} + |\eta|^\beta + 1 \right) |\psi(\eta)| |\alpha_0(\xi/h)| |\tilde{r}(\eta, \xi)|
\end{aligned}$$

by the trivial bound $|\eta|^{\beta-1} \leq |\eta|^\beta + 1$. Hence, by Cauchy-Schwarz inequality we get

$$\begin{aligned}
2h^2 |\Re \langle \alpha_\psi | W r \rangle| &\leq C \|\psi\|_{L^2(\mathbb{R}^3)} \|r\|_{L^2(\mathbb{R}^6)} \times \\
&\quad \times \left(\int_{\mathbb{R}^3} d\xi \left(|\xi|^{2\beta} + |\xi|^2 \right) |\alpha_0(\xi/h)|^2 \right)^{1/2} \\
+ C \left(\|W|\psi|^2\|_{L^1(\mathbb{R}^3)}^{1/2} + \|\psi\|_{L^2(\mathbb{R}^3)} \right) &\left[\left(\int_{\mathbb{R}^6} d\eta d\xi |\eta|^\beta |\tilde{r}|^2 \right)^{1/2} + \|r\|_{L^2(\mathbb{R}^6)} \right] \times \\
&\quad \times \left(\int_{\mathbb{R}^3} d\xi |\xi|^2 |\alpha_0(\xi/h)|^2 \right)^{1/2} \\
&\leq Ch^{5/2} \left(\|\psi\|_{L^2}^2 + \|r\|_{L^2}^2 + \|W|\psi|^2\|_{L^1} + \|W|r|^2\|_{L^1} \right)
\end{aligned}$$

where we have estimated

$$\int_{\mathbb{R}^6} d\eta d\xi |\eta|^\beta |\tilde{r}|^2 \leq C \|W|r|^2\|_{L^1(\mathbb{R}^6)}.$$

The two terms depending on r can then be absorbed in the corresponding positive ones coming from the estimate of $\langle r | \mathfrak{h} | r \rangle$ by adding a $\frac{1}{2}$ prefactor for h small enough, while the other two can be included in the $A_0 h^2$ remainder up to the change of the constant C in A_0 .

The quadratic expression in ξ is bounded from below by means of Assumption 2:

$$\begin{aligned}
&\int_{\mathbb{R}^3} d\eta \langle r(\eta, \cdot) | -h^2 \Delta_\xi + V(\cdot/h) + E_0 | r(\eta, \cdot) \rangle_{L_\xi^2(\mathbb{R}^3)} \\
&\geq \int_{\mathbb{R}^3} d\eta \langle r(\eta, \cdot) | -h^2 \varepsilon \Delta_\xi + g | r(\eta, \cdot) \rangle_{L_\xi^2(\mathbb{R}^3)} \\
&= g \|r\|_{L^2(\mathbb{R}^6)}^2 + h^2 \varepsilon \|\nabla_\xi r\|_{L^2(\mathbb{R}^6)}^2. \quad (70)
\end{aligned}$$

Lemma 6. *Let $\mu = -E_0 + h^2 D$, $D \in \mathbb{R}$, and let Γ an admissible BCS state with upper-right entry α as in (61), such that $\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq C_\Gamma h$. Then, there exists a finite constant C such that*

$$|\text{Tr } \mathfrak{h} \alpha \bar{\alpha} \alpha \bar{\alpha} - \text{Tr } \mathfrak{h} \alpha_\psi \bar{\alpha}_\psi \alpha_\psi \bar{\alpha}_\psi| \leq Ch^2 \left(\|\nabla \psi\|_{L^2}^4 + A_0^2 \right). \quad (71)$$

Proof. We first rewrite the quartic term via

$$\alpha\bar{\alpha}\alpha\bar{\alpha} - \alpha_\psi\bar{\alpha}_\psi\alpha_\psi\bar{\alpha}_\psi = r\bar{\alpha}\alpha\bar{\alpha}_\psi + \alpha_\psi\bar{\alpha}\alpha\bar{r} + r\bar{\alpha}\alpha\bar{r} + \alpha_\psi(\bar{\alpha}\alpha - \bar{\alpha}_\psi\alpha_\psi)\bar{\alpha}_\psi,$$

so that the cyclicity of trace and triangle inequality yields

$$\begin{aligned} |\mathrm{Tr} \, \mathfrak{h}\alpha\bar{\alpha}\alpha\bar{\alpha} - \mathrm{Tr} \, \mathfrak{h}\alpha_\psi\bar{\alpha}_\psi\alpha_\psi\bar{\alpha}_\psi| &\leq \left\| \mathfrak{h}^{1/2}r\bar{\alpha}\alpha\bar{\alpha}_\psi\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} + \left\| \mathfrak{h}^{1/2}\alpha_\psi\bar{\alpha}\alpha\bar{r}\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} \\ &+ \left\| \mathfrak{h}^{1/2}r\bar{\alpha}\alpha\bar{r}\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} + \left\| \mathfrak{h}^{1/2}\alpha_\psi(\bar{\alpha}\alpha - \bar{\alpha}_\psi\alpha_\psi)\bar{\alpha}_\psi\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1}. \end{aligned} \quad (72)$$

To estimate this four terms, we apply Hölder inequality:

$$\begin{aligned} \left\| \mathfrak{h}^{1/2}\alpha_\psi\bar{\alpha}\alpha\bar{r}\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} &\leq \left\| \mathfrak{h}^{1/2}\alpha_\psi \right\|_{\mathfrak{S}^6} \|\alpha\|_{\mathfrak{S}^6}^2 \left\| \mathfrak{h}^{1/2}r \right\|_{\mathfrak{S}^2}; \\ \left\| \mathfrak{h}^{1/2}r\bar{\alpha}\alpha\bar{\alpha}_\psi\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} &\leq \left\| \mathfrak{h}^{1/2}r \right\|_{\mathfrak{S}^2} \|\alpha\|_{\mathfrak{S}^6}^2 \left\| \mathfrak{h}^{1/2}\alpha_\psi \right\|_{\mathfrak{S}^6}; \\ \left\| \mathfrak{h}^{1/2}r\bar{\alpha}\alpha\bar{r}\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} &= \left\| \alpha\bar{r}\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^2}^2 \leq \|\alpha\|_{\mathfrak{S}^\infty}^2 \left\| \mathfrak{h}^{1/2}r \right\|_{\mathfrak{S}^2}^2; \\ \left\| \mathfrak{h}^{1/2}\alpha_\psi(\bar{\alpha}\alpha - \bar{\alpha}_\psi\alpha_\psi)\bar{\alpha}_\psi\mathfrak{h}^{1/2} \right\|_{\mathfrak{S}^1} &\leq \|\alpha\bar{\alpha} - \bar{\alpha}_\psi\alpha_\psi\|_{\mathfrak{S}^{3/2}} \left\| \mathfrak{h}^{1/2}\alpha_\psi \right\|_{\mathfrak{S}^6}^2. \end{aligned}$$

Plugging the above bounds in (72), we obtain

$$\begin{aligned} |\mathrm{Tr} \, \mathfrak{h}\alpha\bar{\alpha}\alpha\bar{\alpha} - \mathrm{Tr} \, \mathfrak{h}\alpha_\psi\bar{\alpha}_\psi\alpha_\psi\bar{\alpha}_\psi| &\leq 2 \left\| \mathfrak{h}^{1/2}\alpha_\psi \right\|_{\mathfrak{S}^6} \|\alpha\|_{\mathfrak{S}^6}^2 \left\| \mathfrak{h}^{1/2}r \right\|_{\mathfrak{S}^2} \\ &+ \|\alpha\|_{\mathfrak{S}^6}^2 \left\| \mathfrak{h}^{1/2}r \right\|_{\mathfrak{S}^2}^2 + \|\bar{\alpha}\alpha - \bar{\alpha}_\psi\alpha_\psi\|_{\mathfrak{S}^{3/2}} \left\| \mathfrak{h}^{1/2}\alpha_\psi \right\|_{\mathfrak{S}^6}^2. \end{aligned} \quad (73)$$

By (68) and the condition on the BCS energy of Γ , we deduce the inequality

$$\begin{aligned} \left(\frac{1}{2}g - Dh^2 \right) \|r\|_{L^2}^2 + h^2 \left[\langle \tilde{r} | -\frac{1}{4}\Delta_\eta - \varepsilon\Delta_\xi + \frac{1}{2}W | \tilde{r} \rangle_{L^2(\mathbb{R}^6)} \right] \\ \leq Ch \left[1 + \|\psi\|_{L^2}^2 + hA_0 \right], \end{aligned} \quad (74)$$

with A_0 defined in Proposition 3. This, for h small enough (e.g., smaller than $\sqrt{g/(4D)}$), gives a bound on $\|r\|_{L^2}^2$ as well as its Sobolev norms in terms of the norm of ψ . Hence, we have

$$\begin{aligned} \|\bar{\alpha}\alpha - \bar{\alpha}_\psi\alpha_\psi\|_{\mathfrak{S}^{3/2}} &= \|\bar{\alpha}_\psi r + \bar{r}\alpha_\psi + \bar{r}r\|_{\mathfrak{S}^{3/2}} \\ &\leq 2 \|\alpha_\psi\|_{\mathfrak{S}^6} \|r\|_{\mathfrak{S}^2} + \|r\|_{\mathfrak{S}^2}^2 \leq Ch \left[\|\psi\|_{L^6}^2 + \|\psi\|_{L^2}^2 + 1 + hA_0 \right], \end{aligned}$$

by the monotonicity of Schatten norms, Lemma 1 and (74). Similarly, by Sobolev inequality

$$\begin{aligned} \|\alpha\|_{\mathfrak{S}^6}^2 &\leq C \left(\|\alpha_\psi\|_{\mathfrak{S}^6}^2 + \|r\|_{\mathfrak{S}^2}^2 \right) \leq Ch \left[\|\psi\|_{L^6}^2 + \|\psi\|_{L^2}^2 + 1 + hA_0 \right] \\ &\leq Ch \left[\|\nabla\psi\|_{L^2}^2 + \|\psi\|_{L^2}^2 + 1 + hA_0 \right]. \end{aligned} \quad (75)$$

To conclude, we have to estimate the norms of $\mathfrak{h}^{1/2} \alpha_\psi$ but, for any operator T , one has

$$\begin{aligned} \left\| \mathfrak{h}^{1/2} T \right\|_{\mathfrak{S}^{2n}} &= \left\| T^\dagger \mathfrak{h} T \right\|_{\mathfrak{S}^n}^{1/2} \\ &\leq \left(h^2 \|T^\dagger(-\Delta)T\|_{\mathfrak{S}^n} + h^2 \|T^\dagger WT\|_{\mathfrak{S}^n} + \mu \|T^\dagger T\|_{\mathfrak{S}^n} \right)^{1/2} \\ &\leq h \left(\frac{1}{2} \|\nabla_\eta T\|_{\mathfrak{S}^{2n}} + \|\nabla_\xi T\|_{\mathfrak{S}^{2n}} + \left\| W^{1/2} T \right\|_{\mathfrak{S}^{2n}} \right) + (E_0 - h^2 D) \|T\|_{\mathfrak{S}^{2n}}. \end{aligned}$$

Applying this inequality to estimate the norms above and using once more the monotonicity of Schatten norms, Proposition 3, Lemmas 1 and 2 and Sobolev inequality, we obtain

$$\begin{aligned} \left\| \mathfrak{h}^{1/2} \alpha_\psi \right\|_{\mathfrak{S}^6} &\leq h \left[\frac{1}{2} \|\nabla_\eta \tilde{\alpha}_\psi\|_{\mathfrak{S}^2} + \|\nabla_\xi \tilde{\alpha}_\psi\|_{\mathfrak{S}^2} + \left\| W^{1/2} \alpha_\psi \right\|_{\mathfrak{S}^2} \right] + E_0 \|\alpha_\psi\|_{\mathfrak{S}^6} \\ &\leq Ch^{1/2} \left[\|W|\psi|^2\|_{L^1}^{1/2} + \|\psi\|_{L^6} + A_0 + h \|\nabla\psi\|_{L^2} \right] \\ &\leq Ch^{1/2} \left[\|\nabla\psi\|_{L^2} + \|W|\psi|^2\|_{L^1}^{1/2} + A_0 \right], \end{aligned}$$

$$\begin{aligned} \left\| \mathfrak{h}^{1/2} r \right\|_{\mathfrak{S}^2} &\leq h \left[\frac{1}{2} \|\nabla_\eta r\|_{\mathfrak{S}^2} + \|\nabla_\xi r\|_{\mathfrak{S}^2} + \left\| W^{1/2} r \right\|_{\mathfrak{S}^2} \right] + E_0 \|r\|_{\mathfrak{S}^2} \\ &\leq Ch^{1/2} \left[1 + \|\psi\|_{L^2} + h^{1/2} \sqrt{A_0} \right], \end{aligned}$$

as follows from the a priori estimate (74). Putting together all the bounds found so far, we get the result.

In order to complete the proof of the lower bound, we need a last ingredient.

Lemma 7. *Let $\mu = -E_0 + h^2 D$, $D \in \mathbb{R}$, and let Γ an admissible BCS state with upper-right entry α as in (61), such that $\mathcal{E}_\mu^{\text{BCS}}[\Gamma] \leq C_\Gamma h$. Then, there exists a finite constant C such that*

$$\int_{\mathbb{R}^3} d\eta \{ |\nabla\psi|^2 + W|\psi|^2 + |\psi|^2 + |\psi|^4 \} \leq C. \quad (76)$$

Proof. Let us denote for short

$$\mathcal{E} := \int_{\mathbb{R}^3} d\eta \{ |\nabla\psi|^2 + W|\psi|^2 + |\psi|^2 + |\psi|^4 \}.$$

Combining Lemma 6 with (40), we get

$$\mathrm{Tr} \mathfrak{h} \alpha \bar{\alpha} \alpha \bar{\alpha} \geq g_{\mathrm{BCS}} h \|\psi\|_{L^4}^4 - Ch^2 \mathcal{E}^2, \quad (77)$$

so that, by Lemma 5, we find

$$C_{\Gamma} h \geq \mathcal{E}_{\mu}^{\mathrm{BCS}}[\Gamma] \geq h \mathcal{E}_D^{\mathrm{GP}}(\psi) - Ch^2 (\mathcal{E}^2 + 1), \quad (78)$$

where we used once more the estimate on $\|r\|_{L^2}$ following from (74). Since there exists a positive constant $c > 0$ such that $\mathcal{E}_D^{\mathrm{GP}}(\psi) \geq c\mathcal{E} - D\|\psi\|_{L^2}^2$, we get

$$\mathcal{E} \leq \frac{1}{c} \left(C_{\gamma} + D \|\psi\|_{L^2}^2 \right) + O(h).$$

However, such a bound gives a control on the norms $\|W|\psi|^2\|_{L^1}$ and $\|\psi\|_{L^4}$, which can be used as in the proof of Proposition 2 to get an estimate of $\|\psi\|_{L^2}^2$, i.e., one obtains that there exists a finite constant such that

$$\|\psi\|_{L^2}^2 \leq C, \quad (79)$$

which in turn yields the result.

The estimate (78) together with (76) gives the energy lower bound (22). The combination of Lemmas 4 to 7 provides the proof of the remaining statements about the decomposition of α .

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