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Nicolas Rougerie, Dominique Spehner

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# INTERACTING BOSONS IN A DOUBLE-WELL POTENTIAL : LOCALIZATION REGIME

NICOLAS ROUGERIE AND DOMINIQUE SPEHNER

**ABSTRACT.** We study the ground state of a large bosonic system trapped in a symmetric double-well potential, letting the distance between the two wells increase to infinity with the number of particles. In this context, one should expect an interaction-driven transition between a delocalized state (particles are independent and all live in both wells) and a localized state (particles are correlated, half of them live in each well). We start from the full many-body Schrödinger Hamiltonian in a large-filling situation where the on-site interaction and kinetic energies are comparable. When tunneling is negligible against interaction energy, we prove a localization estimate showing that the particle number fluctuations in each well are strongly suppressed. The modes in which the particles condense are minimizers of nonlinear Schrödinger-type functionals.

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## 1. INTRODUCTION

The Mott insulator/superfluid phase transition manifests itself by an interaction-driven drastic change in transport properties of a quantum system. Under conditions where the non-interacting system would be conducting, repulsive interactions can induce an insulating behavior if they dominate tunneling effects of electrons between ions in a crystal (in solid state systems), or of atoms between the wells of a magneto-optic trapping potential (in cold atomic gases). Signatures of the transition have been observed experimentally in cold Bose gases trapped by periodic lattice potentials at low integer fillings (a few atoms per site) [5, 23, 21]. They include a sudden change in the fluctuations of the numbers of particles on each site and the relative phases at some critical value of the ratio between the tunneling and interaction energies [18].

In this paper, we mathematically investigate the case of bosons confined in a double-well potential in a large filling situation, i.e. when one has many particles per well. This situation corresponds to current experiments in cold atom physics, the trapped atoms forming an external Bose-Josephson junction [16, 24, 46]. Like in the multiple-well case, one expects a transition between a delocalized and a localized regimes, the latter occurring when the interactions between particles are stronger than the energy needed for a particle to tunnel from one well into another. In the double-well situation this transition is not, however, expected to be a sharp transition. Instead, one expects for large atom numbers a wide transition regime in which the particle numbers and relative phase fluctuations change smoothly (Josephson regime).

In theoretical studies of the Mott transition, it is customary to use a tight-binding approximation and work with a Hubbard model [18, 30]. This relies on assuming that only the ground state of each potential well is occupied. At low filling (few particles per well), this is certainly reasonable for the interaction energy within one well will usually be smaller than the gap above the well's ground state energy. The physics is then reduced to particles hopping/tunneling between wells and subject to on-site interactions. In a large filling situation, it is not so clear that one can rely on such a simplified model: the interactions between particles on a given site can (and will) change the mode in which particles condense. Nevertheless, some conditions of applicability of the two-mode approximation have been worked out [40] and the two-mode Hubbard model has been used extensively in the physics literature to study external Bose-Josephson junctions (see for instance [17]) and has been successful in explaining experimental results with a hundred up to thousand atoms per well [20, 16]. The problem of going beyond the Bose-Hubbard description, which has been also considered in the physics literature (see for example [19]), does not seem to have previously been studied from a mathematical standpoint.

We here start from the full many-body Schrödinger Hamiltonian

$$H_N = \sum_{j=1}^N (-\Delta_j + V_N(x_j)) + \frac{\lambda}{N-1} \sum_{1 \leq i < j \leq N} w(x_i - x_j) \quad (1.1)$$

for  $N$  interacting particles in  $\mathbb{R}^d$  ( $d = 1, 2, 3$ ) and consider the large  $N$  limit of its ground state in the case where  $V_N$  is a symmetric double-well potential. As appropriate for bosons, we consider the action of  $H_N$  on the symmetric tensor product space

$$\mathfrak{H}^N := \bigotimes_{\text{sym}}^N L^2(\mathbb{R}^d) \simeq L_{\text{sym}}^2(\mathbb{R}^{dN})$$

and study its lowest eigenvalue and associated eigenfunction.

The first sum in the Hamiltonian (1.1) describes the kinetic and potential energies of the bosons in presence of the external trapping potential  $V_N$ , with  $x_j \in \mathbb{R}^d$  and  $\Delta_j$  standing for the position of the  $j$ -th particle and the corresponding Laplacian. The second sum in (1.1) describes interactions among the particles, assumed to be repulsive. The fixed coupling constant  $\lambda > 0$  is multiplied by a scaling factor of order  $1/N$ , in such a way that interactions have a leading order effect in the limit  $N \rightarrow \infty$ , while the ground state energy per particle remains bounded (mean-field regime). The choice of fixing the range of the potential (mean-field limit) is mostly out of simplicity. One should certainly expect our results to remain true in a dilute limit (see e.g. [47, Chapter 7] or [48, Chapter 5] for a discussion of the distinction).

We will not aim at a great generality for the interaction potential  $w$ . In what follows, we denote by  $\hat{w}$  its Fourier transform,  $\|w\|_\infty = \sup_{x \in \mathbb{R}^d} |w(x)|$  its sup norm and by  $B(0, R)$  a ball of  $\mathbb{R}^d$  of radius  $R$  centered at the origin.

**Assumption 1.1 (The interaction potential).**

*The interaction potential  $w$  is positive, of positive type, symmetric, and bounded with compact support:*

$$w > 0, \quad \hat{w} \geq 0, \quad w(x) = w(-x), \quad \|w\|_\infty < \infty, \quad \text{supp}(w) \subset B(0, R_w) \quad (1.2)$$

for some  $R_w > 0$ .

It is well-known (see [31, 33, 47, 49] and references therein) that if the one-body potential  $V_N \equiv V$  in (1.1) does not depend on  $N$  and  $V(x)$  goes to infinity when  $|x| \rightarrow \infty$ , the lowest eigenvalue  $E(N)$  of the Hamiltonian (1.1) is given in the large  $N$  limit by

$$\lim_{N \rightarrow \infty} \frac{E(N)}{N} = e_H(\lambda), \quad (1.3)$$

where  $e_H(\lambda)$  is the Hartree energy, i.e., the minimum of the functional

$$\mathcal{E}_H^\lambda[u] = \int_{\mathbb{R}^d} (|\nabla u|^2 + V|u|^2) dx + \frac{\lambda}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u(x)|^2 w(x-y) |u(y)|^2 dx dy \quad (1.4)$$

under the constraint  $\|u\|_{L^2}^2 = \int_{\mathbb{R}^d} |u|^2 = 1$ . The Hartree functional  $\mathcal{E}_H^\lambda[u]$  is obtained from the energy of the mean-field state  $u^{\otimes N}$  describing  $N$  independent particles in the same state  $u$  as

$$\mathcal{E}_H^\lambda[u] = \frac{1}{N} \langle u^{\otimes N} | H_N | u^{\otimes N} \rangle.$$

The rationale behind (1.3) is that the ground state  $\Psi_N \in \mathfrak{H}^N$  of the  $N$ -body Hamiltonian  $H_N$  roughly behaves as

$$\Psi_N \underset{N \rightarrow \infty}{\approx} (u_H^\lambda)^{\otimes N} \quad (1.5)$$

where  $u_H^\lambda$  is the minimizer of the Hartree functional. Note that the latter is, under Assumption 1.1, unique modulo a constant phase and can be chosen to be positive.

The situation changes when the trapping potential  $V_N$  in the Hamiltonian (1.1) is allowed to depend on  $N$ , which is the case of interest in this work. We shall consider a model with a symmetric double-well potential:

$$V_N(x) = \min \{ V(x - \mathbf{x}_N), V(x + \mathbf{x}_N) \}, \quad (1.6)$$

where  $V$  is a fixed radial potential and the two localization centers  $\pm \mathbf{x}_N = \pm(L_N/2, 0, \dots, 0)$  are along the first coordinate axis. We can with our methods deal with rather general radial confining potentials, but shall for simplicity stick to the model case of a power-law potential:

$$V(x) = |x|^s, \quad s \geq 2. \quad (1.7)$$

To mimic a potential with two deep and well-separated wells, we let the inter-well distance

$$L_N = 2|\mathbf{x}_N| \rightarrow \infty$$

in the limit  $N \rightarrow \infty$ . By scaling, this situation is equivalent to the one where the distance  $L_N$  stays fixed and the range of the interaction goes to 0, but the potential barrier  $V_N(0)$  goes to infinity.

In the following, the coupling constant  $\lambda$  is kept fixed and we will often omit it in the upper index to simplify notation. We denote by  $\mathcal{E}_{H-}[u]$  and  $\mathcal{E}_{H+}[u]$  the functionals (1.4) in which  $V_N$  is replaced by the left and right potential wells, given respectively by

$$V_N^-(x) = V(x + \mathbf{x}_N), \quad V_N^+(x) = V(x - \mathbf{x}_N).$$

Obviously, the positive minimizers  $u_{H\pm}$  of  $\mathcal{E}_{H\pm}[u]$  are equal to the same fixed function  $u_H$  modulo a translation by  $\pm \mathbf{x}_N$  and the corresponding Hartree energies are equal,

$$\mathcal{E}_{H\pm}[u_{H\pm}] := \inf_{\|u\|_{L^2}=1} \{\mathcal{E}_{H\pm}[u]\} = e_H.$$

When the inter-well distance  $L_N$  is very large,  $u_{H-}$  and  $u_{H+}$  become almost orthogonal to one another since they are localized in far-apart potential wells.

In the case of a single particle with Hamiltonian  $H_1 = -\Delta + V_1$ , it is well-known that the lowest energy state  $\Psi_1$  is close in the limit  $L_1 \rightarrow \infty$  to the symmetric superposition

$$\Psi_1 \approx C_{\text{dloc}}^1 \left( \frac{u_- + u_+}{\sqrt{2}} \right), \quad (1.8)$$

where  $u_{\pm}$  is the ground state of  $-\Delta + V_1^{\pm}$  and  $C_{\text{dloc}}^1$  is a normalization factor. More precisely, denoting by  $e$  the lowest eigenvalue of the Hamiltonian  $-\Delta + V$  in a single well, it can be shown [3, 13, 14, 8, 25, 26, 27, 28, 41] that the spectrum of  $H_1$  in an interval of length of order one centered around  $e$  consists of exactly two eigenvalues, which converge to  $e$  as  $L_N \rightarrow \infty$ , and that the eigenfunction  $\Psi_1$  associated to the lowest of these eigenvalues satisfies

$$\left\| \Psi_1 - \frac{u_- + u_+}{\sqrt{2}} \right\| \rightarrow 0$$

as  $L_1 \rightarrow \infty$ . This embodies the fact that a particle in the ground state of  $H_1$  has equal probabilities of being in the left or right well, i.e., the ground state (1.8) is delocalized over the two wells. Extensions of this result to nonlinear models are given in [11, 12].

When there is more than one particle, the situation may change completely due to the repulsive interactions. If both  $N$  and  $L_N$  are large, one should expect a transition between:

- A regime where a delocalized ground state akin to (1.5) is preferred, occurring when  $L_N$  is not too large. Actually, if  $L_N$  is small enough so that tunneling dominates over interactions, a reasonable approximation is to replace the Hartree minimizer in (1.5) by a symmetric superposition,

in analogy with (1.8). This leads to the heuristic

$$\Psi_N \approx \Psi_{\text{dloc}} = C_{\text{dloc}}^N \left( \frac{u_{\text{H-}} + u_{\text{H+}}}{\sqrt{2}} \right)^{\otimes N} \quad (1.9)$$

with the normalization factor

$$C_{\text{dloc}}^N = (1 + \langle u_{\text{H-}}, u_{\text{H+}} \rangle)^{-N/2} \rightarrow 1$$

when  $L_N \rightarrow \infty$ . In the  $N$ -body state  $\Psi_{\text{dloc}}$ , all particles are independent and identically distributed in the same quantum state, delocalized over the two wells.

• A regime where a localized state emerges to reduce on-site interactions, occurring for larger inter-well distances  $L_N$ . An ansatz for such a state can be taken of the form (hereafter we assume that  $N$  is even)<sup>1</sup>

$$\Psi_N \approx \Psi_{\text{loc}} = C_{\text{loc}}^N u_{\text{H-}}^{\otimes N/2} \otimes_{\text{sym}} u_{\text{H+}}^{\otimes N/2}. \quad (1.10)$$

As above, the normalization factor  $C_{\text{loc}}^N \rightarrow 1$  when  $L_N \rightarrow \infty$ , with small corrections of the order of  $\langle u_{\text{H-}}, u_{\text{H+}} \rangle$ . The ansatz  $\Psi_{\text{loc}}$  is a correlated state where half of the particles live in the left well  $V_N^-$  and the other half in the right well  $V_N^+$ . Note that the ansatz (1.10) involving two one-body wave functions has a kinship with states used to describe two component Bose-Einstein condensates, see e.g. [2, 38, 39, 44]. The physics is however very different, and so shall our analysis be.

In this paper, we focus on the regime where localization prevails. Note that this should *not* be interpreted as (1.10) being very close to the true ground state, even in the sense of reduced density matrices (see Remark 2.5 and Section 2.3 below). The simple ansatz (1.10) is in fact motivated by what happens very deep in the localization regime. In the regime close to the transition, which is our concern here, localization is not as strong as in (1.10) and one should be careful about what it actually means.

We formulate localization as follows. Denote by  $a^*(u)$  and  $a(u)$  the bosonic creation and annihilation operators<sup>2</sup> in a mode  $u \in L^2(\mathbb{R}^d)$ . Let

$$\mathcal{N}_- = a^*(u_{\text{H-}})a(u_{\text{H-}}) \quad \text{and} \quad \mathcal{N}_+ = a^*(u_{\text{H+}})a(u_{\text{H+}}) \quad (1.11)$$

be the number operators in the modes  $u_{\text{H-}}$  and  $u_{\text{H+}}$  localized in the left and right wells, respectively. We say that the system is localized if, in the large  $N$  limit, the variance of  $\mathcal{N}_{\pm}$  satisfies<sup>3</sup>

$$\left\langle \Psi_N \left| \left( \mathcal{N}_{\pm} - \frac{N}{2} \right)^2 \right| \Psi_N \right\rangle \ll N \quad (1.12)$$

with  $\Psi_N$  the ground state of the many-body Hamiltonian. Then the fluctuations of  $\mathcal{N}_-$  and  $\mathcal{N}_+$  are reduced with respect to the case of independent particles (1.9), where they would be of order  $N$  since

$$\langle u^{\otimes N} | \mathcal{N}_{\pm}^2 | u^{\otimes N} \rangle - \langle u^{\otimes N} | \mathcal{N}_{\pm} | u^{\otimes N} \rangle^2 = N \langle u_{\text{H}\pm}, u \rangle$$

<sup>1</sup>The definition of the symmetrized tensor product  $\otimes_{\text{sym}}$  is recalled below, see (2.10).

<sup>2</sup>The definition is recalled below, see (4.3).

<sup>3</sup>By symmetry of the potential  $V_N$ , it is easy to see that the expectation of  $\mathcal{N}_{\pm}$  in the ground state  $\Psi_N$  is  $\langle \Psi_N | \mathcal{N}_{\pm} | \Psi_N \rangle = N/2$ . Thus the quantity in the left-hand side of (1.11) is the variance of  $\mathcal{N}_{\pm}$ .

for any  $u \in L^2(\mathbb{R}^d)$ . The reduced fluctuations in (1.12) constitute a violation of the central limit theorem and show the occurrence of strong correlations, akin to those of (1.10), in the ground state of the system.

Our main result in this paper shows that, for a fixed  $\lambda$ , localization in the sense of (1.12) occurs when  $N \rightarrow \infty$  and  $L_N \rightarrow \infty$  satisfy

$$\log N \leq 2(1 - \varepsilon)A\left(\frac{L_N}{2}\right) \quad (1.13)$$

for some arbitrarily small fixed  $\varepsilon > 0$ , where

$$A(r) = \int_0^r \sqrt{V(r')} dr' \quad (1.14)$$

is the Agmon distance (at zero energy) from semiclassical analysis [1]. In the model case (1.7) we have

$$A(r) = \left(1 + \frac{s}{2}\right)^{-1} r^{1+s/2}. \quad (1.15)$$

Note that, although the localized and delocalized states  $\Psi_{\text{loc}}$  and  $\Psi_{\text{dloc}}$  in (1.9) and (1.10) have very different physical properties, distinguishing them in the large  $N$  limit is not as easy as one might think. Actually, as we shall see in Section 2.1, the difference between the interaction energies per particle in the states  $\Psi_{\text{loc}}$  and  $\Psi_{\text{dloc}}$  is of order  $1/N$ . This is of the same order as the next-to-leading order term in the large  $N$  expansion of the ground state energy in a single well, due to Bogoliubov fluctuations [6, 9, 50, 22, 35, 15, 43, 35]. Indeed, if the potential  $V_N \equiv V$  in (1.1) is independent of  $N$ , one can go beyond (1.3) and prove that

$$\frac{E(N)}{N} = e_{\text{H}}(\lambda) + N^{-1}e_{\text{B}}(\lambda) + o(N^{-1}), \quad (1.16)$$

where  $e_{\text{B}}(\lambda)$  is the ground state energy of the Bogoliubov Hamiltonian, obtained from  $H_N$  by a suitable expansion around the condensed state  $u_{\text{H}}^{\otimes N}$  (see Section 4 below for more details). We will prove that Bogoliubov fluctuations, even though they must be taken into account in the analysis of the problem, do not play an important role in deciding which of the localized and delocalized states has the smallest energy.

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## 2. MAIN RESULTS AND DISCUSSION

**2.1. Heuristics.** The order of magnitude (as a function of  $N$ ) of the inter-well distance  $L_N$  at which the localized state (1.10) has a lower energy than the delocalized state (1.9) can be derived heuristically as follows. Let us consider the *tunneling energy*

$$\begin{aligned} T_N &= \langle u_{\text{H}-} | (-\Delta + V_N) | u_{\text{H}+} \rangle \\ &= \left\langle \frac{u_{\text{H}-} + u_{\text{H}+}}{\sqrt{2}} \middle| (-\Delta + V_N) \middle| \frac{u_{\text{H}-} + u_{\text{H}+}}{\sqrt{2}} \right\rangle \\ &\quad - \frac{1}{2} \langle u_{\text{H}-} | (-\Delta + V_N) | u_{\text{H}-} \rangle - \frac{1}{2} \langle u_{\text{H}+} | (-\Delta + V_N) | u_{\text{H}+} \rangle. \end{aligned} \quad (2.1)$$

Recall the variational equations satisfied by  $u_{H\pm}$ :

$$[-\Delta + V_N^\pm + \lambda w * |u_{H\pm}|^2] u_{H\pm} = \mu u_{H\pm} \quad (2.2)$$

with  $*$  denoting convolution and  $\mu$  the chemical potential (Lagrange multiplier),

$$\mu = e_H + \frac{\lambda}{2} \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_{H\pm}(x)|^2 w(x-y) |u_{H\pm}(y)|^2 dx dy . \quad (2.3)$$

Inserting (2.2) in (2.1) we obtain

$$T_N = \int_{\mathbb{R}^d} u_{H-} V_t^+ u_{H+} = \int_{\mathbb{R}^d} u_{H+} V_t^- u_{H-} , \quad (2.4)$$

where  $V_t^\pm$  are the tunneling potentials

$$V_t^\pm = V_N - V_N^\pm - \lambda w * |u_{H\pm}|^2 + \mu . \quad (2.5)$$

From (2.4) one can derive that  $T_N \leq 0$  for large enough inter-well distances  $L_N$  (see Proposition 3.3 below). Going back to (2.1), this is equivalent to the symmetric delocalized state  $(u_{H+} + u_{H-})/\sqrt{2}$  having a lower one-body (i.e., kinetic and potential) energy than the states  $u_{H-}$  and  $u_{H+}$  localized in the left and right wells.

Actually, we recall that the energy of  $N$  bosons in a state  $\Psi \in \mathfrak{H}^N$  is given by

$$\langle \Psi | H_N | \Psi \rangle = E_\Psi^{(\text{kin+pot})} + E_\Psi^{(\text{int})} , \quad (2.6)$$

where the energy components are

$$E_\Psi^{(\text{kin+pot})} = \text{Tr} [(-\Delta + V_N) \gamma_\Psi^{(1)}] , \quad E_\Psi^{(\text{int})} = \frac{\lambda}{2(N-1)} \text{Tr} [w \gamma_\Psi^{(2)}] \quad (2.7)$$

and the  $k$ -body density matrices  $\gamma_\Psi^{(k)}$  are defined by

$$\gamma_\Psi^{(k)} = \frac{N!}{(N-k)!} \text{Tr}_{k+1 \rightarrow N} [|\Psi\rangle\langle\Psi|] \quad (2.8)$$

or, equivalently [32, Section 1],

$$\left\langle v_1 \otimes_{\text{sym}} \cdots \otimes_{\text{sym}} v_k, \gamma_\Psi^{(k)} u_1 \otimes_{\text{sym}} \cdots \otimes_{\text{sym}} u_k \right\rangle = k! \langle \Psi | a^*(u_1) \cdots a^*(u_k) a(v_1) \cdots a(v_k) | \Psi \rangle \quad (2.9)$$

for any  $k = 1, \dots, N$  and  $u_1, v_1, \dots, u_k, v_k \in \mathfrak{H}$ . Hereafter, the symmetric tensor product  $\otimes_{\text{sym}}$  is defined by<sup>4</sup>

$$\begin{aligned} \Psi_1 \otimes_{\text{sym}} \Psi_2(x_1, \dots, x_N) &:= \frac{1}{\sqrt{N_1! N_2! N!}} \\ &\sum_{\sigma \text{ permutation of } \{1, \dots, N\}} \Psi_1(x_{\sigma(1)}, \dots, x_{\sigma(N_1)}) \Psi_2(x_{\sigma(N_1+1)}, \dots, x_{\sigma(N)}) \end{aligned} \quad (2.10)$$

for any  $\Psi_1 \in \mathfrak{H}^{N_1}$  and  $\Psi_2 \in \mathfrak{H}^{N_2}$  with  $N = N_1 + N_2$ .

---

<sup>4</sup>Note that  $\Psi_1 \otimes_{\text{sym}} \Psi_2$  is not normalized even if this is the case for  $\Psi_1$  and  $\Psi_2$ , for instance  $u \otimes_{\text{sym}} u = \sqrt{2} u^{\otimes 2}$ .



A simple calculation shows that the 1-body density matrix  $\gamma_{\text{dloc}}^{(1)}$  and  $\gamma_{\text{loc}}^{(1)}$  in the delocalized and localized states  $\Psi_{\text{dloc}}$  and  $\Psi_{\text{loc}}$  are given by

$$\gamma_{\text{dloc}}^{(1)} \simeq \frac{N}{2} (|u_{\text{H}-}\rangle\langle u_{\text{H}-}| + |u_{\text{H}+}\rangle\langle u_{\text{H}+}| + |u_{\text{H}-}\rangle\langle u_{\text{H}+}| + |u_{\text{H}+}\rangle\langle u_{\text{H}-}|) \quad (2.11)$$

$$\gamma_{\text{loc}}^{(1)} \simeq \frac{N}{2} (|u_{\text{H}-}\rangle\langle u_{\text{H}-}| + |u_{\text{H}+}\rangle\langle u_{\text{H}+}|), \quad (2.12)$$

up to small corrections of order  $N\langle u_{\text{H}-}, u_{\text{H}+} \rangle$ . These can be neglected in the limit  $L_N \rightarrow \infty$ . One then infers from (2.6), (2.11), and (2.12) that

$$E_{\text{dloc}}^{(\text{kin}+\text{pot})} - E_{\text{loc}}^{(\text{kin}+\text{pot})} = NT_N < 0. \quad (2.13)$$

As a result of tunneling between the two wells,  $\Psi_{\text{dloc}}$  has a lower one-body energy than  $\Psi_{\text{loc}}$ .

On the other hand,  $\Psi_{\text{loc}}$  has a lower interaction energy than  $\Psi_{\text{dloc}}$ . Indeed, it is easy to see that the 2-body density matrices of both states have ranges in the 3-dimensional subspace with basis  $\{|u_{\text{H}+}^{\otimes 2}\rangle, |u_{\text{H}-}^{\otimes 2}\rangle, |u_{\text{H}-} \otimes_{\text{sym}} u_{\text{H}+}\rangle\}$ . Since  $u_{\text{H}-}$  and  $u_{\text{H}+}$  are well-separated in space and  $w$  is short-ranged, one can neglect in the limit  $L_N \rightarrow \infty$  all the matrix elements of  $w$  in this basis save for the two elements

$$\langle u_{\text{H}\pm}^{\otimes 2}, w u_{\text{H}\pm}^{\otimes 2} \rangle = \langle u_{\text{H}}^{\otimes 2}, w u_{\text{H}}^{\otimes 2} \rangle = \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_{\text{H}}|^2(x) w(x-y) |u_{\text{H}}|^2(y) dx dy$$

corresponding to on-site interactions (see Remark 3.4 below). The first equality follows from the translation invariance and parity of  $w$ . By using (1.11), (2.9), and the commutation relations of  $a$  and  $a^*$  one finds

$$\langle u_{\text{H}\pm}^{\otimes 2}, \gamma_{\Psi}^{(2)} u_{\text{H}\pm}^{\otimes 2} \rangle = \langle \Psi | \mathcal{N}_{\pm} (\mathcal{N}_{\pm} - 1) | \Psi \rangle.$$

We infer from (2.7) that

$$E_{\Psi}^{(\text{int})} = \frac{\lambda}{2(N-1)} \langle u_{\text{H}}^{\otimes 2}, w u_{\text{H}}^{\otimes 2} \rangle \langle \Psi | (\mathcal{N}_{+} (\mathcal{N}_{+} - 1) + \mathcal{N}_{-} (\mathcal{N}_{-} - 1)) | \Psi \rangle. \quad (2.14)$$

The interaction energies of the delocalized and localized states are thus given by

$$E_{\text{dloc}}^{(\text{int})} = \left(1 + \frac{1}{N-2}\right) E_{\text{loc}}^{(\text{int})} = \frac{\lambda N}{4} \langle u_{\text{H}}^{\otimes 2}, w u_{\text{H}}^{\otimes 2} \rangle \quad (2.15)$$

The localized state thus favors the interaction energy, but only by a small amount,  $O(N^{-1})$  in the energy per particle.

We deduce from this discussion that the limits of large  $N$  and  $L_N$  (with fixed  $\lambda$ ) for which the localized state (1.10) has a lower energy than the delocalized state is given by

$$\text{Localization regime: } N \rightarrow \infty, \quad N^{-1} \gg |T_N| \quad (2.16)$$

We warn the reader that while this limit is obtained by comparing the energies of the two ground states  $\Psi_{\text{loc}}$  for zero tunneling and  $\Psi_{\text{dloc}}$  for vanishing interactions, the true ground state of  $H_N$  differs significantly from both  $\Psi_{\text{loc}}$  and  $\Psi_{\text{dloc}}$  when  $N^{-2} \ll |T_N| \ll 1$  (see Remark 2.5 and Section 2.3 below). Although a better definition would be given by the localization criterion (1.12), we hereafter refer to the limit (2.16) as the “localization regime” since we are able to prove (1.12) in this limit. We do not claim optimality however, see the better estimates of the ground state in Section 2.3 below.

As we shall later see, due to the presence of the non-linearity we are not able to evaluate exactly the order of magnitude of  $|T_N|$ , but we get in Proposition 3.3 a rather precise estimate: for any  $\varepsilon > 0$ ,

$$c_\varepsilon \exp\left(-2(1+\varepsilon)A\left(\frac{L_N}{2}\right)\right) \leq |T_N| \leq C_\varepsilon \exp\left(-2(1-\varepsilon)A\left(\frac{L_N}{2}\right)\right), \quad (2.17)$$

where  $A(r)$  is the Agmon distance (1.14) associated with the single-well potential  $V$  and  $c_\varepsilon$  and  $C_\varepsilon$  are positive constants depending only on  $\varepsilon$ . In view of (2.17) and since  $A(L_N/2) \rightarrow \infty$  as  $L_N \rightarrow \infty$ , the localization condition (2.16) is satisfied when for any  $\varepsilon > 0$  and fixed  $\lambda$ ,

$$\boxed{\text{Localization: } N \rightarrow \infty, \quad L_N \rightarrow \infty, \quad \log N \leq 2(1-\varepsilon)A\left(\frac{L_N}{2}\right)}. \quad (2.18)$$

In the sequel, when we will write that (1.13) or (2.18) holds, this will always mean that it does so for some  $\varepsilon > 0$  that one can choose arbitrarily small, independently of  $N$ .

**2.2. Main theorem.** One difficulty is apparent from the previous discussion: we are trying to capture a transition governed by a correction of order  $N^{-1}$  to the ground state energy per particle. On-site fluctuations are responsible for another correction of the same order of magnitude, cf (1.16). The intuition discussed above is nevertheless correct and a localized state will be preferred in the regime (2.18). A rigorous proof of this fact requires a detailed analysis taking into account on-site Bogoliubov fluctuations.

To state our main result we recall that the single-well Hartree energy  $e_H(\lambda)$  at coupling constant  $\lambda$  is defined as the minimum of the energy functional (1.4) with  $V$  the single-well potential (1.7). The Bogoliubov energy  $e_B(\lambda)$  is obtained as the lowest eigenvalue of the second quantization of the Hessian of  $\mathcal{E}_H^\lambda$  around its minimum, see Section 4 for details.

**Theorem 2.1 (Localized Regime).**

Let  $\lambda \geq 0$  be a fixed constant. In the limit (1.13), we have

- (Energy asymptotics): the ground state energy  $E(N)$  of  $H_N$  satisfies

$$\boxed{\frac{E(N)}{N} = e_H\left(\Delta_N \frac{\lambda}{2}\right) + \frac{2}{N} e_B\left(\frac{\lambda}{2}\right) + o(N^{-1})} \quad (2.19)$$

where

$$\Delta_N = 1 - \frac{1}{N-1}. \quad (2.20)$$

- (Particle number fluctuations): the ground state  $\Psi_N$  of  $H_N$  satisfies

$$\boxed{\left\langle \Psi_N \left| \left( \mathcal{N}_+ - \frac{N}{2} \right)^2 \right| \Psi_N \right\rangle + \left\langle \Psi_N \left| \left( \mathcal{N}_- - \frac{N}{2} \right)^2 \right| \Psi_N \right\rangle \ll N} \quad (2.21)$$

where  $\mathcal{N}_\pm$  are the particle number operators in the left and right wells, defined in (1.11).

*Remark 2.2* (Composition of the energy).

The energy expansion (2.19) is a first signature of a transition to a localized state. It coincides (up to errors of order  $o(N^{-1})$ ) with the ground state energy of two independent bosonic gases localized infinitely far apart in the left and right wells, having  $N/2$  particles each. Note that, since the coupling constant in the Hamiltonian (1.1) is  $\lambda(N-1)^{-1}$  instead of  $\lambda(N/2-1)^{-1}$ , the

parameter  $\lambda$  should be renormalized as  $\lambda \rightarrow \lambda \Delta_N/2$ , so that the ground state energy of each gas is equal to

$$(N/2)e_H(\Delta_N \lambda/2) + e_B(\lambda/2) + o(1).$$

The energy in the right-hand side of (2.19) is therefore equal to the sum of the lowest energies of the two gases in the left and right wells, up to errors of order  $o(1)$ . Indeed (2.19) can be obtained using as trial state a refinement of (1.10), taking into account on-site Bogoliubov fluctuations.

In the regime (1.13) one can see that the delocalized ansatz (1.9), supplemented by the appropriate Bogoliubov fluctuations, has a larger energy per particle, by an amount  $O(N^{-1})$ . Indeed, the first term in (2.19) then becomes  $e_H(\frac{\Delta}{2})$  while the second one is unchanged at leading order<sup>5</sup> and the tunneling contribution is negligible.  $\diamond$

*Remark 2.3* (Strong correlations).

To appreciate that (2.21) indeed is a signature of correlations, the following considerations are helpful. First note that  $\mathcal{N}_-$  and  $\mathcal{N}_+$  could be seen as random variables, and that, roughly speaking,

$$\mathcal{N}_- = \sum_{j=1}^N X_j$$

where  $X_j$  is a random variable which takes the value 1 if particle  $j$  is in the  $-$  well and 0 if it is in the  $+$  well. Each  $X_j$  has mean  $1/2$  so that

$$\langle \Psi_N | \mathcal{N}_- | \Psi_N \rangle = \frac{N}{2}.$$

Now, if correlations between particles could be neglected, the  $X_j$ 's would be independent random variables. Using the central limit theorem, one would expect the variance

$$\left\langle \Psi_N \left| \left( \mathcal{N}_- - \frac{N}{2} \right)^2 \right| \Psi_N \right\rangle$$

to scale like  $N$  when  $N \rightarrow \infty$ . Our result (2.21) rules this out, and thus the  $X_j$ 's cannot be independent. Note that weakly correlated particles usually also satisfy central limit theorems, see for example [4, 7]. Thus, (2.21) implies that the bosons in the double-well potential must be strongly correlated in the localized regime. In contrast, in the delocalized regime one expects weak correlations, and thus particle number fluctuations of the order of  $\sqrt{N}$ .  $\diamond$

*Remark 2.4* (More general single-well potentials  $V$ ).

As mentioned in the Introduction, the results of Theorem 2.1 and the estimate (2.17) on the tunneling energy  $T_N$  are in fact valid for more general single-well potentials  $V(x)$ , not necessarily given by power laws. For instance, one can easily generalize all the estimates of Section 3 and the proof in the subsequent sections to radial potentials  $V(r)$  satisfying the following assumptions:

- (a)  $V(r) \geq 0$  and  $V(r)$  is increasing on  $(r_0, \infty)$  for some fixed  $r_0 > 0$ ;
- (b)  $\lim_{r \rightarrow \infty} \frac{d}{dr} \sqrt{V(r)}$  exists and belongs to  $(0, \infty]$ ;
- (c)  $V'(r)/V''(r) \rightarrow \infty$ ,  $V(r)/V'(r) \rightarrow \infty$  and  $A(r)/\sqrt{V(r)} \rightarrow \infty$  when  $r \rightarrow \infty$ , with  $A(r)$  the Agmon distance (1.14) associated to  $V$ ;

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<sup>5</sup>This is not so easy to show, see the expressions in [22].

(d)  $\lim_{r \rightarrow \infty} \frac{rV'(r)}{V(r)} = s$  exists and belongs to  $[2, \infty]$ .

◇

*Remark 2.5* (Ground state in the localization regime).

The heuristic arguments presented in Section 2.1 to identify the localization regime are very rough since we have merely compared the energies of two states  $\Psi_{\text{loc}}$  and  $\Psi_{\text{dloc}}$ , corresponding respectively to the true ground states in the absence of tunneling ( $L_N = \infty$ ) and for vanishing interactions ( $\lambda = 0$ ). It turns out that the ground state of the many-body Hamiltonian (1.1) is not close to the purely localized ansatz (1.10) in the whole localization regime  $|T_N| \ll N^{-1}$ . In fact, its one-body density matrix  $\gamma_{\Psi_N}^{(1)}$  does not even have two macroscopic eigenvalues of order  $N$ , and a fortiori is not close to the diagonal density matrix  $\gamma_{\text{loc}}^{(1)}$  given by (2.12). As we will see in the next subsection and Appendix C, closeness to  $\gamma_{\text{loc}}^{(1)}$  should be expected to hold for lower tunneling energies  $|T_N| \ll N^{-2}$  only. For higher  $|T_N|$ ,  $\gamma_{\Psi_N}^{(1)}$  is instead expected to be close to the density matrix  $\gamma_{\text{dloc}}^{(1)}$  of the *delocalized* state, given by (2.11).

Even if Theorem 2.1 does not provide a full characterization of the ground state, it captures its most physically important feature, namely the reduced fluctuations of particle numbers in each well (squeezing), which implies as mentioned before the presence of strong correlations between particles (such correlations are of course not seen in the one-body density matrix). One may conjecture from heuristic arguments (see the next subsection) that this property holds for smaller inter-well distances  $L_N$  than assumed in this theorem, up to tunneling energies  $|T_N| \ll 1$ . Proving this is, however, out of reach from the methods presented in Section 6. ◇

**2.3. More precise heuristics.** The properties of the ground state of interacting bosons in a symmetric double-well potential have been studied extensively in the physics literature (see e.g. the review articles [20, 30]). We summarize them in Table 1 and derive them heuristically in this subsection and in Appendix C, neglecting on-site Bogoliubov fluctuations as in Section 2.1.

The *main conjectures* we wish to argue for in this subsection are that

- localization in the sense of (2.21) holds when the tunneling energy satisfies  $|T_N| \ll 1$  (compare with (2.16)).
- this is essentially sharp, i.e. (2.21) fails for  $|T_N| \gg 1$ .

Proving these conjectures remains out of reach of our present method, for this would require much finer estimates of the tunneling contribution to the ground-state energy.

Instead of investigating the many-body Hamiltonian  $H_N$ , most studies in the physics literature deal with the simpler two-mode Bose-Hubbard Hamiltonian, which is obtained by restricting  $H_N$  to the subspace  $\mathfrak{H}_{\text{BH}} \subset \mathfrak{H}^N$  spanned by the  $N + 1$  Fock states

$$|n, N - n\rangle = \frac{1}{\sqrt{n!(N - n)!}} (a_-^*)^n (a_+^*)^{N - n} |0\rangle = C_n u_{\text{H}-}^{\otimes n} \otimes_{\text{sym}} u_{\text{H}+}^{\otimes (N - n)}$$

where  $n = 0, \dots, N$ ,  $|0\rangle \in \mathfrak{H}^N$  denotes the vacuum state,  $a_- = a(u_{\text{H}-})$  and  $a_+ = a(u_{\text{H}+})$  are the annihilation operators in the states  $u_{\text{H}-}$  and  $u_{\text{H}+}$  minimizing the Hartree functionals in the

Limit	<i>Fock regime</i> $N \rightarrow \infty,  T_N  \ll N^{-2}$	<i>Josephson regime</i> $N \rightarrow \infty, N^{-2} \ll  T_N  \ll 1$	<i>Rabi regime</i> $N \rightarrow \infty, 1 \ll  T_N $
expected ground state	Fock state $\Psi_{\text{loc}}$	Squeezed state $\Psi_{\text{sq}}$	Coherent state $\Psi_{\text{dloc}}$
particle number fluctuations	$\langle (\Delta \mathcal{N}_-)^2 \rangle = O(1)$	$\langle (\Delta \mathcal{N}_-)^2 \rangle \ll N$	$\langle (\Delta \mathcal{N}_-)^2 \rangle = O(N)$
tunneling factor	$\langle u_{H-}, \gamma_{\Psi_N}^{(1)} u_{H+} \rangle = O(1)$	$\langle u_{H-}, \gamma_{\Psi_N}^{(1)} u_{H+} \rangle \simeq \frac{N}{2}$	$\langle u_{H-}, \gamma_{\Psi_N}^{(1)} u_{H+} \rangle = \frac{N}{2}$

TABLE 1. Expected properties of the ground state of the many-body Hamiltonian (1.1) in the limits  $N \rightarrow \infty$ ,  $L_N \rightarrow \infty$  (see e.g. [30, 20]). Here  $|T_N|$  is the tunneling energy, decaying with  $L_N$  roughly as  $e^{-2A(L_N/2)}$ , where  $A(r)$  is the Agmon distance (see (2.17)). We prove rigorously in this paper the reduced particle number fluctuations in the limit  $N \rightarrow \infty$ ,  $|T_N| \ll N^{-1}$ , that is, from the Fock regime up to the middle of the Josephson regime.

left and right wells, and  $C_n$  is a normalization factor<sup>6</sup>. The energy of a general state in  $\mathfrak{H}_{\text{BH}}$ ,

$$|\Psi\rangle = \sum_{n=0}^N c_n |n, N-n\rangle, \quad (2.22)$$

can be evaluated as we now explain. First, since  $H_N$  is invariant under the exchange of the two wells (thanks to the symmetry of  $V_N$ ), its non-degenerate ground state is invariant under the exchange of  $u_{H+}$  and  $u_{H-}$ , i.e., it satisfies  $c_{N-n} = c_n$  for any  $n = 0, \dots, N$ .

By using (2.7) and the fact that the one-body density matrix  $\gamma_{\Psi}^{(1)}$  has a two-dimensional range spanned by  $u_{H-}$  and  $u_{H+}$ , the kinetic and potential energies of the state (2.22) reads

$$E_{\Psi}^{(\text{kin+pot})} = e_+ \langle u_{H+}, \gamma_{\Psi}^{(1)} u_{H+} \rangle + e_- \langle u_{H-}, \gamma_{\Psi}^{(1)} u_{H-} \rangle + 2T_N \text{Re} \langle u_{H+}, \gamma_{\Psi}^{(1)} u_{H-} \rangle$$

with  $e_{\pm} = \langle u_{H\pm}, (-\Delta + V_N) u_{H\pm} \rangle$ . From (2.9) and the identity  $c_n = c_{N-n}$  one concludes that

$$\langle u_{H\pm}, \gamma_{\Psi}^{(1)} u_{H\pm} \rangle = \langle \Psi | a_{\pm}^* a_{\pm} | \Psi \rangle = \frac{N}{2}. \quad (2.23)$$

Calculating on the other hand

$$\langle u_{H+}, \gamma_{\Psi}^{(1)} u_{H-} \rangle = \langle \Psi | a_+^* a_- | \Psi \rangle,$$

one gets

$$E_{\Psi}^{(\text{kin+pot})} = E_{\text{loc}}^{(\text{kin+pot})} + 2T_N \sum_{n=0}^N \sqrt{n(N-n+1)} \text{Re} \{ \overline{c_n} c_{n-1} \} \quad (2.24)$$

with  $E_{\text{loc}}^{(\text{kin+pot})} = (e_+ + e_-)N/2$ .

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<sup>6</sup> A few (mainly numerical) works in the physics literature go beyond the two-mode approximation. For instance, perturbative and exact diagonalization approaches have been used in Ref. [19] to include also the first excited state in each well.

By arguing as in Section 2.1, discarding all matrix elements of the interaction  $w$  save for those between  $u_{H\pm}^{\otimes 2}$  and  $u_{H\pm}^{\otimes 2}$ , one obtains from (2.14) the interaction energy

$$E_{\Psi}^{(\text{int})} = U_N \left( \frac{N(N-2)}{4} + \left\langle (\Delta \mathcal{N}_-)^2 \right\rangle_{\Psi} \right), \quad U_N = \frac{\lambda \langle u_H^{\otimes 2}, w u_H^{\otimes 2} \rangle}{N-1} \quad (2.25)$$

with

$$\left\langle (\Delta \mathcal{N}_{\pm})^2 \right\rangle_{\Psi} = \left\langle \Psi \left| (\mathcal{N}_{\pm} - N/2)^2 \right| \Psi \right\rangle$$

the square fluctuation of  $\mathcal{N}_{\pm} = a_{\pm}^* a_{\pm}$ . Thus, the total energy of a state of the form (2.22) is given by

$$E_{\Psi} = E_{\Psi}^{(\text{kin+pot})} + E_{\Psi}^{(\text{int})} = E_{\text{loc}} + 2T_N \sum_{n=0}^N \sqrt{n(N-n+1)} \text{Re} \{ \overline{c_n} c_{n-1} \} + U_N \left\langle (\Delta \mathcal{N}_-)^2 \right\rangle_{\Psi},$$

where  $E_{\text{loc}}$  is the energy of the localized state, see Section 2.1. From these considerations, we moreover deduce that the problem of finding the state  $\Psi$  in the subspace  $\mathfrak{H}_{\text{BH}}$  with minimal energy  $E_{\Psi}$  is equivalent to determining the ground state of the following two-mode Bose-Hubbard Hamiltonian acting on  $\mathfrak{H}_{\text{BH}}$

$$H_{\text{BH}} = e_+ \mathcal{N}_+ + e_- \mathcal{N}_- + T_N (a_-^* a_+ + a_+^* a_-) + \frac{U_N}{2} (a_+^* a_+^* a_+ a_+ + a_-^* a_-^* a_- a_-).$$

Note that  $\mathcal{N}_- + \mathcal{N}_+ = N\mathbb{1}$  (here  $\mathbb{1}$  denotes the identity operator) since we are neglecting all Bogoliubov excitations outside the one-particle subspace spanned by  $u_{H-}$  and  $u_{H+}$ .

To obtain the transition values of Table 1, consider a trial state  $\Psi$  given by

$$c_n = \frac{1}{\mathcal{Z}_N} e^{-(n-N/2)^2/\sigma_N^2} \quad (2.26)$$

with  $\sigma_N$  setting the scale of the particle number fluctuations and  $\mathcal{Z}_N$  a normalization constant. Assuming squeezed particle number fluctuations,  $1 \ll \sigma_N \ll N^{1/2}$ , simple calculations and estimates give, to leading order in  $N$ ,

$$E_{\Psi}^{(\text{kin+pot})} + E_{\Psi}^{(\text{int})} \approx E_{\text{loc}} + T_N N \left( 1 - \frac{1}{2\sigma_N^2} \right) + U_N \frac{\sigma_N^2}{4}. \quad (2.27)$$

On the other hand, from the computations of Section 2.1 we have

$$E_{\text{dloc}} \approx E_{\text{loc}} + T_N N + \frac{\lambda N}{4} \langle u_H^{\otimes 2}, w u_H^{\otimes 2} \rangle.$$

To minimize (2.27) in  $\sigma_N$ , we pick (recall that  $T_N < 0$  and  $\lambda = O(1)$  by convention)

$$\sigma_N \propto N^{1/2} |T_N|^{1/4} \ll N^{1/2} \text{ if } |T_N| \ll 1.$$

and obtain, for two fixed numbers  $a_1, a_2 > 0$

$$E_{\Psi} - E_{\text{dloc}} = a_1 |T_N|^{1/2} - a_2 < 0 \text{ if } |T_N| \ll 1$$

and the other way around if  $|T_N| \gg 1$ . One can similarly show that the state  $\Psi$  has a smaller energy than  $\Psi_{\text{loc}}$  when  $|T_N| \gg N^{-2}$  and the other way around if  $|T_N| \ll N^{-2}$ . This leads to the transitional values of Table 1. A more precise guess (spin-squeezed state) can be made for the ground state in the Josephson regime, see Appendix C.

Further note that, both the trial state above and the spin-squeezed state discussed in Appendix C have tunneling factors close to that of the delocalized state (as indicated in Table 1). This

implies that their one-body density matrix are close to that of the delocalized state to leading order in  $N$ , and we expect the same for the true ground state.

**2.4. Organization of the proofs.** The rest of the paper is organized as follows:

- Section 3 contains useful estimates on the Hartree minimizers to be used throughout the paper, in particular sharp decay estimates.
- Section 4 recalls those elements of Bogoliubov's theory we shall need in the proofs of our main results, following mainly [22, 35].
- Section 5 is concerned with the construction of a trial state having energy (2.19), thus providing the desired upper bound on the ground state energy.
- In Section 6 we present the core of the proof of our main theorem, namely the energy lower bound and the estimates on particle number fluctuations that follow from it.
- Appendix A contains, for the convenience of the reader, elements of proofs for the results on Bogoliubov's theory we use in the paper. We make no claim of originality here and refer to [22, 35, 50] for full details.
- We present in Appendix B the proof of a lemma used in Section 6 about the optimal way of distributing particles between the two wells.
- Finally, some details on squeezed states are given in Appendix C.

### 3. BOUNDS ON THE MINIMIZERS OF THE MEAN-FIELD FUNCTIONALS

**3.1. Hartree minimizer in a single well.** The Hartree functional that we shall study is

$$\mathcal{E}_H[u] = \int_{\mathbb{R}^d} \left( |\nabla u|^2 + V|u|^2 + \frac{\lambda}{2} |u|^2 w * |u|^2 \right), \quad (3.1)$$

where  $V(x)$  is the single well potential (1.7). We shall denote the minimizer of  $\mathcal{E}_H[u]$  by  $u_H$ . We will later apply the results of this section to  $u_{H-}$  and  $u_{H+}$ , that are just translates of  $u_H$ .

Given Assumption 1.1 on the interaction  $w$ , the existence and uniqueness of the minimizer of the Hartree functional (3.1) under the unit mass constraint is an easy exercise. In fact, since  $w$  is assumed to be of positive type, the functional (3.1) is strictly convex in  $|u|^2$ . It follows from the identity  $|\nabla u|^2 = (\nabla|u|)^2 + |u|^2(\nabla\varphi)^2$  with  $u = |u|e^{i\varphi}$  that  $\mathcal{E}_H[u] \geq \mathcal{E}_H[|u|]$ , with equality if and only if  $\varphi$  is constant. Thus the minimizer  $u_H$  is unique up to a constant phase factor, which can be chosen such that  $u_H > 0$ . One can also show that  $u_H$  is radial (see e.g. [37] for details on these claims). By exploiting the elliptic character of the variational equation satisfied by  $u_H$  (see (2.2)), one shows in the usual way that  $u_H$  is a smooth function.

**Proposition 3.1 (Decay estimates on the Hartree minimizer).**

Let  $V(x) = |x|^s$  with  $s \geq 2$ ,  $A(r)$  be the Agmon distance (1.14), and

$$\alpha = \begin{cases} \frac{2d-2+s}{4s} & \text{if } s > 2 \\ \frac{2d-2+s}{4s} - \frac{\mu}{2s} & \text{if } s = 2, \end{cases} \quad (3.2)$$

with  $\mu$  the chemical potential in (2.2).

For any  $0 < \varepsilon < 1$ , and any  $|x| \geq R_0$  large enough,  $u_H$  satisfies the pointwise estimates

$$c_\varepsilon \frac{e^{-A(|x|)}}{V(x)^{\alpha+\varepsilon}} \leq u_H(x) \leq C_\varepsilon \frac{e^{-A(|x|)}}{V(x)^{\alpha-\varepsilon}}, \quad (3.3)$$

where  $c_\varepsilon > 0$  and  $C_\varepsilon > 0$  are two constants depending only on  $\varepsilon$ .

In the special case of a harmonic trap  $V(x) = |x|^2$ , this shows that  $u_H(x)$  decays like a Gaussian when  $|x| \rightarrow \infty$ :

$$u_H(x) \sim C \exp\left(-\frac{1}{2}|x|^2\right) \quad (3.4)$$

up to some power-law corrections.

*Proof.* We set, for some number  $\beta \in \mathbb{R}$ ,

$$f(x) = \exp(-A(|x|)) V(x)^{-\beta/s} = \exp\left(-\left(1 + \frac{s}{2}\right)^{-1} |x|^{1+s/2}\right) |x|^{-\beta}. \quad (3.5)$$

Then, setting  $r = |x|$ ,

$$\Delta f(x) = \left[r^s + \left(2\beta - \frac{s}{2} - d + 1\right) r^{s/2-1} + (\beta^2 + 2\beta - d) r^{-2}\right] f(x). \quad (3.6)$$

Since  $|u_H|^2$  decays at infinity and  $w$  has compact support,  $w * |u_H|^2$  also decays at infinity. We deduce that, for  $r$  large enough,

$$(-\Delta f + V + \lambda w * |u_H|^2 - \mu) f \geq 0 \quad (\text{respectively } \leq 0) \quad (3.7)$$

if one picks  $\beta = s\alpha - \varepsilon$  (respectively  $\beta = s\alpha + \varepsilon$ ). The result is obtained by using the above functions as super/sub-solutions for the variational equation (4.6) and a maximum principle argument.

Pick first  $\beta = s\alpha - \varepsilon$ , define  $R_-$  to be some radius large enough for (3.7) and

$$r^s > \mu - \lambda w * |u_H|^2(x) \quad (3.8)$$

to hold whenever  $r \geq R_-$ . Let  $f_-$  be equal to  $f$  outside  $B(0, R_-)$  and smoothly extended to a function bounded away from 0 inside  $B(0, R_-)$ . Further set

$$C_\varepsilon = \max_{|x| < R_-} \left\{ \frac{u_H(x)}{f_-(x)} \right\} > 0$$

and

$$g_- = u_H - C_\varepsilon f_-.$$

The latter being a smooth function, decaying at infinity, it must reach a global maximum. We have the following alternative:

- (1) Either  $g_-$  reaches its maximum at a point  $x_0$  inside  $B(0, R_-)$ , then by construction

$$u_H(x) - C_\varepsilon f_-(x) \leq u_H(x_0) - C_\varepsilon f_-(x_0) \leq 0$$

for all  $x$ .

- (2) Or  $g_-$  reaches its maximum at some point  $x_0$  outside  $B(0, R_-)$ . Then, according to (3.7) and the variational equation (2.2), we have

$$(-\Delta + V + \lambda w * |u_H|^2 - \mu) g_-(x_0) = -C_\varepsilon (-\Delta + V + \lambda w * |u_H|^2 - \mu) f_-(x_0) \leq 0$$

But  $\Delta g_-(x_0) \leq 0$  because  $x_0$  is a maximum of  $g_-$ , thus

$$(|x_0|^s + \lambda w * |u_H|^2(x_0) - \mu) g_-(x_0) \leq 0$$

and this implies  $g_-(x_0) \leq 0$  upon inserting (3.8). Hence

$$u_H(x) - C_\varepsilon f_-(x) \leq u_H(x_0) - C_\varepsilon f_-(x_0) \leq 0$$

for all  $x$  again.



In both cases one has  $g_-(x) \leq g(x_0) \leq 0$  for all  $x \in \mathbb{R}^d$ , which yields the upper bound in (3.3) because  $f_-(x) = f(x)$  for  $|x|$  large enough.

The lower bound in (3.3) is proven similarly, picking now  $\beta = s\alpha + \varepsilon$ , defining  $f_+$  similarly as before and setting

$$c_\varepsilon = \min_{|x| < R_+} \left\{ \frac{u_H(x)}{f_+(x)} \right\}, \quad g_+ = u_H - c_\varepsilon f_+.$$

The latter function, being smooth and decaying at infinity, must reach a global minimum or else be everywhere positive. In the latter case there is nothing to prove, while in the former one can argue exactly as above, switching some signs where appropriate.  $\square$

The pointwise estimates (3.3) yield a simple but useful corollary, namely a control of the mean-field potential generated by  $|u_H|^2$  via  $w$ ,

$$h_{\text{mf}} := w * |u_H|^2. \quad (3.9)$$

**Lemma 3.2 (Local control of the mean-field potential).**

For any  $\eta > 0$ , there is a constant  $C_\eta > 0$  such that

$$h_{\text{mf}} \leq C_\eta |u_H|^{2-\eta}. \quad (3.10)$$

Note that if  $w$  was a contact potential  $w = \delta_0$ , (3.10) would be an equality with  $\eta = 0$ ,  $C_\eta = 1$ . What the lemma says is that the decay of the mean-field potential is not much worse than in the case of purely local interactions.

*Proof.* Since  $w$  is bounded with a compact support included in the ball  $B(0, R_w)$ , one has

$$h_{\text{mf}}(x) = \int_{\mathbb{R}^d} w(y) |u_H(x-y)|^2 dy \leq \|w\|_\infty |B(0, R_w)| \sup_{y \in B(0, R_w)} |u_H(x-y)|^2.$$

Let  $\varepsilon \in (0, 1)$  be such that

$$\frac{1+\varepsilon}{(1-\varepsilon)^2} = \left(1 - \frac{\eta}{2}\right)^{-1}.$$

We can use the following estimate on the Hartree minimizer, which is less precise than (3.3):

$$c_\varepsilon \exp(-(1+\varepsilon)A(|x|)) \leq u_H(x) \leq C_\varepsilon \exp(-(1-\varepsilon)A(|x|)) \quad x \in \mathbb{R}^d, \quad (3.11)$$

where  $c_\varepsilon > 0$  and  $C_\varepsilon > 0$  are two constants depending on  $\varepsilon$ . Therefore, we have for any  $x \in \mathbb{R}^d$ ,  $|x| \geq R_w$ ,

$$\begin{aligned} \sup_{y \in B(0, R_w)} \frac{|u_H(x-y)|}{|u_H(x)|^{1-\eta/2}} &\leq C'_\varepsilon \sup_{y \in B(0, R_w)} \exp\left(-(1-\varepsilon)A(|x-y|) + (1+\varepsilon)\left(1 - \frac{\eta}{2}\right)A(|x|)\right) \\ &\leq C'_\varepsilon \exp\left(-(1-\varepsilon)(A(|x|) - R_w) - (1-\varepsilon)A(|x|)\right) \end{aligned} \quad (3.12)$$

for some  $C'_\varepsilon > 0$ . It is easy to check that the exponential in the second line of (3.12) is bounded in  $x$ , which yields the desired result.  $\square$

A further consequence of Proposition 3.1 is the estimate on the tunneling energy announced in (2.17). Let  $u_{H-}(x) = u_H(x + \mathbf{x}_N)$  and  $u_{H+}(x - \mathbf{x}_N)$  be the Hartree minimizers corresponding to the left and right trapping potentials  $V_N^-$  and  $V_N^+$ , respectively.

**Proposition 3.3 (Bounds on tunneling terms).**

For any  $\varepsilon > 0$ , one can find some positive constants  $c_\varepsilon$ ,  $C_\varepsilon$ , and  $L_\varepsilon > 0$  such that for any  $L_N > L_\varepsilon$ ,

$$c_\varepsilon \exp\left(-2(1+\varepsilon)A\left(\frac{L_N}{2}\right)\right) \leq \int_{\mathbb{R}^d} u_{H-} u_{H+} \leq C_\varepsilon \exp\left(-2(1-\varepsilon)A\left(\frac{L_N}{2}\right)\right). \quad (3.13)$$

Moreover, the tunneling energy defined in (2.1) is negative for  $N$  large enough and satisfies

$$c_\varepsilon \exp\left(-2(1+\varepsilon)A\left(\frac{L_N}{2}\right)\right) \leq |T_N| \leq C_\varepsilon \exp\left(-2(1-\varepsilon)A\left(\frac{L_N}{2}\right)\right). \quad (3.14)$$

In fact, since we know the rate of decay of the Hartree minimizer down to polynomial corrections, we could reach a similar precision in the estimates (3.13) and (3.14). We do not state this explicitly for conciseness. We will, however, need this information to prove that  $T_N < 0$  and get the lower bound on  $|T_N|$  in (3.14).

*Proof.* We use the bounds (3.3), suitably translated by  $\pm \mathbf{x}_N$ . For the first estimate, the polynomial correction to the rate of decay obtained in (3.3) is not relevant and one can just calculate integrals of the form

$$I_a = \int_{\mathbb{R}^d} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx \quad (3.15)$$

with  $a = ((1+s/2)^{-1} \pm \varepsilon)$ , the  $\pm \varepsilon$  being used to absorb any additional polynomial term.

On the one hand, for  $|x| \geq CL_N$  with a large enough constant  $C > 0$  we have, by the triangle inequality

$$|x - \mathbf{x}_N|^{1+s/2} + |x + \mathbf{x}_N|^{1+s/2} \geq 2|x|^{1+s/2} \left(1 - \frac{1}{2C}\right)^{1+s/2}.$$

Thus, provided  $C$  is chosen large enough we obtain

$$\begin{aligned} \int_{\{|x| \geq CL_N\}} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx &\leq \int_{\{|x| \geq CL_N\}} e^{-2a(1-\frac{1}{2C})^{1+s/2}|x|^{1+s/2}} dx \\ &\leq e^{-a(1-\frac{1}{2C})^{1+s/2}C^{1+s/2}L_N^{1+s/2}} \int_{\{|x| \geq CL_N\}} e^{-a(1-\frac{1}{2C})^{1+s/2}|x|^{1+s/2}} dx \\ &\leq e^{-3(1-\varepsilon)A\left(\frac{L_N}{2}\right)} \end{aligned}$$

which is much smaller than the precision we aim at in the desired result.

There remains to estimate the part of the integral located where  $|x| \leq CL_N$ . We write  $x = (x_1, \dots, x_d)$  and note that the function

$$\begin{aligned} |x - \mathbf{x}_N|^{1+s/2} + |x + \mathbf{x}_N|^{1+s/2} &= \left( \left| x_1 - \frac{L_N}{2} \right|^2 + |x_2|^2 + \dots + |x_d|^2 \right)^{1/2+s/4} \\ &\quad + \left( \left| x_1 + \frac{L_N}{2} \right|^2 + |x_2|^2 + \dots + |x_d|^2 \right)^{1/2+s/4} \end{aligned}$$

is even and convex in  $x_1$ . It thus takes its absolute minimum at  $x_1 = 0$  and we have

$$\begin{aligned} |x - \mathbf{x}_N|^{1+s/2} + |x + \mathbf{x}_N|^{1+s/2} &\geq 2 \left( \frac{L_N}{2} \right)^{1+s/2} \left( 1 + \frac{4|x_2|^2}{L_N^2} + \dots + \frac{4|x_d|^2}{L_N^2} \right)^{1/2+s/4} \\ &\geq 2 \left( \frac{L_N}{2} \right)^{1+s/2} + 2 \left( |x_2|^{1+s/2} + \dots + |x_d|^{1+s/2} \right) \end{aligned}$$

and it follows that

$$\int_{\{|x| \leq CL_N\}} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx \leq CL_N e^{-2(1+\varepsilon)A\left(\frac{L_N}{2}\right)},$$

where we separate the integrals in  $x_2, \dots, x_d$ , which are all convergent. The prefactor  $L_N$  comes from the integral in  $x_1$  and can be absorbed in the exponential, changing slightly the value of  $\varepsilon$ , to obtain the upper bound in (3.13). For the lower bound we simply note that

$$\int_{\mathbb{R}^d} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx \geq \int_{\{|x| \leq L_N^\gamma\}} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx$$

for any  $\gamma$ . In particular, taking  $\gamma < 1$ , we have by a Taylor expansion

$$|x - \mathbf{x}_N|^{1+s/2} + |x + \mathbf{x}_N|^{1+s/2} = 2 \left( \frac{L_N}{2} \right)^{1+s/2} + O\left(L_N^{\gamma+s/2}\right) \leq 2 \left( \frac{L_N}{2} \right)^{1+s/2} (1 + o(1))$$

on the relevant integration domain, thus

$$\int_{\mathbb{R}^d} e^{-a|x-\mathbf{x}_N|^{1+s/2}-a|x+\mathbf{x}_N|^{1+s/2}} dx \geq e^{-2(1-\varepsilon)A\left(\frac{L_N}{2}\right)} L_N^{d\gamma}$$

and we can again absorb the last factor  $L_N^{d\gamma}$  in the exponential, changing slightly  $\varepsilon$ .

For the second estimate (3.14), we use the expression (2.4):

$$T_N = \int_{\mathbb{R}^d} u_{H-} V_t^+ u_{H+} = \int_{\mathbb{R}^d} u_{H-} (V_N - V_N^+) u_{H+} + \int_{\mathbb{R}^d} u_{H-} (\mu - \lambda w * |u_{H+}|^2) u_{H+}.$$

To get the bounds (3.14) one can estimate exactly as above, absorbing any polynomial growth coming from  $V_N - V_N^+$  into exponential factors. To prove that  $T_N < 0$ , a little more care is needed, and we use the full information contained in (3.3), namely that we know the rate of decay up to polynomial corrections.

Estimating as previously, keeping track of polynomial factors, we obtain, for any  $\varepsilon > 0$ ,

$$\begin{aligned} c_\varepsilon L_N^{1-2\alpha-\varepsilon} \exp\left(-2A\left(\frac{L_N}{2}\right)\right) &\leq \left| \int_{\mathbb{R}^d} u_{H-} (\mu - \lambda w * |u_{H+}|^2) u_{H+} \right| \\ &\leq C_\varepsilon L_N^{1-2\alpha+\varepsilon} \exp\left(-2A\left(\frac{L_N}{2}\right)\right) \end{aligned} \quad (3.16)$$

where  $\alpha$  is defined in (3.2). On the other hand, since  $V_N - V_N^+$  is negative by definition we have for any  $\gamma$

$$\int_{\mathbb{R}^d} u_{H-} (V_N - V_N^+) u_{H+} \leq \int_{\{|x| \leq L_N^\gamma\}} u_{H-} (V_N - V_N^+) u_{H+}.$$

Taking  $\gamma < 1$  we have, on the latter integration domain,

$$V_N - V_N^+ = 4s \mathbf{1}_{\{x_1 < 0\}} x_1 \left( \frac{L_N}{2} \right)^{s/2-1} (1 + o(1))$$

using a Taylor expansion. Putting this together with (3.3) and arguing as above we deduce that

$$\int_{\mathbb{R}^d} u_{H-} (V_N - V_N^+) u_{H+} \leq -C_\varepsilon L_N^{1+s/2-2\alpha-\varepsilon} \exp\left(-2A\left(\frac{L_N}{2}\right)\right).$$

Comparing with (3.16) we see that  $T_N < 0$  for  $N$  large enough as we claimed and one deduces the lower bound on  $|T_N|$ .  $\square$

*Remark 3.4* (Bounds on the off-site interaction energies).

One can show in a similar way that the off-site terms appearing in the interaction energy of the localized and delocalized states in Sec. 2.1,

$$\langle u_{H-} \otimes u_{H+}, w u_{H-} \otimes u_{H+} \rangle, \langle u_{H-}^{\otimes 2}, w u_{H+}^{\otimes 2} \rangle, \langle u_{H\pm}^{\otimes 2}, w u_{H-} \otimes u_{H+} \rangle$$

are of the order of  $\exp(-2(1-\varepsilon)A(L_N/2))$  in the limit  $L_N \rightarrow \infty$  (this follows immediately from (3.13) and  $\|w\|_\infty < \infty$  for the last two terms, and comes from the fact that  $w$  has compact support for the first term).  $\diamond$

**3.2. Hartree energy and minimizer in a perturbed well.** In the sequel, we shall be lead to consider a perturbation of the previous Hartree functional. This comes about when estimating tunneling effects in energy lower bounds. Essentially, we perturb the functional by a relatively small potential in a region far away from the bottom of the well, and we prove that this does not change much the Hartree energy and minimizer.

Consider

$$\mathcal{E}_{H,\delta_N}[u] = \int_{\mathbb{R}^d} \left( |\nabla u|^2 + V_{\delta_N}(x)|u|^2 + \frac{\lambda}{2}|u|^2 w * |u|^2 \right). \quad (3.17)$$

where the perturbed potential is of the form

$$V_{\delta_N}(x) = V(x)(1 - \delta_N(x)) \quad , \quad |\delta_N(x)| \leq \delta \mathbf{1}_{|x^1 - \frac{L_N}{2}| \leq \ell}(x) \quad (3.18)$$

for some constant  $\delta > 0$  independent of  $N$ . Here,  $x^1$  is the first coordinate of  $x$ , and we thus perturb the original potential in a strip of width  $\ell$  centered at a distance  $L_N/2$  from the origin. The choice of  $\ell$  will be discussed later, the point being that if  $\ell \ll L_N$  we do not perturb the problem much.

We denote by  $u_{H,\delta_N}$  and  $e_{H,\delta_N}$  respectively the unique positive minimizer and the minimum of the above functional. They satisfy properties very similar to those of the unperturbed analogues. In particular, one has the same estimates on  $u_{H,\delta_N}$  as in (3.11) in terms of the Agmon distance associated to the *unperturbed* potential  $V(r)$ :

**Lemma 3.5 (Pointwise estimates for the perturbed minimizer).**

For any  $0 < \varepsilon < 1$ , one can find some constant  $C_\varepsilon$ ,  $c_\varepsilon$ , and  $L_\varepsilon > 0$  such that for all  $L_N > L_\varepsilon$  and  $x \in \mathbb{R}^d$ ,

$$c_\varepsilon \exp(-(1+\varepsilon)A(|x|)) \leq u_{H,\delta_N}(x) \leq C_\varepsilon \exp(-(1-\varepsilon)A(|x|)) \quad (3.19)$$

*Proof.* One only needs minor modifications to the arguments in the proof of Proposition 3.1.  $\square$

We next prove that the difference between the trapping energies in the perturbed and unperturbed potentials  $V$  and  $V_{\delta_N}$ ,

$$\int_{\mathbb{R}^d} V_{\delta_N} |u_H|^2$$

is of the order of the tunneling energy to some power arbitrary close to one.

**Lemma 3.6 (Difference in the trapping energies).**

For any  $0 < \eta < 1$ , one can find some constant  $C_\eta$ ,  $c_\eta$ , and  $L_\eta > 0$  such that for all  $L_N > L_\eta$ ,

$$\int_{\mathbb{R}^d} V|\delta_N||u_H|^2 \leq C_\eta|T_N|^{1-\eta} \quad , \quad \int_{\mathbb{R}^d} V|\delta_N||u_{H,\delta_N}|^2 \leq C_\eta|T_N|^{1-\eta} . \quad (3.20)$$

*Proof.* Using (3.18), bounding  $V(r)$  by  $e^{\varepsilon A(r)}$  for large  $r$  and using the pointwise estimates (3.3), we have for large enough  $L_N$

$$\begin{aligned} \int_{\mathbb{R}^d} V|\delta_N|u_H^2 &\leq \delta \int_{\{|x^1 - \frac{L_N}{2}| \leq \ell\}} V|u_H|^2 \leq C_\varepsilon^2 \delta \int_{\{|x^1 - \frac{L_N}{2}| \leq \ell\}} \exp\left(-2(1-\varepsilon)A(|x|)\right) dx \\ &\leq 2C_\varepsilon^2 \delta \ell e^{-2(1-\varepsilon)A(L_N/2-\ell)} \int_{\mathbb{R}^{d-1}} \exp\left(-2(1-\varepsilon) \int_{\frac{L_N}{2}-\ell}^{((L_N/2-\ell)^2+|x^\perp|^2)^{1/2}} \sqrt{V(r)} dr\right) dx^\perp . \end{aligned}$$

Arguing similarly as in the proof of Proposition 3.3, the last integral can be bounded from above by a polynomial function of  $\frac{L_N}{2} - \ell$  and thus by  $e^{\varepsilon A(L_N/2)}$  for large enough  $L_N$ . We also have

$$A\left(\frac{L_N}{2}\right) - A\left(\frac{L_N}{2} - \ell\right) \leq \ell \sqrt{V\left(\frac{L_N}{2}\right)} \leq \frac{\varepsilon}{2(1-\varepsilon)} A\left(\frac{L_N}{2}\right) .$$

Collecting the above bounds and using the lower bound on the tunneling energy in (3.14), we get the desired result. One proceeds similarly for the proof of the second inequality in (3.20), by relying on Lemma 3.5.  $\square$

We can now prove the announced result that  $u_{H,\delta_N}$  is close to  $u_H$  for large  $L_N$ . We could probably prove stronger estimates, but we refrain from doing so for shortness.

**Proposition 3.7 (Difference between perturbed and unperturbed minimizers).**

For any  $\eta > 0$ , one can find constants  $C_\eta$ ,  $c_\eta$ , and  $L_\eta > 0$  such that if  $L_N \geq L_\eta$ , then

$$|e_H - e_{H,\delta_N}| \leq C_\eta|T_N|^{1-\eta} \quad (3.21)$$

and

$$\|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)} \leq C_\eta|T_N|^{1/2-\eta} . \quad (3.22)$$

*Proof.* We proceed in several steps:

**Step 1.** We clearly have

$$e_{H,\delta_N} = \mathcal{E}_{H,\delta_N}[u_{H,\delta_N}] = \mathcal{E}_H[u_{H,\delta_N}] + \int_{\mathbb{R}^d} V\delta_N|u_{H,\delta_N}|^2 \geq e_H - \int_{\mathbb{R}^d} V|\delta_N||u_{H,\delta_N}|^2$$

and similarly

$$e_H \geq e_{H,\delta_N} - \int_{\mathbb{R}^d} V|\delta_N||u_H|^2 .$$

The bound (3.21) follows from these inequalities and from Lemma 3.5. Thus  $e_{H,\delta_N} \rightarrow e_H$  when  $L_N \rightarrow \infty$ . Let  $e_{H,\delta_N}^\eta$  be the minimum of the energy functional (3.17) in which the potential  $V_{\delta_N}$  is replaced by a perturbed potential  $V_{\delta_N} + \eta W$ , where  $W \in L^\infty(\mathbb{R}^d)$  is a bounded potential. By the same argument as above,  $e_{H,\delta_N}^\eta$  converges to  $e_H$  when  $(L_N^{-1}, \eta) \rightarrow (0, 0)$ . But  $e_{H,\delta_N}^\eta$  is a concave function of  $\eta$  (as infimum of an affine functional), so we deduce that its derivative

with respect to  $\eta$  converges to the corresponding derivative for  $\delta_N = 0$  when  $L_N \rightarrow \infty$ . These derivatives are given by

$$\left. \frac{\partial e_{H,\delta_N}^\eta}{\partial \eta} \right|_{\eta=0} = \int_{\mathbb{R}^d} W |u_{H,\delta_N}|^2 \rightarrow \left. \frac{\partial e_H^\eta}{\partial \eta} \right|_{\eta=0} = \int_{\mathbb{R}^d} W |u_H|^2 .$$

This being so for any  $W \in L^\infty(\mathbb{R}^d)$ , we deduce that

$$|u_{H,\delta_N}|^2 \rightarrow |u_H|^2 \quad , \quad L_N \rightarrow \infty$$

in the  $L^\infty$  weak-\* topology. In particular, since by Assumption 1.1 the interaction potential  $w$  is bounded,

$$w * |u_{H,\delta_N}|^2(x) \rightarrow w * |u_H|^2(x) \quad (3.23)$$

for almost all  $x \in \mathbb{R}^d$ . Furthermore, by the dominated convergence theorem,

$$\int_{\mathbb{R}^d} |u_{H,\delta_N}|^2 w * |u_{H,\delta_N}|^2 = \int_{\mathbb{R}^d} \hat{w}(k) \left| \int_{\mathbb{R}^d} e^{ikx} |u_{H,\delta_N}|^2 \right|^2 \rightarrow \int_{\mathbb{R}^d} |u_H|^2 w * |u_H|^2 . \quad (3.24)$$

As a result, the chemical potentials  $\mu_{\delta_N}$  and  $\mu$  associated to  $u_{H,\delta_N}$  and  $u_H$ , respectively, satisfy (see (2.3))

$$\mu_{\delta_N} \rightarrow \mu \quad \text{when} \quad L_N \rightarrow \infty . \quad (3.25)$$

**Step 2.** The Hartree minimizer  $u_H$  is an eigenfunction with zero eigenvalue of the mean-field Hamiltonian

$$H_{\text{mf}} = -\Delta + V + \lambda w * |u_H|^2 - \mu .$$

Since it is positive,  $u_H$  must be in fact the ground state of this Hamiltonian, which is non degenerate. Similarly,  $u_{H,\delta_N}$  is the non-degenerate ground state of the perturbed Hamiltonian

$$H_{\text{mf},\delta_N} = -\Delta + V_{\delta_N} + \lambda w * |u_{H,\delta_N}|^2 - \mu_{\delta_N} .$$

By using Lemma 3.5 and (3.24), we have

$$\mu_{\delta_N} = \langle u_{H,\delta_N}, (H_{\text{mf},\delta_N} + \mu_{\delta_N}) u_{H,\delta_N} \rangle = \langle u_{H,\delta_N}, (H_{\text{mf}} + \mu) u_{H,\delta_N} \rangle + o(1)$$

and since  $H_{\text{mf}}$  has a non-degenerate ground state we deduce

$$\mu_{\delta_N} \geq \mu + c \|P^\perp u_{H,\delta_N}\|^2 + o(1) ,$$

where  $c > 0$  is the spectral gap of  $H_{\text{mf}}$  and  $P^\perp$  the orthogonal projector onto  $u_H$ . One concludes from this inequality and from (3.25) that

$$\|u_{H,\delta_N} - u_H\|_{L^2(\mathbb{R}^d)} \rightarrow 0 \quad \text{when} \quad L_N \rightarrow \infty . \quad (3.26)$$

**Step 3.** It follows from Assumption 1.1 on  $w$  that the Hessian of  $\mathcal{E}_H$  at  $u_H$  is non degenerate (see the related discussions in [35, Section 2]). Since we already know (3.26), for  $L_N$  sufficiently large so that  $\|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)}$  is small enough, one has

$$\mathcal{E}_H[u_{H,\delta_N}] \geq \mathcal{E}_H[u_H] + a \|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)}^2$$

for some fixed constant  $a > 0$ . Hence

$$\begin{aligned} e_{H,\delta_N} - \int_{\mathbb{R}^d} V \delta_N |u_{H,\delta_N}|^2 &= \mathcal{E}_H[u_{H,\delta_N}] \geq \mathcal{E}_H[u_H] - \int_{\mathbb{R}^d} V \delta_N |u_H|^2 + a \|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)}^2 \\ &\geq e_{H,\delta_N} - \int_{\mathbb{R}^d} V \delta_N |u_H|^2 + a \|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)}^2 . \end{aligned}$$

Hence, one infers from Lemma 3.6 that for any  $0 < \eta < 1$  and  $L_N$  large enough,

$$\|u_H - u_{H,\delta_N}\|_{L^2(\mathbb{R}^d)}^2 \leq a^{-1} \int_{\mathbb{R}^d} V \delta_N (|u_H|^2 - |u_{H,\delta_N}|^2) \leq 2a^{-1} C_\eta T_N^{1-2\eta}$$

which is the desired result.  $\square$

#### 4. ELEMENTS OF BOGOLIUBOV THEORY

Here we recall elements of Bogoliubov's theory that are needed in the rest of the paper, following mainly [35, 42]. See also [9, 15, 50, 22, 52] for other recent discussions.

**4.1. Bogoliubov Hamiltonian.** For clarity we first recall how the Bogoliubov Hamiltonian is constructed.

*Second quantized formalism.* Bogoliubov's approximation for the spectrum of a large bosonic system is usually described in a grand-canonical setting where the particle number is not fixed. This means that the Hamiltonian (1.1) is extended to the Fock space

$$\mathcal{F} = \mathcal{F}(\mathfrak{H}) := \mathbb{C} \oplus \mathfrak{H} \oplus \mathfrak{H}^2 \oplus \dots \oplus \mathfrak{H}^N \oplus \dots \quad (4.1)$$

in the usual way

$$\mathbb{H} = 0 \oplus H_1 \oplus H_2 \oplus \dots \oplus H_N \oplus \dots \quad (4.2)$$

with (note the value of the coupling constant)

$$H_M = \sum_{j=1}^M (-\Delta_j + V(x_j)) + \frac{\lambda}{N-1} \sum_{1 \leq i < j \leq M} w(x_i - x_j).$$

It is convenient to express this Hamiltonian by using standard bosonic annihilation and creation operators. We denote by  $u_i$ ,  $i = 0, 1, \dots$ , the vectors of an orthonormal basis of  $\mathfrak{H} = L^2(\mathbb{R}^d)$  with  $u_0 = u_H$  the Hartree ground state corresponding to  $H_N$ , i.e. the minimizer of the functional (1.4). Let  $a_i^* = a^*(u_i)$  and  $a_i = a_i(u_i)$  be respectively the annihilation and creation operators in the mode  $u_i$ , defined by

$$\begin{aligned} (a_i^* \Psi)(x_1, \dots, x_{M+1}) &= (u_i \otimes_{\text{sym}} \Psi)(x_1, \dots, x_{M+1}) \in \mathfrak{H}^{M+1} \\ (a_i \Psi)(x_1, \dots, x_{M-1}) &= \sqrt{M} \int_{\mathbb{R}^d} \bar{u}_i(x) \Psi(x, x_1, \dots, x_{M-1}) dx \in \mathfrak{H}^{M-1} \end{aligned} \quad (4.3)$$

for any  $\Psi \in \mathfrak{H}^M$ , where the symmetrized tensor product is defined in (2.10). Then we have

$$\mathbb{H} - \mu \sum_{i=0}^{\infty} a_i^* a_i = \sum_{i,j=0}^{\infty} (h_{ij} - \delta_{ij} \mu) a_i^* a_j + \frac{\lambda}{2(N-1)} \sum_{i,j,k,l=0}^{\infty} w_{ijkl} a_i^* a_j^* a_k a_l \quad (4.4)$$

with  $\delta_{ij} = 1$  if  $i = j$  and 0 otherwise and

$$\begin{aligned} h_{ij} &= \langle u_i | -\Delta + V | u_j \rangle \\ w_{ijkl} &= \langle u_i \otimes u_j | w | u_k \otimes u_l \rangle = w_{jilk} = \overline{w_{klji}}. \end{aligned}$$

*Bogoliubov's Hamiltonian.* Bogoliubov's approximation consists in replacing  $a_0^*$  and  $a_0$  by  $\sqrt{N}$  in the expression in the right-hand side of (4.4) and then dropping all terms that are more than quadratic in the operators  $a_i^*, a_i$ ,  $i = 1, 2, \dots$ . As explained in [35], this amounts to second-quantizing the Hessian at  $u_H$  of the Hartree functional (1.4). Non-degeneracy of this Hessian is required and the assumption  $\hat{w} \geq 0$  is a convenient way of ensuring this.

Removing a constant (coming from terms involving only  $a_0^*, a_0$ ) one ends up with the quadratic Hamiltonian

$$\mathbb{H}^B := \sum_{i,j=1}^{\infty} (h_{ij} - \mu \delta_{ij}) a_i^* a_j + \frac{\lambda}{2} \sum_{i,j=1}^{\infty} \left( w_{00ij} a_i a_j + \overline{w}_{00ij} a_i^* a_j^* + 2(w_{0i0j} + w_{0ij0}) a_i^* a_j \right). \quad (4.5)$$

Here, we have used the variational equation satisfied by  $u_H$ ,

$$(-\Delta + V)u_H + \lambda(w * |u_H|^2)u_H = \mu u_H, \quad (4.6)$$

to discard the linear terms in  $a_i^*$  and  $a_i$  and we have neglected terms of the order of  $1/\sqrt{N}$ .

The above Hamiltonian acts on the Fock space of elementary excitations, namely the Fock space

$$\mathcal{F}_{\perp} = \mathcal{F}(\mathfrak{H}_{\perp}) := \mathbb{C} \oplus \mathfrak{H}_{\perp} \oplus \dots \oplus (\mathfrak{H}_{\perp})^N \oplus \dots$$

associated to the Hilbert space

$$\mathfrak{H}_{\perp} = \{u_H\}^{\perp}. \quad (4.7)$$

We denote by  $e_B$  the lowest eigenvalue of  $\mathbb{H}^B$  and write the associated eigenstate as

$$\Phi^B = \phi_0^B \oplus \phi_1^B \oplus \dots \oplus \phi_n^B \oplus \dots \quad (4.8)$$

with  $\phi_n^B \in (\mathfrak{H}_{\perp})^n$ . It is well-known that  $\Phi^B$  is a quasi-free state, i.e., is entirely characterized via Wick's theorem in terms of its generalized one-body density matrix. Given a state  $\Gamma$  on  $\mathfrak{H}_{\perp}^N$ , the latter is an operator combining the usual one-body density matrix

$$\langle u, \gamma_{\Gamma}^{(1)} v \rangle = \text{Tr}[a^*(v)a(u)\Gamma]$$

with the pairing density matrix defined by

$$\langle u, \alpha_{\Gamma} J v \rangle = \text{Tr}[a(v)a(u)\Gamma],$$

where  $J$  is the complex conjugation and  $u, v$  are arbitrary vectors in  $\mathfrak{H}$ . Note that  $\gamma_{\Gamma}^{(1)}$  is a (self-adjoint) non-negative operator on  $\mathfrak{H}_{\perp}$ , whereas  $\alpha_{\Gamma}$  should be interpreted as an operator from  $J\mathfrak{H}_{\perp}$  to  $\mathfrak{H}_{\perp}$  satisfying  $\alpha_{\Gamma}^* = J\alpha_{\Gamma}J$ .

*Remark 4.1* (Bogoliubov's energy at small coupling).

One can show that

$$-C\lambda^2 \leq e_B \leq 0 \quad (4.9)$$

for some  $\lambda$ -independent constant  $C > 0$ . The upper bound follows by simply taking the vacuum as a trial state. A sketch of the proof of the lower bound is given in Appendix A. Hence the Bogoliubov energy  $e_B$  goes rapidly to 0 when  $\lambda \rightarrow 0$  and may be safely dropped when  $\lambda$  is small.  $\diamond$



**4.2. Useful results.** The proofs of our main results rely heavily on recent results of [22, 35, 50] on the Bogoliubov fluctuations in the case of a single well potential  $V_N \equiv V$ . We summarize them here, and give for completeness some elements of proof in Appendix A.

In this paper, the main application of Bogoliubov's theory will be to provide a control of quantum fluctuations out of the condensate. As in [35], we write any  $N$ -body wave function  $\Psi_N \in \mathfrak{H}^N$  as

$$\Psi_N = \sum_{j=0}^N u_{\text{H}}^{\otimes(N-j)} \otimes_{\text{sym}} \varphi_j \quad (4.10)$$

with  $\varphi_j \in (\mathfrak{H}_{\perp})^j$ . The convention here is that  $\varphi_0$  is simply a number. Then one can define the unitary map

$$U_N : \Psi_N \mapsto \varphi_0 \oplus \dots \oplus \varphi_N \quad (4.11)$$

which sends  $\mathfrak{H}^N$  to the truncated Fock space  $\mathcal{F}_{\perp}^{\leq N}$ . Let  $H_N$  be the  $N$ -body Hamiltonian (1.1) with a potential  $V_N \equiv V$  independent of  $N$ . We denote by

$$\mathbb{H}_N := U_N (H_N - N e_{\text{H}}(\lambda)) U_N^* \quad (4.12)$$

the corresponding Hamiltonian on  $\mathcal{F}_{\perp}^{\leq N}$  after subtraction of the mean field contribution. The following results show that  $\mathbb{H}_N$  is closely related to the Bogoliubov Hamiltonian (4.5) in the limit  $N \rightarrow \infty$ . We denote by  $d\Gamma(h^{\perp})$  the second quantization of the one-body Hamiltonian  $h^{\perp} = P^{\perp}(-\Delta + V)P^{\perp}$  acting on  $\mathfrak{H}_{\perp}$ , where  $P^{\perp}$  is the orthogonal projector onto  $\{u_{\text{H}}\}^{\perp}$ . Let

$$\mathcal{N}^{\perp} = \mathcal{N} - a^*(u_{\text{H}})a(u_{\text{H}})$$

be the particle number operator in  $\mathfrak{H}_{\perp}$ , with  $\mathcal{N}$  the total particle number operator.

**Proposition 4.2 (Control of fluctuations out of the condensate).**

Let  $e_{\text{B}} < 0$  be the lowest eigenvalue of  $\mathbb{H}^{\text{B}}$ . For  $N$  large enough, there is a constant  $C > 0$  such that, as operators on  $\mathcal{F}_{\perp}^{\leq N}$ ,

$$\mathbb{H}_N \geq C \left( d\Gamma(h^{\perp}) - C \right) \quad (4.13)$$

and

$$\mathbb{H}_N \geq e_{\text{B}} + N^{-1}(\mathcal{N}^{\perp})^2 - CN^{-2/5}. \quad (4.14)$$

A lower bound on the first eigenvalue  $E_N$  of  $H_N$  follows easily from (4.12) and (4.14). A matching upper bound can be obtained by using a trial state:

**Proposition 4.3 (Upper bound for the single-well many-body energy).**

Let  $E_N$  be the ground state energy of (1.1) with  $V_N \equiv V$  and consider the  $N$ -body wave function

$$\Psi_N := c_M \sum_{j=0}^M u_{\text{H}}^{\otimes(N-j)} \otimes_{\text{sym}} \phi_j^{\text{B}},$$

where  $\phi_j^{\text{B}}$  is the component in  $(\mathfrak{H}_{\perp})^j$  of the ground state of  $\mathbb{H}^{\text{B}}$  (cf. (4.8)),  $c_M$  a normalization constant, and  $M \propto N^{1/5}$  when  $N \rightarrow \infty$ . Then for any  $\varepsilon > 0$ , there is a constant  $C_{\varepsilon} > 0$  such that

$$E_N \leq \langle \Psi_N | H_N | \Psi_N \rangle \leq N e_{\text{H}} + e_{\text{B}} + C_{\varepsilon} N^{-2/5+\varepsilon}. \quad (4.15)$$

We conclude this section with a mild decay estimate for the Bogoliubov ground state.

**Lemma 4.4 (Decay of the Bogoliubov ground state).**

Let  $\Phi^B$  be the ground state of  $\mathbb{H}^B$  on  $\mathcal{F}_\perp$ . Then  $\gamma_{\Phi^B}^{(1)}$  is trace-class and  $\alpha_{\Phi^B}$  is Hilbert-Schmidt. Let  $\rho_{\Phi^B}(x) = \gamma_{\Phi^B}^{(1)}(x, x)$  be the one-body density of  $\Phi^B$ . Then there is a constant  $C > 0$  such that

$$\int_{\mathbb{R}^d} V \rho_{\Phi^B} \leq C. \quad (4.16)$$

Note that, according to the first statement, the mean number of particles which are not condensed,

$$\text{Tr} [\gamma_{\Phi^B}^{(1)}] = \int_{\mathbb{R}^d} \rho_{\Phi^B}(x) dx = \sum_{j=1}^{\infty} j \|\phi_j^B\|^2,$$

is finite in the limit  $N \rightarrow \infty$ .

A sketch of the proofs of the last three results, following mostly [35], is provided in Appendix A for the convenience of the reader.

**5. ENERGY UPPER BOUND**

To prove the energy upper bound in the localized regime we use a trial state where exactly half of the particles is localized in each well:

$$\Psi_{\text{loc}} := \Psi'_- \otimes \Psi'_+ \quad , \quad \Psi'_-, \Psi'_+ \in \mathfrak{H}^{N/2}, \quad (5.1)$$

where the states  $\Psi'_-$  and  $\Psi'_+$  describe Bose condensates with  $N' = N/2$  particles localized in the  $V_N^-$  and  $V_N^+$  wells, respectively, together with their Bogoliubov fluctuations. We define them as follows: let

$$H_{N'} := \sum_{j=1}^{N'} (-\Delta_j + V(x_j)) + \frac{\lambda'}{N' - 1} \sum_{1 \leq i < j \leq N'} w(x_i - x_j)$$

be the Hamiltonian associated to  $N' = N/2$  particles in the single-well potential  $V$  with a renormalized  $N$ -dependent coupling constant  $\lambda'$  such that

$$\frac{\lambda'}{N' - 1} = \frac{\lambda}{N - 1},$$

and let

$$\mathcal{E}_H^{\lambda'}[u] = \int_{\mathbb{R}^d} (|\nabla u|^2 + V|u|^2 + \frac{\lambda'}{2}|u|^2 w * |u|^2)$$

be the corresponding energy functional. We denote by  $u_H^{\lambda'}$  the minimizer of  $\mathcal{E}_H^{\lambda'}[u]$  with unit  $L^2$ -norm and by

$$\Phi^{B, \lambda'} = \phi_0^{B, \lambda'} \oplus \dots \oplus \phi_j^{B, \lambda'} \oplus \dots \in \mathcal{F}(\{u_H^{\lambda'}\}^\perp)$$

the ground state of the Bogoliubov Hamiltonian obtained from  $H_{N'}$  by the procedure described in the previous section. We then define, as in Proposition 4.3, the normalized wave-function

$$\Psi' := c_{N'} \sum_{j=0}^M (u_H^{\lambda'})^{\otimes (N'-j)} \otimes_{\text{sym}} \phi_j^{B, \lambda'} \in \mathfrak{H}^{N'} \quad (5.2)$$

with  $M \propto N^{1/5}$  and  $c_{N'}$  a normalization factor. Then, let

$$\Psi'_- := \Psi'(\cdot - \mathbf{x}_N) \quad , \quad \Psi'_+ = \Psi'(\cdot + \mathbf{x}_N) \quad (5.3)$$

where the translation by  $\pm \mathbf{x}_N$  is understood to act on each of the coordinate vectors  $x_j$ ,  $j = 1, \dots, N'$ , in the argument of the function. Similarly, we denote by  $\Phi_-^{B, \lambda'}$  and  $\Phi_+^{B, \lambda'}$  the translates of the Bogoliubov ground state  $\Phi^{B, \lambda'}$ .

We shall prove the following, which gives the desired energy upper bound on the ground state energy  $E(N)$  of the  $N$ -body Hamiltonian (1.1) in the double well:

**Proposition 5.1 (Energy of the localized state).**

Let  $\Psi_{\text{loc}}$  be the trial state defined in (5.1). In the localized regime (1.13) we have

$$\frac{E(N)}{N} \leq N^{-1} \langle \Psi_{\text{loc}} | H_N | \Psi_{\text{loc}} \rangle \leq e_H \left( \Delta_N \frac{\lambda}{2} \right) + \frac{2}{N} e_B \left( \frac{\lambda}{2} \right) + o(|T_N|) + o(N^{-1}) \quad (5.4)$$

where  $\Delta_N$  and  $T_N$  are given by (2.20) and (2.1).

*Proof.* Note that (5.1) is not fully symmetric under particle exchange, only  $\Psi'_-$  and  $\Psi'_+$  are. We thus start with:

**Step 1: (5.1) is an admissible trial state.** It is well-known (see e.g. [36, Section 3.2]) that the ground state energy of the  $N$ -body Hamiltonian (1.1) acting on the unsymmetrized Hilbert space  $\mathfrak{H}^{\otimes N}$  coincides with the bosonic ground state energy  $E(N)$ . Note that  $\Psi_{\text{loc}}$  is normalized since  $\Psi'_-$  and  $\Psi'_+$  are. Hence (5.1) is an admissible trial state for computing an upper bound on  $E(N)$  and the first inequality holds. There remains to evaluate the energy of  $\Psi_{\text{loc}}$ .

**Step 2: main terms.** To compute the energy we recall that (2.6)-(2.7) hold with a non-symmetrized state  $\Psi \in \mathfrak{H}^{\otimes N}$  provided we take as definitions (compare with (2.8))

$$\gamma_{\Psi}^{(1)} = \sum_{j=1}^N \text{Tr}_{\bar{j}} [|\Psi\rangle\langle\Psi|] \quad , \quad \gamma_{\Psi}^{(2)} = \sum_{1 \leq j < k \leq N} \text{Tr}_{\{j,k\}} [|\Psi\rangle\langle\Psi|] \quad ,$$

where  $\text{Tr}_{\bar{j}}$  (respectively  $\text{Tr}_{\{j,k\}}$ ) stands for the partial trace with respect to all particles but the  $j$ -th (respectively all particles but the  $j$ -th and the  $k$ -th). Another advantage of the unsymmetrized trial state (5.1), apart from the fact that it is normalized when  $\Psi'_{\pm}$  are normalized, is that one can easily compute its one- and two-body density matrices using these definitions: we easily find

$$\gamma_{\Psi_{\text{loc}}}^{(1)} = \gamma_{\Psi'_-}^{(1)} + \gamma_{\Psi'_+}^{(1)} \quad , \quad \gamma_{\Psi_{\text{loc}}}^{(2)} = \gamma_{\Psi'_-}^{(2)} + \gamma_{\Psi'_+}^{(2)} + \gamma_{\Psi'_-}^{(1)} \otimes \gamma_{\Psi'_+}^{(1)} \quad .$$

We insert this in (2.6) and use  $V_N \leq V_N^{\pm}$  to obtain

$$\begin{aligned} \langle \Psi_{\text{loc}} | H_N | \Psi_{\text{loc}} \rangle &\leq \text{Tr} \left[ (-\Delta + V_N^-) \gamma_{\Psi'_-}^{(1)} \right] + \frac{\lambda}{2(N-1)} \text{Tr} \left[ w \gamma_{\Psi'_-}^{(2)} \right] \\ &\quad + \text{Tr} \left[ (-\Delta + V_N^+) \gamma_{\Psi'_+}^{(1)} \right] + \frac{\lambda}{2(N-1)} \text{Tr} \left[ w \gamma_{\Psi'_+}^{(2)} \right] \\ &\quad + \frac{\lambda}{2(N-1)} \text{Tr} \left[ w \gamma_{\Psi'_-}^{(1)} \otimes \gamma_{\Psi'_+}^{(1)} \right] \quad . \end{aligned} \quad (5.5)$$

The first two lines are identical and are estimated as follows

$$\begin{aligned} \text{Tr} \left[ (-\Delta + V_N^{\pm}) \gamma_{\Psi'_{\pm}}^{(1)} \right] + \frac{\lambda}{2(N-1)} \text{Tr} \left[ w \gamma_{\Psi'_{\pm}}^{(2)} \right] &= \text{Tr} \left[ (-\Delta + V) \gamma_{\Psi'}^{(1)} \right] + \frac{\lambda'}{2(N'-1)} \text{Tr} \left[ w \gamma_{\Psi'}^{(2)} \right] \\ &= \langle \Psi' | H_{N'} | \Psi' \rangle \\ &\leq N' e_H(\lambda') + e_B(\lambda') + o(1) \quad , \end{aligned}$$

where the last inequality follows from Proposition 4.3. The last expression gives the desired upper bound in (5.4), because

$$\lambda' = \frac{\Delta_N \lambda}{2} = \frac{\lambda}{2} + O(N^{-1})$$

and the discrepancy between  $e_B(\lambda')$  and  $e_B(\lambda/2)$  can be easily included in the  $o(1)$  term (it is in fact of order  $N^{-1}$ , as follows from considerations similar to those discussed in Appendix A). Hence there only remains to estimate the error term on the third line of (5.5), which describes interactions between the particles in the left well with those in the right well.

**Step 3: bound on the interactions between particles in different wells.** Let

$$P'_\pm = |u_{H\pm}^{\lambda'}\rangle\langle u_{H\pm}^{\lambda'}| \quad \text{and} \quad Q'_\pm = 1 - P'_\pm$$

be the orthogonal projectors onto the span of  $u_{H\pm}^{\lambda'} = u_H^{\lambda'}(\mp \mathbf{x}_N)$  and its orthogonal, respectively. It follows from the definition of  $\Psi_-$  that

$$P'_- \gamma_{\Psi_-}^{(1)} P'_- = \left( \frac{N}{2} - \text{Tr} \left[ \gamma_{\Phi_-^{B,\lambda'}}^{(1)} \right] \right) P'_- \quad , \quad Q'_- \gamma_{\Psi_-}^{(1)} Q'_- = \gamma_{\Phi_-^{B,\lambda'}}^{(1)} .$$

Note that, strictly speaking, we only get in the one- and two-body density matrices of  $\Psi_-$  the contribution from  $\Phi_-^{B,\lambda'}$  living on  $j$ -particle sectors with  $j \leq M$ . Using Wick's theorem, one can easily see that  $\|\phi_j^{B,\lambda'}\|^2$  decays very rapidly with  $j$ , and the contribution from the rest thus yields a very small remainder, that we ignore (see similar considerations in Equation (A.3) below). It is in fact sufficient at this stage to notice that

$$P'_- \gamma_{\Psi_-}^{(1)} P'_- \leq C N P'_- \quad , \quad Q'_- \gamma_{\Psi_-}^{(1)} Q'_- \leq C \gamma_{\Phi_-^{B,\lambda'}}^{(1)} \quad (5.6)$$

for some constant  $C > 0$ . Since  $\gamma_{\Psi_-}^{(1)}$  is a positive self-adjoint operator we have that, as operators,

$$P'_- \gamma_{\Psi_-}^{(1)} Q'_- + Q'_- \gamma_{\Psi_-}^{(1)} P'_- \leq P'_- \gamma_{\Psi_-}^{(1)} P'_- + Q'_- \gamma_{\Psi_-}^{(1)} Q'_- . \quad (5.7)$$

Similar formulas holds for  $\gamma_{\Psi_+}^{(1)}$ . Writing

$$\text{Tr} \left[ w \gamma_{\Psi_-}^{(1)} \otimes \gamma_{\Psi_+}^{(1)} \right] = \text{Tr} \left[ w (P'_- + Q'_-) \gamma_{\Psi_-}^{(1)} (P'_- + Q'_-) \otimes (P'_+ + Q'_+) \gamma_{\Psi_+}^{(1)} (P'_+ + Q'_+) \right] ,$$

expanding, inserting (5.6) and (5.7), we thus get the bound

$$\begin{aligned} \text{Tr} \left[ w \gamma_{\Psi_-}^{(1)} \otimes_s \gamma_{\Psi_+}^{(1)} \right] &\leq 4C^2 N^2 \text{Tr} \left[ w P'_- \otimes P'_+ \right] + 8C^2 N \text{Tr} \left[ w P'_- \otimes \gamma_{\Phi_+^{B,\lambda'}}^{(1)} \right] \\ &\quad + 4C^2 \text{Tr} \left[ w \gamma_{\Phi_-^{B,\lambda'}}^{(1)} \otimes \gamma_{\Phi_+^{B,\lambda'}}^{(1)} \right] , \end{aligned} \quad (5.8)$$

where we use that objects in the  $V_N^-$  well are the images of those in the  $V_N^+$  well under the mirror symmetry  $(x^1, x^2, \dots, x^N) \mapsto (-x^1, x^2, \dots, x^N)$  to group some terms. Since  $w$  is bounded and  $\gamma_{\Phi_-^{B,\lambda'}}^{(1)}, \gamma_{\Phi_+^{B,\lambda'}}^{(1)}$  are trace-class, the last term is of order one. Recalling that this must be divided by  $N - 1$  to get the contribution to the energy, this is much smaller than the level of precision we aim at.

For the other two terms we use Lemma 3.2: for any trace-class operator  $\gamma$  on  $\mathfrak{H}$  and any  $0 < \eta < 1$ , we have

$$\begin{aligned} \text{Tr} [w P'_- \otimes \gamma] &= \iint_{\mathbb{R}^d \times \mathbb{R}^d} |u_{\text{H}-}^{\lambda'}(x)|^2 w(x-y) \gamma(y, y) dx dy \\ &\leq C_\eta \int_{\mathbb{R}^d} |u_{\text{H}-}^{\lambda'}(y)|^{2-\eta} \gamma(y, y) dy \end{aligned}$$

where we identify  $\gamma$  and its kernel. In particular, for the first term of the right-hand side of (5.8), we obtain

$$\text{Tr} [w P'_- \otimes P'_+] \leq C_\eta \int_{\mathbb{R}^d} |u_{\text{H}-}^{\lambda'}(x)|^{2-\eta} |u_{\text{H}+}^{\lambda'}(x)|^2 dx .$$

Then we recall that  $u_{\text{H}\pm}^{\lambda'} = u_{\text{H}}^{\lambda'}(\cdot \mp \mathbf{x}_N)$ . Using the decay estimate (3.3) we have

$$u_{\text{H}-}^{1-\eta}(x) u_{\text{H}+}(x) \leq C_\varepsilon^2 \exp \left( -2(1-\varepsilon)(A(|x - \mathbf{x}_N|) + A(|x + \mathbf{x}_N|)) \right) .$$

By the same argument as in the proof of (3.13) and by using (1.13), we conclude that

$$N^2 \text{Tr} [w P'_- \otimes P'_+] \leq C'_\varepsilon N^2 e^{-4(1-\varepsilon)A(L_N/2)} \ll 1$$

as desired. Finally, for the second term in the right-hand side of (5.8) we write

$$\begin{aligned} \text{Tr} \left[ w P'_- \otimes \gamma_{\Phi_+^{\text{B}, \lambda'}}^{(1)} \right] &\leq C_\eta \int_{\mathbb{R}^d} |u_{\text{H}-}^{\lambda'}(x)|^{2-\eta} \rho_{\Phi_+^{\text{B}, \lambda'}}(x) dx \\ &\leq C_\eta \int_{\mathbb{R}^d} \frac{|u_{\text{H}-}^{\lambda'}|^{2-\eta}}{1 + V_N^+} (1 + V_N^+) \rho_{\Phi_+^{\text{B}, \lambda'}} \\ &\leq C_\eta \sup_{\mathbb{R}^d} \frac{|u_{\text{H}-}^{\lambda'}|^{2-\eta}}{1 + V_N^+} \int_{\mathbb{R}^d} (1 + V_N^+) \rho_{\Phi_+^{\text{B}, \lambda'}} . \end{aligned}$$

Then, using the decay estimate (3.3) again and the fact that  $V(r) \rightarrow \infty$  as  $r \rightarrow \infty$ , we easily see that

$$\sup_{\mathbb{R}^d} \frac{|u_{\text{H}-}^{\lambda'}|^{2-\eta}}{1 + V_N^+} \rightarrow 0 \text{ when } N \rightarrow \infty$$

whereas Lemma 4.4 ensures that

$$\int_{\mathbb{R}^d} (1 + V_N^+) \rho_{\Phi_+^{\text{B}, \lambda'}} \leq C$$

uniformly in  $N$ . We thus have

$$N \text{Tr} [w P'_- \otimes \gamma_{\Phi_+^{\text{B}}}^{(1)}] \ll N$$

in the limit  $N \rightarrow \infty$ , which concludes the proof since this term gets divided by  $N - 1$  in the energy expansion (5.5).  $\square$

## 6. ENERGY LOWER BOUND AND LOCALIZATION ESTIMATE

In this section, we prove the lower bound corresponding to (5.5) by a suitable localization procedure. The fluctuations of the number of particles in each well will be estimated in the course of the proof. We first split in Sec. 6.1 the many-body Hamiltonian into two parts corresponding to the left and right wells. For the state of the system we follow the procedure of localization in Fock space presented in [32] (see also [49, Section 5]) to obtain a lower bound in Sec. 6.2 in terms of all the possible ways of distributing the particles in the two wells.

**6.1. Geometric localization procedure.** Let us first introduce two smooth localization functions,  $\chi_-$  and  $\chi_+$ , such that

$$\chi_+^2 + \chi_-^2 = 1$$

and

$$\begin{aligned} \text{supp}(\chi_-) &\subset \left\{ x \in \mathbb{R}^d \mid x^1 \leq \ell \right\} \\ \text{supp}(\chi_+) &\subset \left\{ x \in \mathbb{R}^d \mid x^1 \geq -\ell \right\}, \end{aligned}$$

where  $\ell$  is a localization length satisfying  $1 \ll \ell \ll L_N$ . Clearly, one can assume that

$$\chi_+(x^1, x^2, \dots, x^d) = \chi_-(-x^1, x^2, \dots, x^d) \quad , \quad |\nabla \chi_-| + |\nabla \chi_+| \leq C\ell^{-1} \mathbf{1}_{\{|x^1| \leq \ell\}}$$

for any  $(x^1, \dots, x^d) \in \mathbb{R}^d$ . Next, we define some cut-off functions  $\eta_{\pm}$  along the  $x^1$ -direction satisfying

$$\eta_-(x) = \begin{cases} 0 & \text{for } x^1 \leq 0 \\ 1 & \text{for } 0 \leq x^1 \leq \ell \\ 0 & \text{for } x^1 \geq 2\ell. \end{cases} \quad , \quad \eta_+(x) = \begin{cases} 0 & \text{for } x^1 \geq 0 \\ 1 & \text{for } -\ell \leq x^1 \leq 0 \\ 0 & \text{for } x^1 \leq -2\ell \end{cases}$$

and we consider the two modified potentials

$$\begin{aligned} \tilde{V}_N^+ &= V_N^+ + (V_N^- - V_N^+) \eta_+ - |\nabla \chi_-|^2 - |\nabla \chi_+|^2 \\ \tilde{V}_N^- &= V_N^- + (V_N^+ - V_N^-) \eta_- - |\nabla \chi_-|^2 - |\nabla \chi_+|^2. \end{aligned} \quad (6.1)$$

Modulo a small perturbation in the strip  $\{x \in \mathbb{R}^d \mid -2\ell \leq x^1 \leq 2\ell\}$ , these two potentials mimic the left and right potentials  $V_N^{\pm}$ . More precisely,

$$0 \leq \delta_N^{\pm} := \frac{V_N^{\pm} - \tilde{V}_N^{\pm}}{V_N^{\pm}} \leq \|\delta_N^{\pm}\|_{\infty} \mathbf{1}_{-2\ell \leq x^1 \leq 2\ell} \quad (6.2)$$

and it is easy to show that  $\|\delta_N^{\pm}\|_{\infty} \rightarrow 0$  as  $L_N \rightarrow \infty$  when  $V(x) = |x|^s$ . We have the simple lemma

**Lemma 6.1 (Localizing the Hamiltonian).**

Let  $\tilde{H}_1^{\pm}$  be the one-body Hamiltonian with the modified potential (6.1),

$$\tilde{H}_1^{\pm} := -\Delta + \tilde{V}_N^{\pm}.$$

For any  $\Psi \in \mathfrak{H}^N$ , one has

$$\langle \Psi | H_N | \Psi \rangle \geq \sum_{s=\pm} \left( \text{Tr}_{\mathfrak{H}} \left[ \tilde{H}_1^s \chi_s \gamma_{\Psi}^{(1)} \chi_s \right] + \frac{\lambda}{2(N-1)} \text{Tr}_{\mathfrak{H}^2} \left[ w \chi_s^{\otimes 2} \gamma_{\Psi}^{(2)} \chi_s^{\otimes 2} \right] \right). \quad (6.3)$$

*Proof.* We split the one-body Hamiltonian using the IMS formula [10, Theorem 3.2]

$$-\Delta = \chi_-(-\Delta)\chi_- + \chi_+(-\Delta)\chi_+ - |\nabla\chi_-|^2 - |\nabla\chi_+|^2.$$

Using also  $\chi_+^2 + \chi_-^2 = 1$  and

$$V_N(x) = V_N^\pm(x) + (V_N^\mp - V_N^\pm)(x)\eta_\pm(x) \text{ if } x \in \text{supp}(\chi_\pm),$$

this yields

$$-\Delta + V_N = \chi_- \tilde{H}_1^- \chi_- + \chi_+ \tilde{H}_1^+ \chi_+. \quad (6.4)$$

As for the two-body part we note that since  $w \geq 0$  we have, for all  $\Psi \in \mathfrak{H}^2$ ,

$$\begin{aligned} \langle \Psi, w\Psi \rangle &= \iint (\chi_+^2(x) + \chi_-^2(x)) (\chi_+^2(y) + \chi_-^2(y)) w(x-y) |\Psi(x,y)|^2 dx dy \\ &\geq \iint \chi_-^2(x) \chi_-^2(y) w(x-y) |\Psi(x,y)|^2 dx dy + \iint \chi_+^2(x) \chi_+^2(y) w(x-y) |\Psi(x,y)|^2 dx dy \end{aligned}$$

and thus, as an operator on the two-body space,

$$w \geq \chi_-^{\otimes 2} w \chi_-^{\otimes 2} + \chi_+^{\otimes 2} w \chi_+^{\otimes 2}. \quad (6.5)$$

Inserting this into the expressions (2.7) of the energies and using the cyclicity of the trace, we get (6.3).  $\square$

Now we want to see the localized density matrices  $\chi_\pm^{\otimes 2} \gamma_\Psi^{(2)} \chi_\pm^{\otimes 2}$  as the reduced density matrices of two states living on the Fock spaces  $\mathcal{F}(\chi_\pm \mathfrak{H})$ . This is a well-known procedure, recalled in [32, Section 3] and [47, 49, Chapter 5]. It is used repeatedly in [33, 34]. To any  $N$ -body state  $\Gamma = |\Psi\rangle\langle\Psi|$  (this applies to mixed states also) we associate some localized states  $G^-$  and  $G^+$  in the Fock space  $\mathcal{F}(\mathfrak{H}) = \mathbb{C} \oplus \mathfrak{H} \oplus \mathfrak{H}^2 \oplus \dots$ , of the form

$$G^\pm = G_0^\pm \oplus G_1^\pm \oplus \dots \oplus G_N^\pm \oplus 0 \oplus \dots, \quad (6.6)$$

with the crucial property that their reduced density matrices satisfy (here we use the convention  $\text{Tr}_{n+1 \rightarrow n}[G_n^\pm] = G_n^\pm$ )

$$\chi_\pm^{\otimes n} \gamma_\Psi^{(n)} \chi_\pm^{\otimes n} = (G^\pm)^{(n)} := \sum_{k=n}^N \frac{k!}{(k-n)!} \text{Tr}_{n+1 \rightarrow k} [G_k^\pm], \quad (6.7)$$

where for any  $1 \leq n \leq N$ ,  $\gamma_\Psi^{(n)}$  is the  $n$ -body reduced density matrix of  $\Psi \in \mathfrak{H}^N$  normalized as in (2.8) and  $\gamma_\Psi^{(0)} = \chi_\pm^{\otimes 0} = 1$ .

The relations (6.7) determine the localized states  $G^\pm$  uniquely and they ensure that  $G^-$  and  $G^+$  are (mixed) states on the Fock spaces  $\mathcal{F}(\chi_- \mathfrak{H})$  and  $\mathcal{F}(\chi_+ \mathfrak{H})$ , respectively:

$$\sum_{k=0}^N \text{Tr} [G_k^-] = \sum_{k=0}^N \text{Tr} [G_k^+] = 1. \quad (6.8)$$

An important property is that

$$\text{Tr}_{\mathfrak{H}^k} [G_k^-] = \text{Tr}_{\mathfrak{H}^{N-k}} [G_{N-k}^+] \text{ for all } k = 0, \dots, N, \quad (6.9)$$

that is, the probability of having  $k$  particles  $\chi_-$ -localized is equal to the probability of having  $N - k$  particles  $\chi_+$ -localized.

Let us now anticipate a little bit on the forthcoming energy lower bounds. Using the previous constructions, they will be expressed in terms of all the possible ways of distributing  $n$  particles in one well and  $N - n$  particles in the other well. The energy of such a configuration will be bounded from below by applying the expansion of Proposition 4.3, leading to an approximate value in terms of  $R(n)$  and  $R(N - n)$  where

$$R(n) := ne_H \left( \lambda \frac{n-1}{N-1} \right) + e_B \left( \lambda \frac{n-1}{N-1} \right) \quad (6.10)$$

is (to subleading order) the energy of  $n$  particles in one well. The key estimate allowing to conclude the proof is contained in Proposition B.1, see Appendix B, which confirms that it is more favorable to distribute the particles evenly between the two wells.

**6.2. Lower bound and corollaries.** We now complete the proof of the energy estimate in Theorem 2.1:

**Step 1: splitting the energy.** Let us define the  $n$ -body Hamiltonians

$$\begin{aligned} \tilde{H}_n^\pm &:= \sum_{j=1}^n \left( -\Delta_j + \tilde{V}_N^\pm(x_j) \right) + \frac{\lambda}{N-1} \sum_{1 \leq i < j \leq n} w(x_i - x_j) \\ H_n^\pm &:= \sum_{j=1}^n \left( -\Delta_j + V_N^\pm(x_j) \right) + \frac{\lambda}{N-1} \sum_{1 \leq i < j \leq n} w(x_i - x_j) . \end{aligned} \quad (6.11)$$

Combining (6.3) and (6.7) we obtain the lower bound

$$\langle \Psi | H_N | \Psi \rangle \geq \sum_{n=1}^N \text{Tr}_{\mathfrak{H}^n} \left[ \tilde{H}_n^+ G_n^+ + \tilde{H}_n^- G_n^- \right] . \quad (6.12)$$

The rationale in the following is to apply a mean-field approximation in each term of the sum in the right-hand side of (6.12) and to approximate the Hartree energies for the perturbed Hamiltonians  $\tilde{H}_n^\pm$  by those of the unperturbed ones  $H_n^\pm$ , relying on the considerations of Section 3.2.

**Step 2: mean-field approximation and a-priori bound.** We first perform a mean-field approximation in each term of the sum in the right-hand side of (6.12). We regard the operators  $\tilde{H}_n^\pm$  as  $n$ -body Hamiltonians in mean-field scaling with effective  $n$ -dependent coupling constant

$$\lambda_n = \lambda \frac{n-1}{N-1} .$$

Let  $\tilde{u}_{H^\pm}^{\lambda_n}$  be the (unique) minimizer with unit  $L^2$ -norm of the energy functionals  $\tilde{\mathcal{E}}_{H^\pm}^{\lambda_n}[u]$  obtained by replacing  $V$  by the perturbed potentials  $\tilde{V}_N^\pm$  and  $\lambda$  by  $\lambda_n$  in (1.4), and let  $\tilde{e}_H(\lambda_n)$  be the corresponding Hartree energy (recall that these energies are the same for the left and right potentials wells because  $\tilde{V}_N^-$  and  $\tilde{V}_N^+$  are related to each other by the mirror symmetry  $(x^1, x^\perp) \mapsto (-x^1, x^\perp)$ ). For  $n = 1$ ,  $\lambda_n = 0$  and  $\tilde{u}_{H^\pm}^0$  and  $\tilde{e}_H(0) = \inf \{ \text{spec}(\tilde{h}_\pm) \}$  denote respectively the ground state and lowest eigenvalue of the one-body Hamiltonian  $\tilde{h}_\pm = -\Delta + \tilde{V}_N^\pm$ . Applying Proposition 4.2 to the functionals  $\tilde{\mathcal{E}}_{H^\pm}^{\lambda_n}[u]$  and recalling (4.12), we may bound from below each term in the sum of (6.12) by

$$(n\tilde{e}_H(\lambda_n) - C^2) (\text{Tr}[G_n^+] + \text{Tr}[G_n^-]) + C \left\langle d\Gamma(\tilde{h}_+^\perp) \right\rangle_{G_n^+} + C \left\langle d\Gamma(\tilde{h}_-^\perp) \right\rangle_{G_n^-} ,$$



where

$$\left\langle d\Gamma(\tilde{h}_{\pm}^{\perp}) \right\rangle_{G_n^{\pm}} := \text{Tr}_{\mathfrak{H}^n} \left[ d\Gamma(\tilde{h}_{\pm}^{\perp}) G_n^{\pm} \right],$$

$d\Gamma(\tilde{h}_{\pm}^{\perp})$  being the second quantized operator corresponding to the one-body Hamiltonian

$$\tilde{h}_{\pm}^{\perp} := \tilde{P}_{\pm}^{\perp} \left( -\Delta + \tilde{V}_N^{\pm} \right) \tilde{P}_{\pm}^{\perp}$$

with  $\tilde{P}_{\pm}^{\perp}$  the orthogonal projector onto  $\{\tilde{u}_{H_{\pm}}^{\lambda_n}\}^{\perp}$ . In view of (6.2), one can apply Proposition 3.7 to the perturbed potentials  $\tilde{V}_N^{\pm}$  to conclude that  $\tilde{e}_H(\lambda_n)$  is very close to the Hartree energies  $e_H(\lambda_n)$  for the unperturbed potentials  $V_N^{\pm}$ , with errors of the order of  $|T_N|^{1-\eta}$ . Hence, using also (6.8) and (6.9), we obtain from (6.12)

$$\begin{aligned} \langle \Psi | H_N | \Psi \rangle &\geq \sum_{n=0}^N \left( n e_H(\lambda_n) + (N-n) e_H(\lambda_{N-n}) \right) \text{Tr}[G_n^+] \\ &\quad + C \sum_{n=1}^N \left( \left\langle d\Gamma(\tilde{h}_{+}^{\perp}) \right\rangle_{G_n^+} + \left\langle d\Gamma(\tilde{h}_{-}^{\perp}) \right\rangle_{G_n^-} \right) - C^2 + O(N|T_N|^{1-\eta}) \end{aligned} \quad (6.13)$$

for any  $0 < \eta < 1$ . By Proposition 3.3,  $|T_N|^{1-\eta} \ll C_{\eta}^{1-\eta} e^{-2(1-2\eta)A(L_N/2)}$ , so that  $N|T_N|^{1-\eta}$  converges to zero in the limit (1.13). Thus the term  $O(N|T_N|^{1-\eta})$  can be absorbed in the constant  $C^2$ .

The quantity inside the parenthesis in the first line of (6.13) gives for large  $n$  and  $(N-n)$  the ground state energy when one distributes  $n$  particles in the left potential well  $V_N^-$  and  $(N-n)$  particles in the right potential well  $V_N^+$ , the two wells being infinitely far apart (so that particles in different wells do not interact). It is shown in Appendix B that it is more favorable to distribute the particles evenly between the two wells: We have for any  $n = 0, \dots, N$ ,

$$n e_H(\lambda_n) + (N-n) e_H(\lambda_{N-n}) \geq N e_H \left( \lambda_{\frac{N}{2}} \right) = N e_H \left( \Delta_N \frac{\lambda}{2} \right)$$

with  $\Delta_N$  given by (2.20). Thus, using (6.8) again,

$$\langle \Psi | H_N | \Psi \rangle \geq N e_H \left( \Delta_N \frac{\lambda}{2} \right) + C \sum_{n=1}^N \left( \left\langle d\Gamma(\tilde{h}_{+}^{\perp}) \right\rangle_{G_n^+} + \left\langle d\Gamma(\tilde{h}_{-}^{\perp}) \right\rangle_{G_n^-} \right) - C'. \quad (6.14)$$

Choosing  $\Psi$  to be the ground state of  $H_N$  and combining with the energy upper bound of Proposition 5.1, we obtain the leading term of the large  $N$  expansion of  $E_N$ ,

$$E_N = N e_H \left( \Delta_N \frac{\lambda}{2} \right) + O(1),$$

together with the following a priori bound that will be used below in the estimate of the next-to-leading order terms:

$$0 \leq \sum_{n=1}^N \left\langle d\Gamma(\tilde{h}_{+}^{\perp}) \right\rangle_{G_n^+} + \sum_{n=1}^N \left\langle d\Gamma(\tilde{h}_{-}^{\perp}) \right\rangle_{G_n^-} \leq C''. \quad (6.15)$$

**Step 3: error made by removing the tildes in the lower bound (6.12).** We now use the a priori bound (6.15) to show that one can replace  $\tilde{H}_n^{\pm}$  by  $H_n^{\pm}$  in (6.12), making a small error.

We first notice that according to (6.7) and (6.11),

$$\sum_{n=1}^N \text{Tr} \left[ (H_n^+ - \tilde{H}_n^+) G_n^+ \right] = \text{Tr}_{\mathfrak{H}} \left[ \delta_N^+ V_N^+ (G^+)^{(1)} \right] ,$$

where  $\delta_N^+$  is defined in (6.2). Projecting onto the subspace generated by  $\tilde{u}_{H^+}$  and its orthogonal, the last trace can be expressed as a sum of three terms,

$$\text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+ \delta_N^+ V_N^+ \tilde{P}_+ (G^+)^{(1)} \right] + 2\text{Re} \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+ \delta_N^+ V_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] + \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+^\perp \delta_N^+ V_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] .$$

Since

$$0 \leq (G^+)^{(1)} = \chi_+ \gamma_\Psi^{(1)} \chi_+ \leq \text{Tr} \left[ \chi_+ \gamma_\Psi^{(1)} \chi_+ \right]$$

and  $\text{Tr} \gamma_\Psi^{(1)} = N$ , the first term is bounded for any  $0 < \eta < 1$  by

$$0 \leq \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+ \delta_N^+ V_N^+ \tilde{P}_+ (G^+)^{(1)} \right] \leq N \int_{\{|x^1| \leq 2\ell\}} |\tilde{u}_{H^+}|^2 \delta_N^+ V_N^+ = O(N|T_N|^{1-\eta})$$

by virtue of Lemma 3.6. Thus this term converges to zero in the limit (1.13). One deals with the third term by using the identity

$$0 \leq \delta_N^+ V_N^+ = \tilde{\delta}_N^+ \tilde{V}_N^+ \quad \text{with} \quad \tilde{\delta}_N^+ = \frac{\delta_N^+}{1 - \delta_N^+} .$$

This gives

$$\begin{aligned} 0 \leq \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+^\perp \delta_N^+ V_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] &\leq \|\tilde{\delta}_N^+\|_\infty \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+^\perp \tilde{V}_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] \\ &\leq \|\tilde{\delta}_N^+\|_\infty \text{Tr}_{\mathfrak{H}} \left[ \tilde{h}_+^\perp (G^+)^{(1)} \right] \\ &= \|\tilde{\delta}_N^+\|_\infty \sum_{n=1}^N \left\langle d\Gamma(\tilde{h}_+^\perp) \right\rangle_{G_n^+} , \end{aligned}$$

where we used  $-\Delta \geq 0$  in the second inequality. Since  $\|\delta_N^+\|_\infty \rightarrow 0$  this term converges to zero too, thanks to the a priori bound (6.15). Finally, the second term can be treated similarly because the Cauchy-Schwarz inequality gives

$$\left| \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+ \delta_N^+ V_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] \right|^2 \leq \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+ \delta_N^+ V_N^+ \tilde{P}_+ (G^+)^{(1)} \right] \text{Tr}_{\mathfrak{H}} \left[ \tilde{P}_+^\perp \delta_N^+ V_N^+ \tilde{P}_+^\perp (G^+)^{(1)} \right] .$$

Hence

$$\sum_{n=1}^N \text{Tr} \left[ (H_n^+ - \tilde{H}_n^+) G_n^+ \right] = o(1) .$$

The proof for  $H_n^-$  and  $\tilde{H}_n^-$  is the same.

**Step 4: mean-field approximation for the localized energies.** Since we have shown that we can discard the discrepancy between the original and perturbed functionals, the energy lower bound (6.12) yields:

$$\langle \Psi | H_N | \Psi \rangle \geq \sum_{n=1}^N \text{Tr}_{\mathfrak{H}^n} \left[ H_n^+ G_n^+ + H_n^- G_n^- \right] + o(1) . \quad (6.16)$$

We can now apply to each of the  $n$ -body Hamiltonians  $H_n^\pm$  the bound (4.14) of Proposition 4.2, which includes the corrections to the Hartree energies given by Bogoliubov's theory. We denote by

$$\mathcal{N}_-^\perp := \mathcal{N} - a^*(u_{H-}^{\lambda_n})a(u_{H-}^{\lambda_n}) \quad , \quad \mathcal{N}_+^\perp := \mathcal{N} - a^*(u_{H+}^{\lambda_n})a(u_{H+}^{\lambda_n}) \quad (6.17)$$

the operators counting the number of particles orthogonal to  $u_{H-}^{\lambda_n}$  and  $u_{H+}^{\lambda_n}$ , respectively, with  $\mathcal{N}$  the total particle number operator. Thus we get

$$\begin{aligned} \langle \Psi | H_N | \Psi \rangle &\geq \sum_{n=1}^N \left( n e_H(\lambda_n) + e_B(\lambda_n) - C n^{-2/5} \right) \left( \text{Tr}[G_n^+] + \text{Tr}[G_n^-] \right) \\ &\quad + \sum_{n=1}^N \frac{1}{n} \left( \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} + \left\langle \left( \mathcal{N}_+^\perp \right)^2 \right\rangle_{G_n^+} \right) + o(1) , \end{aligned}$$

where  $e_H(0) = \inf\{\text{spec}(-\Delta + V_N)\}$  and  $e_B(0) = 0$  in the term  $n = 1$ . We next use as before the relation (6.9) to reduce this to

$$\begin{aligned} \langle \Psi | H_N | \Psi \rangle &\geq \sum_{n=0}^N \left( E_{n,N-n}^{\text{loc}} - C \left( n^{-2/5} \mathbf{1}_{\{n>0\}} + (N-n)^{-2/5} \mathbf{1}_{\{n<N\}} \right) \right) \text{Tr}[G_n^+] \\ &\quad + \sum_{n=1}^N \frac{1}{n} \left( \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} + \left\langle \left( \mathcal{N}_+^\perp \right)^2 \right\rangle_{G_n^+} \right) + o(1) , \end{aligned}$$

where

$$E_{n,N-n}^{\text{loc}} = n e_H(\lambda_n) + e_B(\lambda_n) + (N-n) e_H(\lambda_{N-n}) + e_B(\lambda_{N-n}) \quad (6.18)$$

is the ground state energy up to  $o(1)$  in the case of infinitely far apart wells with  $n$  particles in the left well and  $(N-n)$  particles in the right well (here we set  $e_B(\lambda_n) := 0$  for  $n = 0$ ). As before, the energy is minimized by choosing the same number  $n = N/2$  of particles in each well. More precisely, one has (see Proposition B.1 in Appendix B)

$$E_{n,N-n}^{\text{loc}} \geq E_{\frac{N}{2}, \frac{N}{2}}^{\text{loc}} + \frac{C}{N} \left( n - \frac{N}{2} \right)^2 , \quad (6.19)$$

so that by (6.8),

$$\begin{aligned} \langle \Psi | H_N | \Psi \rangle &\geq E_{\frac{N}{2}, \frac{N}{2}}^{\text{loc}} + \frac{C}{N} \sum_{n=0}^N \left( \left( n - \frac{N}{2} \right)^2 - N n^{-2/5} \mathbf{1}_{\{n>0\}} - N (N-n)^{-2/5} \mathbf{1}_{\{n<N\}} \right) \text{Tr}[G_n^+] \\ &\quad + \sum_{n=1}^N \frac{1}{n} \left( \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} + \left\langle \left( \mathcal{N}_+^\perp \right)^2 \right\rangle_{G_n^+} \right) + o(1) . \end{aligned}$$

Going back to (6.18) and using  $e_B(\lambda_{N/2}) = e_B(\lambda/2) + o(1)$ , we see that the term  $E_{\frac{N}{2}, \frac{N}{2}}^{\text{loc}}$  yields the desired first two terms in (2.19). To complete the energy lower bound, it thus suffices to notice that, for  $N$  large enough and any  $n = 0, \dots, N$

$$\left( n - \frac{N}{2} \right)^2 - N n^{-2/5} \mathbf{1}_{\{n>0\}} - N (N-n)^{-2/5} \mathbf{1}_{\{n<N\}} \geq \frac{1}{2} \left( n - \frac{N}{2} \right)^2 - c N^{3/5}$$

for some  $c > 0$ , so that

$$\begin{aligned} \langle \Psi | H_N | \Psi \rangle &\geq N e_H \left( \Delta_N \frac{\lambda}{2} \right) + 2e_B \left( \frac{\lambda}{2} \right) + o(1) \\ &\quad + \frac{C}{2N} \sum_{n=1}^N \left( n - \frac{N}{2} \right)^2 \text{Tr}[G_n^+] + \sum_{n=1}^N \frac{1}{n} \left( \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} + \left\langle \left( \mathcal{N}_+^\perp \right)^2 \right\rangle_{G_n^+} \right). \end{aligned} \quad (6.20)$$

The energy lower bound follows by discarding the terms on the last line, which are positive. Choosing  $\Psi$  in (6.20) to be the ground state of  $H_N$  and combining with the energy upper bound proved in Proposition 5.1, we get as by-products

$$\sum_{n=1}^N \left( n - \frac{N}{2} \right)^2 \text{Tr}[G_n^+] \ll N \quad (6.21)$$

and, since  $n \leq N$ ,

$$\sum_{n=1}^N \left( \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} + \left\langle \left( \mathcal{N}_+^\perp \right)^2 \right\rangle_{G_n^+} \right) \ll N. \quad (6.22)$$

These estimates provide the control of particle number fluctuations announced in Theorem 2.1, as we discuss next.

**6.3. Control of fluctuations.** We now conclude the proof of (2.21), using the estimates (6.21) and (6.22). The two terms in the right-hand side of (2.21) are estimated similarly, let us discuss only one of them. Let us set

$$\begin{aligned} \mathcal{N}_- &= a^*(u_{H-}) a(u_{H-}) \\ \mathcal{N}_{\chi_-} &= a^*(\chi_- u_{H-}) a(\chi_- u_{H-}). \end{aligned}$$

From (2.9) and the definition (6.7) of the localized state  $G^-$ , we have

$$\left\langle a^*(\chi_- u)^n a(\chi_- v)^n \right\rangle_{\Psi_N} = (n!)^{-1} \left\langle v^{\otimes n}, (G_-)^{(n)} u^{\otimes n} \right\rangle = \left\langle a^*(u)^n a(v)^n \right\rangle_{G^-}$$

for any  $n = 1, \dots, N$  and  $u, v \in \mathfrak{H}$ , so that

$$\left\langle \left( \mathcal{N}_{\chi_-} - \frac{N}{2} \right)^2 \right\rangle_{\Psi_N} = \left\langle \left( \mathcal{N}_- - \frac{N}{2} \right)^2 \right\rangle_{G^-} + \left( \|\chi_- u_{H-}\|_{L^2(\mathbb{R}^d)}^2 - 1 \right) \left\langle \mathcal{N}_- \right\rangle_{G^-}.$$

By (6.17), the operator inequality  $(A + B)^2 \leq 2A^2 + 2B^2$ , and  $\int \chi_-^2 |u_{H-}|^2 \leq 1$ , it follows that

$$\left\langle \left( \mathcal{N}_{\chi_-} - \frac{N}{2} \right)^2 \right\rangle_{\Psi_N} \leq 2 \left\langle \left( \mathcal{N}_- - \frac{N}{2} \right)^2 \right\rangle_{G^-} + 2 \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G^-}.$$

Recalling the decomposition (6.6) and using (6.21) and (6.22) this gives

$$\begin{aligned} \left\langle \left( \mathcal{N}_{\chi_-} - \frac{N}{2} \right)^2 \right\rangle_{\Psi_N} &\leq 2 \sum_{n=1}^N \left( n - \frac{N}{2} \right)^2 \text{Tr}[G_n^-] + 2 \sum_{n=1}^N \left\langle \left( \mathcal{N}_-^\perp \right)^2 \right\rangle_{G_n^-} \\ &\ll N. \end{aligned} \quad (6.23)$$

To conclude the proof of (2.21), there only remains to remove the cut-offs function  $\chi_-$ . To this end we prove the following simple lemma

**Lemma 6.2 (Removing cut-offs functions).**

For any  $N$ -body bosonic state  $\Gamma_N$ , one can find a constant  $C > 0$  such that

$$\left| \langle \mathcal{N}_- \rangle_{\Gamma_N} - \langle \mathcal{N}_{\chi_-} \rangle_{\Gamma_N} \right| \leq CN \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2 \quad (6.24)$$

and

$$\left| \langle \mathcal{N}_-^2 \rangle_{\Gamma_N} - \langle \mathcal{N}_{\chi_-}^2 \rangle_{\Gamma_N} \right| \leq CN^2 \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2. \quad (6.25)$$

*Proof.* We denote

$$\begin{aligned} \mathcal{O}_1 &= |u_{H-}\rangle \langle u_{H-}| - |\chi_- u_{H-}\rangle \langle \chi_- u_{H-}| \\ \mathcal{O}_2 &= (|u_{H-}\rangle \langle u_{H-}|)^{\otimes 2} - (|\chi_- u_{H-}\rangle \langle \chi_- u_{H-}|)^{\otimes 2}. \end{aligned}$$

Clearly it suffices to prove that

$$\left| \text{Tr} [\mathcal{O}_1 \gamma_{\Gamma_N}^{(1)}] \right| \leq CN \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2, \quad \left| \text{Tr} [\mathcal{O}_2 \gamma_{\Gamma_N}^{(2)}] \right| \leq CN^2 \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2,$$

where  $\gamma_{\Gamma_N}^{(1)}$  and  $\gamma_{\Gamma_N}^{(2)}$  are respectively the one- and two-body density matrices of  $\Gamma_N$ , see (2.9). But

$$\left| \text{Tr} [\mathcal{O}_1 \gamma_{\Gamma_N}^{(1)}] \right| \leq \text{Tr} [\gamma_{\Gamma_N}^{(1)}] \|\mathcal{O}_1\|_{\mathfrak{S}^\infty}$$

and

$$\left| \text{Tr} [\mathcal{O}_2 \gamma_{\Gamma_N}^{(2)}] \right| \leq \text{Tr} [\gamma_{\Gamma_N}^{(2)}] \|\mathcal{O}_2\|_{\mathfrak{S}^\infty} \leq 2 \text{Tr} [\gamma_{\Gamma_N}^{(2)}] \|\mathcal{O}_1\|_{\mathfrak{S}^\infty},$$

where  $\mathfrak{S}^\infty$  is the set of compact operators, equipped with the operator norm. Since  $\gamma_{\Gamma_N}^{(1)}$  and  $\gamma_{\Gamma_N}^{(2)}$  have by definition traces  $N$  and  $N(N-1)$ , it suffices to prove that

$$\|\mathcal{O}_1\|_{\mathfrak{S}^\infty} \leq C \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2.$$

But, as a rank-two operator on  $\text{span}\{u_{H-}, \chi_- u_{H-}\}$ ,  $\mathcal{O}_1$  has matrix elements

$$\begin{aligned} \langle u_{H-}, \mathcal{O}_1 u_{H-} \rangle &= 1 - \left( \int_{\mathbb{R}^d} \chi_- |u_{H-}|^2 \right)^2 \\ \langle u_{H-}, \mathcal{O}_1 \chi_- u_{H-} \rangle &= \int_{\mathbb{R}^d} \chi_- |u_{H-}|^2 \left( 1 - \int_{\mathbb{R}^d} \chi_-^2 |u_{H-}|^2 \right) \\ \langle \chi_- u_{H-}, \mathcal{O}_1 \chi_- u_{H-} \rangle &= \left( \int_{\mathbb{R}^d} \chi_- |u_{H-}|^2 \right)^2 - \left( \int_{\mathbb{R}^d} \chi_-^2 |u_{H-}|^2 \right)^2 \end{aligned}$$

and it is straightforward to see that these are all bounded in absolute value by  $C \int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2$ . Hence, so must be the absolute values of the eigenvalues of  $\mathcal{O}$  and we deduce the result.  $\square$

The final result (2.21) follows from (6.23) and the above lemma, recalling that in the regime of our interest we have

$$\int_{\mathbb{R}^d} \chi_+^2 |u_{H-}|^2 \leq \int_{\{x^1 \geq \frac{L_N}{2} - \ell\}} |u_H|^2(x) = O(|T_N|) \ll N^{-1}, \quad (6.26)$$

as follows from the choice of the cut-off functions and the decay estimates established in Section 3.1.

## APPENDIX A. FLUCTUATIONS OUT OF A BOSE-EINSTEIN CONDENSATE

Let us quickly explain how Proposition 4.2 follows from the arguments of [35]. To this end, we let  $f$  and  $g$  be two smooth truncation functions from  $\mathbb{R}^+$  to  $\mathbb{R}^+$ , satisfying

$$f^2 + g^2 = 1$$

and

$$f(x) = 0 \text{ for } x \geq 1, \quad g(x) = 0 \text{ for } x \leq 1/2.$$

Then, define the operators

$$f_M := f\left(\mathcal{N}^\perp/M\right), \quad g_M := g\left(\mathcal{N}^\perp/M\right) \quad (\text{A.1})$$

on  $\mathcal{F}(\mathfrak{H}_\perp)$ , where  $\mathcal{N}^\perp$  is the number operator

$$\mathcal{N}^\perp := \bigoplus_{j=1}^{\infty} j \mathbb{1}_{(\mathfrak{H}_\perp)^j}.$$

Let us denote by  $\text{d}\Gamma(h^\perp)$  the second quantization of  $h^\perp = P^\perp(-\Delta + V)P^\perp$ , acting on  $\mathcal{F}(\mathfrak{H}_\perp)$ :

$$\text{d}\Gamma(h^\perp) := \bigoplus_{k=0}^{\infty} \sum_{j=0}^k h_j^\perp.$$

Recall that  $\text{d}\Gamma(1)$ , the second quantization of the identity on  $\mathfrak{H}_\perp$ , is just  $\mathcal{N}^\perp$ . We argue as follows:

*Proof of Proposition 4.2.* We first pick some  $M \leq N$ , to be optimized over later, and apply [35, Lemma 6.3] to obtain

$$\mathbb{H}_N \geq f_M \mathbb{H}_N f_M + g_M \mathbb{H}_N g_M - \frac{C}{M^2} \left( \text{d}\Gamma(h^\perp) + C \right),$$

where we also apply the main results of the same paper to show that the first eigenvalue of  $\mathbb{H}_N$  is bounded by a constant (actually, for large  $N$  it converges to the Bogoliubov ground state energy). Next, using [35, Proposition 5.1] to estimate the first term, which lives on the smaller space  $\mathcal{F}^{\leq M}(\mathfrak{H}_\perp)$ , we get

$$\mathbb{H}_N \geq \left( 1 - C\sqrt{\frac{M}{N}} \right) f_M \mathbb{H}^B f_M + g_M \mathbb{H}_N g_M - \frac{C}{M^2} \left( \text{d}\Gamma(h^\perp) + C \right).$$

Next, under our assumption that  $w \geq 0$  we have

$$\mathbb{H}_N \geq \text{d}\Gamma(h^\perp) \geq C\mathcal{N}^\perp$$

and (see [35, Theorem 2.1])

$$\mathbb{H}^B \geq C\text{d}\Gamma(h^\perp + 1) - C. \quad (\text{A.2})$$

Since  $f_M$  and  $g_M$  commute with  $d\Gamma(h^\perp + 1)$  (the latter conserves the particle number), we may borrow a little part of the main terms to control the error in the above:

$$\begin{aligned} \mathbb{H}_N \geq \left(1 - C\sqrt{\frac{M}{N}} - C'M^{-2}\right) f_M \mathbb{H}^B f_M + (1 - C'M^{-2}) g_M d\Gamma(h^\perp) g_M \\ + \frac{C' - C}{M^2} d\Gamma(h^\perp + 1) - \frac{C}{M^2}. \end{aligned}$$

Taking  $C'$  large enough to make the first error term positive, and recalling that  $h^\perp \geq C > 0$  we arrive at

$$\mathbb{H}_N \geq \left(1 - C\sqrt{\frac{M}{N}} - \frac{C}{M^2}\right) f_M \mathbb{H}^B f_M + C \left(1 - \frac{1}{M^2}\right) g_M d\Gamma(h^\perp) g_M - \frac{C}{M^2}.$$

Next we make the choice  $M = N^{1/5}$  to optimize error terms:

$$\mathbb{H}_N \geq \left(1 - CN^{-2/5}\right) f_M \mathbb{H}^B f_M + C \left(1 - N^{-2/5}\right) g_M d\Gamma(h^\perp) g_M - CN^{-2/5}.$$

To obtain the first inequality in Proposition 4.2 we may stop at this stage, inserting (A.2) and using the fact that  $f_M$  and  $g_M$  commute with  $d\Gamma(h^\perp)$ .

We carry on with the proof of (4.14). Since  $e_B$  is bounded and  $g_M$  localizes on particle numbers larger than  $M/2 \gg e_B$ , we clearly have

$$f_M \mathbb{H}^B f_M + g_M d\Gamma(h^\perp) g_M \geq f_M \mathbb{H}^B f_M + C g_M \mathcal{N}^\perp g_M \geq f_M e_B f_M + C \frac{M}{e_B} g_M e_B g_M.$$

Then we may write, on  $\mathcal{F}^{\leq N}(\mathfrak{H}_\perp)$ ,

$$\mathbb{H}_N \geq e_B + N^{-2/5} f_M^2 \mathcal{N}^\perp + C g_M^2 \mathcal{N}^\perp - CN^{-2/5}.$$

Inserting the simple bounds

$$f_M^2 \mathcal{N}^\perp \leq M f_M^2, \quad g_M^2 \mathcal{N}^\perp \leq N g_M^2$$

we get

$$\begin{aligned} \mathbb{H}_N &\geq e_B + N^{-3/5} f_M^2 \left(\mathcal{N}^\perp\right)^2 + CN^{-1} g_M^2 \left(\mathcal{N}^\perp\right)^2 - CN^{-2/5} \\ &\geq e_B + N^{-1} \left(\mathcal{N}^\perp\right)^2 - CN^{-2/5} \end{aligned}$$

which is the desired final result.  $\square$

Now, let us sketch the

*Proof of Proposition 4.3.* This is again implicitly contained in [35]. Using (4.12) we have

$$\langle \Psi_N | H_N | \Psi_N \rangle = c_M \left( N e_H + \langle \Phi_B^M, \mathbb{H}_N \Phi_B^M \rangle \right)$$

where  $\Phi_B^M$  is the projection of the Bogoliubov ground state onto sectors with less than  $M$  particles. Using [35, Proposition 5.1] we obtain

$$\langle \Phi_B^M, \mathbb{H}_N \Phi_B^M \rangle = \langle \Phi_B^M, \mathbb{H}^B \Phi_B^M \rangle + O\left(\sqrt{\frac{M}{N}}\right).$$

Applying then [35, Lemma 6.2] we easily get

$$\langle \Phi_B^M, \mathbb{H}_N \Phi_B^M \rangle = \langle \Phi_B, \mathbb{H}^B \Phi_B \rangle + O(M^{-2}) + O\left(\sqrt{\frac{M}{N}}\right).$$

With  $M \propto N^{1/5}$  this gives

$$\langle \Psi_N | H_N | \Psi_N \rangle = c_M \left( N e_H + e_B + O(N^{-2/5}) \right)$$

and it remains to estimate  $c_M$ . Since this constant normalizes  $\Psi_N$  in  $\mathfrak{H}^N$  and  $\Phi^B$  is a state we have

$$c_M^{-2} = \sum_{j=0}^M \|\phi_j^B\|^2 = 1 - \sum_{j=M}^{\infty} \|\phi_j^B\|^2.$$

But, for any  $\delta > 0$ ,

$$\begin{aligned} \sum_{j=M}^{\infty} \|\phi_j^B\|^2 &\leq \left( \sum_{j=M}^{\infty} j^{-\delta} \|\phi_j^B\|^2 \right)^{1/2} \left( \sum_{j=M}^{\infty} j^{\delta} \|\phi_j^B\|^2 \right)^{1/2} \\ &\leq M^{-\delta/2} \left\langle (\mathcal{N}^\perp)^\delta \right\rangle_{\Phi^B}^{1/2} \leq C_\delta M^{-\delta/2} \end{aligned} \quad (\text{A.3})$$

where we use that  $\left\langle (\mathcal{N}^\perp)^\delta \right\rangle_{\Phi^B}$  is finite for any  $\delta$ . This follows easily from the fact that  $\Phi^B$  is quasi-free, using Wick's theorem. Hence (again with  $M \propto N^{1/5}$ )

$$c_M = 1 + O(N^{-\delta/2})$$

for any  $\delta > 0$ , which completes the proof.  $\square$

Next we turn to the

*Proof of Lemma 4.4.* It follows very closely arguments from [35, Appendix A] and [42]. Details are provided for the convenience of the reader. From the expression (4.5) one can see that the Bogoliubov energy functional can be written as

$$\mathcal{E}_B[\Gamma] := \text{Tr}_{\mathcal{F}_\perp} [\mathbb{H}^B \Gamma] = \text{Tr} \left[ (H_{\text{mf}} - \mu + \lambda K) \gamma_\Gamma^{(1)} \right] + \lambda \text{Re Tr}[K \alpha_\Gamma], \quad (\text{A.4})$$

where

$$H_{\text{mf}} = -\Delta + V + \lambda w * |u_H|^2$$

is the mean-field Hamiltonian and  $K$  the operator on  $\mathfrak{H} = L^2(\mathbb{R}^d)$  whose kernel is given by

$$K(x, y) = u_H(x) w(x - y) u_H(y). \quad (\text{A.5})$$

Note that

$$\langle \psi, K \psi \rangle = \iint_{\mathbb{R}^d \times \mathbb{R}^d} \overline{\psi(x)} u_H(x) w(x - y) u_H(y) \psi(y) dx dy = \int_{\mathbb{R}^d} \hat{w}(k) |\widehat{\psi u_H}(k)|^2 dk,$$

so it follows from our assumption  $\hat{w} \geq 0$  that  $K$  is a positive operator. Since  $w$  is bounded,  $K$  is also trace-class.



The Bogoliubov minimizer  $\Phi^B$  is the ground state of a quadratic Hamiltonian, in particular it is a *pure* quasi-free state. This implies that its one-body and pairing matrices satisfy the relation

$$\alpha_{\Phi^B} \alpha_{\Phi^B}^* = (\alpha_{\Phi^B} J)^2 = \gamma_{\Phi^B}^{(1)} (1 + \gamma_{\Phi^B}^{(1)}) , \quad (\text{A.6})$$

see [35, Appendix A], [51] or [42].

We diagonalize the trace-class operator  $\gamma_{\Phi^B}^{(1)}$  in the form

$$\gamma_{\Phi^B}^{(1)} = \sum_{n \geq 1} c_n |u_n\rangle \langle u_n| \quad , \quad c_n \geq 0 ,$$

and the constraint (A.6) then implies that

$$\alpha_{\Phi^B} = \sum_{n \geq 1} \sqrt{c_n(1+c_n)} |u_n\rangle \langle \overline{u_n}|$$

with  $|\overline{u_n}\rangle := J|u_n\rangle$ . The Bogoliubov energy thus reads

$$e_B = \langle \Phi^B, \mathbb{H}^B \Phi^B \rangle = \sum_{n \geq 1} \left( c_n \langle u_n, (H_{\text{mf}} - \mu) u_n \rangle + \lambda c_n \langle u_n, K u_n \rangle + \lambda \sqrt{c_n(1+c_n)} \text{Re} \langle \overline{u_n}, K u_n \rangle \right) . \quad (\text{A.7})$$

Since  $|\langle \overline{u_n}, K u_n \rangle| \leq \langle u_n, K u_n \rangle$  and  $c - \sqrt{c(1+c)} > -1/2$  for any  $c \in [0, 1]$ , we deduce

$$e_B \geq \sum_{n \geq 1} c_n \langle u_n, (H_{\text{mf}} - \mu) u_n \rangle - \frac{\lambda}{2} \langle u_n, K u_n \rangle = \text{Tr} \left[ (H_{\text{mf}} - \mu) \gamma_{\Phi^B}^{(1)} \right] - \frac{\lambda}{2} \text{Tr}[K] ,$$

where we have used that  $K$  is a positive trace-class operator as noted before. But  $e_B \leq 0$  (see (4.9)), hence

$$\text{Tr} \left[ (H_{\text{mf}} - \mu) \gamma_{\Phi^B}^{(1)} \right] \leq \frac{\lambda}{2} \text{Tr}[K] . \quad (\text{A.8})$$

Recall that  $H_{\text{mf}} - \mu$  is bounded from below on  $\mathfrak{H}_\perp$  by a positive constant  $\kappa > 0$  (since  $u_H$  is the non-degenerate ground state of  $H_{\text{mf}} - \mu$ , see the proof of Proposition 3.7), and that  $\gamma_{\Phi^B}^{(1)}$  lives on this space. Hence we deduce that  $\gamma_{\Phi^B}^{(1)}$  is trace-class. Furthermore,  $\alpha_{\Phi^B}$  is Hilbert-Schmidt because of (A.6). Finally, since both  $-\Delta$  and  $\lambda w * |u_H|^2$  are non-negative, we get

$$\text{Tr} \left[ V \gamma_{\Phi^B}^{(1)} \right] \leq \text{Tr} \left[ H_{\text{mf}} \gamma_{\Phi^B}^{(1)} \right] \leq \frac{\lambda}{2} \text{Tr}[K] + \mu \text{Tr} \left[ \gamma_{\Phi^B}^{(1)} \right] ,$$

which proves (4.16). □

We end this appendix by giving the proof of the lower bound in (4.9). Since  $H_{\text{mf}} \geq 0$  is bounded from below we obtain from (A.8)

$$\text{Tr} \left[ \gamma_{\Phi^B}^{(1)} \right] \leq C\lambda .$$

By using (A.7), the inequality  $|\langle \overline{u_n}, KU_n \rangle| \leq \langle u_n, Ku_n \rangle$  and the positivity of  $K$ , we get

$$\begin{aligned} 0 \geq e_B &\geq \text{Tr} \left[ (H_{\text{mf}} - \mu) \gamma_{\Phi^B}^{(1)} \right] - \lambda \sum_{n \geq 1} \sqrt{c_n(1+c_n)} \langle u_n, Ku_n \rangle \\ &\geq \text{Tr} \left[ (H_{\text{mf}} - \mu) \gamma_{\Phi^B}^{(1)} \right] - \lambda \left( \|K\| \text{Tr} \left[ \gamma_{\Phi^B}^{(1)} \right] \right)^{1/2} \left( \text{Tr}[K] + \|K\| \text{Tr} \left[ \gamma_{\Phi^B}^{(1)} \right] \right)^{1/2} \\ &\geq \text{Tr} \left[ (H_{\text{mf}} - \mu) \gamma_{\Phi^B}^{(1)} \right] - C' \lambda^{3/2} \geq -C' \lambda^{3/2}, \end{aligned}$$

where the second line follows from the Cauchy-Schwarz inequality and the last inequality follows from the fact that  $H_{\text{mf}} - \mu$  is bounded from below by  $\kappa > 0$  on  $\mathfrak{H}_\perp$ . We may bootstrap the argument to get the claimed lower bound.

## APPENDIX B. MINIMAL ENERGY WHEN THE TWO WELLS ARE INFINITELY FAR APART

Let us consider the situation in which the distance  $L$  between the two potential wells is sent to infinity before the number of particles  $N$ . The tunneling energy (2.1) can then be neglected, as well as the interaction energy  $\int |u_{H-}|^2 (w * |u_{H+}|^2)$  between particles in different wells. The problem can thus be mapped into a problem of two independent interacting bosonic gases localized in the left and right wells, with fixed particle numbers  $n$  and  $N - n$ . According to Propositions 4.2 and 4.3, the corresponding lowest energy in the large particle number limits  $n \gg 1$  and  $N - n \gg 1$  reads

$$\begin{aligned} E_{n, N-n}^{\text{loc}} &= n e_H \left( \lambda \frac{n-1}{N-1} \right) + e_B \left( \lambda \frac{n-1}{N-1} \right) \\ &\quad + (N-n) e_H \left( \lambda \frac{N-n-1}{N-1} \right) + e_B \left( \lambda \frac{N-n-1}{N-1} \right), \quad (\text{B.1}) \end{aligned}$$

up to small corrections  $o(1)$ . Here,  $e_H(\lambda)$  and  $e_B(\lambda)$  are the Hartree and Bogoliubov energies corresponding to the Hamiltonian (1.1) with a single well potential  $V_N^+$  or  $V_N^-$ . Since the number of particles in the left and right wells are equal to  $n$  and  $N - n$  instead of  $N$ , the coupling constant  $\lambda$  must be renormalized as indicated in (B.1).

In this appendix, we prove the following very intuitive fact: among all configurations with  $n$  particles in the left well and  $N - n$  particles in the right well, the configuration with the smallest energy is the one with an equal number  $n = N/2$  of particles in each well, which has energy

$$E_{\frac{N}{2}, \frac{N}{2}}^{\text{loc}} = N e_H \left( \Delta_N \frac{\lambda}{2} \right) + 2 e_B \left( \frac{\lambda}{2} \right) + o(N^{-1}) \quad (\text{B.2})$$

with  $\Delta_N$  defined in (2.20). More precisely, we prove the

### Proposition B.1 (Distributing particles evenly is optimal).

There exist an integer  $N_0$  and a constant  $C > 0$  such that for any  $N \geq N_0$  and  $0 \leq n \leq N$ ,

$$E_{n, N-n}^{\text{loc}} \geq E_{\frac{N}{2}, \frac{N}{2}}^{\text{loc}} + \frac{C}{N} \left| n - \frac{N}{2} \right|^2. \quad (\text{B.3})$$

We will use the following well known property of the Hartree energy.

### Lemma B.2 (Scaling and convexity of the Hartree energy).

Let  $e_H(m, \lambda)$  be the minimum of the Hartree functional  $\mathcal{E}_H^\lambda[u]$  given by (1.4) under the constraint

$$\|u\|_{L^2}^2 = m,$$

$$e_H(m, \lambda) := \inf \left\{ \mathcal{E}_H^\lambda[u] \mid \int_{\mathbb{R}^d} |u|^2 = m \right\}. \quad (\text{B.4})$$

For any  $m, \lambda \geq 0$  we have

$$e_H(m, \lambda) = m e_H(1, m\lambda) := m e_H(m\lambda). \quad (\text{B.5})$$

Moreover,  $e_H(m, \lambda)$  is a strictly convex function of  $m$ .

*Proof.* Equation (B.5) follows from a simple scaling argument. To see the convexity of the energy as a function of the mass, we note that  $\mathcal{E}_H^\lambda[u]$  is clearly a strictly convex functional of  $\rho = |u|^2$  (see e.g. [37, Appendix A] for details). We denote by  $\rho_{H,1} = |u_{H,1}|^2$  and  $\rho_{H,2} = |u_{H,2}|^2$  the minimizing densities at masses  $m_1$  and  $m_2 \neq m_1$  and abuse notation by setting  $\mathcal{E}_H^\lambda[\rho_{H,i}] := \mathcal{E}_H^\lambda[u_{H,i}]$ . We then have for any  $0 < t < 1$ ,

$$\begin{aligned} t e_H(m_1, \lambda) + (1-t) e_H(m_2, \lambda) &= t \mathcal{E}_H[\rho_{H,1}] + (1-t) \mathcal{E}_H[\rho_{H,2}] \\ &> \mathcal{E}_H[t\rho_{H,1} + (1-t)\rho_{H,2}] \\ &\geq e_H(tm_1 + (1-t)m_2, \lambda), \end{aligned}$$

where the last inequality comes from

$$\int_{\mathbb{R}^d} (t\rho_{H,1} + (1-t)\rho_{H,2}) = tm_1 + (1-t)m_2.$$

□

*Proof of Proposition B.1.* Using (B.5) we get

$$\begin{aligned} \partial_n \left( n e_H \left( 1, \lambda \frac{n-1}{N-1} \right) \right) &= \partial_n \left( n \frac{N-1}{n-1} e_H \left( \frac{n-1}{N-1}, \lambda \right) \right) \\ &= -\frac{N-1}{(n-1)^2} e_H \left( \frac{n-1}{N-1}, \lambda \right) + \frac{n}{n-1} \frac{\partial e_H}{\partial m} \left( \frac{n-1}{N-1}, \lambda \right) \\ \partial_n^2 \left( n e_H \left( 1, \lambda \frac{n-1}{N-1} \right) \right) &= 2 \frac{N-1}{(n-1)^3} e_H \left( \frac{n-1}{N-1}, \lambda \right) - \frac{2}{(n-1)^2} \frac{\partial e_H}{\partial m} \left( \frac{n-1}{N-1}, \lambda \right) \\ &\quad + \frac{n}{(n-1)(N-1)} \frac{\partial^2 e_H}{\partial m^2} \left( \frac{n-1}{N-1}, \lambda \right). \end{aligned}$$

Since  $\frac{\partial^2 e_H}{\partial m^2}(m, \lambda)$  is strictly positive by Lemma B.2 and  $e_H(m, \lambda)$  and  $\frac{\partial e_H}{\partial m}(m, \lambda)$  are bounded functions of  $m$  on  $[0, 1]$ , we deduce that there is a constant  $C > 0$  such that

$$\partial_n^2 \left( n e_H \left( 1, \lambda \frac{n-1}{N-1} \right) \right) \geq \frac{C}{2N} \quad \text{if } n \geq c_N$$

with  $c_N = O(N^{2/3})$  as  $N \rightarrow \infty$ . Moreover (note that the first eigenvalue of the Bogoliubov Hamiltonian is always non-degenerate),

$$\partial_n^2 e_B \left( \lambda \frac{n-1}{N-1} \right) = \frac{\lambda^2}{(N-1)^2} e_B'' \left( \lambda \frac{n-1}{N-1} \right)$$

is clearly bounded uniformly by a  $O(N^{-2})$ . Thus, for large enough  $N$  one has

$$\partial_n^2 E_{n, N-n}^{\text{loc}} \geq \frac{C}{N} \quad \text{if } n \geq c_N \quad \text{and} \quad N-n \geq c_N.$$

The function  $E_{n,N-n}^{\text{loc}}$  being symmetric around  $n = N/2$ , this implies that it must have a local minimum there. One infers from a second-order Taylor expansion at  $n = N/2$  and the fact that the lower bound on the second derivative is uniform that

$$E_{n,N-n}^{\text{loc}} \geq E_{N/2,N/2}^{\text{loc}} + \frac{C}{N} \left| n - \frac{N}{2} \right|^2 \quad \text{if } n \geq c_N \quad \text{and} \quad N - n \geq c_N.$$

To see that the bounds also holds for  $n < c_N$  or  $N - n < c_N$ , we note that for such  $n$

$$E_{n,N-n}^{\text{loc}} = N e_H(\lambda) + O(N^{2/3}) = N e_H\left(\frac{\lambda}{2}\right) + \frac{CN}{4} + O(N^{2/3}) \geq E_{N/2,N/2}^{\text{loc}} + \frac{C}{N} \left(\frac{N}{2} - n\right)^2,$$

where we have used (B.2) and the fact that  $e_H(1, \lambda)$  is increasing in  $\lambda$ . This completes the proof.  $\square$

### APPENDIX C. SPIN SQUEEZED STATES

In this appendix we define the spin squeezed states and estimate in the large  $N$  limit their energy for the two-mode Bose Hubbard Hamiltonian (see Section 2.3)

$$H_{\text{BH}} = e_+ \mathcal{N}_+ + e_- \mathcal{N}_- + T_N (a_-^* a_+ + a_+^* a_-) + \frac{U_N}{2} (a_+^* a_+^* a_+ a_+ + a_-^* a_-^* a_- a_-).$$

Recall that this Hamiltonian acts on the subspace  $\mathfrak{H}_{\text{BH}} \subset \mathfrak{H}^N$  spanned by the Fock states  $|n, N-n\rangle$ ,  $n = 0, \dots, N$ , and that  $\mathcal{N}_- + \mathcal{N}_+ = N\mathbb{1}$  in this subspace. Omitting terms proportional to the identity,  $H_{\text{BH}}$  can be rewritten as

$$H_{\text{BH}} = (e_+ - e_-) J_z + 2T_N J_x + U_N J_z^2,$$

where  $J_x$  and  $J_z$  are the kinetic momentum operators defined by<sup>7</sup>

$$J_x = \frac{1}{2}(a_-^* a_+ + a_+^* a_-), \quad J_y = \frac{1}{2i}(a_-^* a_+ - a_+^* a_-), \quad J_z = \frac{1}{2}(a_-^* a_- - a_+^* a_+) = \mathcal{N}_- - \frac{N}{2}\mathbb{1}.$$

The total energy of a state  $\Psi \in \mathfrak{H}_{\text{BH}}$  invariant under the exchange of the two wells is thus

$$E_\Psi = \langle \Psi | H_{\text{BH}} | \Psi \rangle = 2T_N \langle \Psi | J_x | \Psi \rangle + U_N \left\langle (\Delta J_z^2) \right\rangle_\Psi. \quad (\text{C.1})$$

An arbitrary state  $\Psi \in \mathfrak{H}_{\text{BH}}$  can be represented geometrically by a 3-dimensional vector with components  $\langle \Psi | J_i | \Psi \rangle$ ,  $i = 1, 2, 3$ , on the Bloch sphere of radius  $N/2$ , together with the corresponding fluctuations (see e.g. [17]).

For vanishing interactions  $U_N = 0$ , the ground state of  $H_{\text{BH}}$  is the delocalized state  $\Psi_{\text{dloc}}$  given by (1.9). This state is a *spin coherent state* centered on the intersection of the Bloch sphere with the  $x$ -axis, i.e., it is an eigenstate of  $J_x$  with the highest eigenvalue  $N/2$  and has fluctuations of the angular momenta in the perpendicular directions equal to  $\langle (\Delta J_y)^2 \rangle_{\text{dloc}} = \langle (\Delta J_z)^2 \rangle_{\text{dloc}} = N/4$ . Increasing  $U_N/|T_N|$  to small non-zero values, it becomes energetically more favorable to decrease the particle number fluctuations  $\langle (\Delta \mathcal{N}_-)^2 \rangle = \langle (\Delta J_z)^2 \rangle$  and thus the interaction energy (second term in the right-hand side of (C.1)), to the expense of increasing a little bit the kinetic and potential energies (first term). One expects that the ground state of  $H_{\text{BH}}$  is a *particle number spin squeezed state* [29]. By definition, such a state has reduced fluctuations of  $J_z$  (i.e., of  $\mathcal{N}_-$ )

<sup>7</sup> It is easy to see that these self-adjoint operators satisfy the usual commutation relations of angular momenta. This implies in particular that  $e^{i\phi_N J_x} J_z e^{-i\phi_N J_x} = \cos \phi_N J_z - \sin \phi_N J_y$ .

and enhanced fluctuations of  $J_y$  as compared to the coherent state  $\Psi_{\text{dloc}}$ , and like the latter it saturates the spin uncertainty inequality, i.e.,

$$\langle (\Delta J_y)^2 \rangle \langle (\Delta J_z)^2 \rangle = \frac{|\langle J_x \rangle|^2}{4}. \quad (\text{C.2})$$

In contrast to coherent states, particles in a squeezed state are correlated.

A spin squeezed state can be obtained by [29]

$$\begin{aligned} |\Psi_{\text{sq}}\rangle &= e^{-i\phi_N J_x} e^{-i\theta_N J_z^2} |\Psi_{\text{dloc}}\rangle \\ &= 2^{-\frac{N}{2}} \sum_{n=0}^N \sqrt{\frac{N!}{n!(N-n)!}} e^{-i\theta_N(n-N/2)^2} e^{-i\phi_N J_x} |n, N-n\rangle, \end{aligned} \quad (\text{C.3})$$

where we have used the components  $c_n = 2^{-N/2} \sqrt{N!/(n!(N-n)!)}$  of  $\Psi_{\text{dloc}}$  in the Fock state basis. The unitary operator  $e^{-i\theta_N J_z^2}$  in (C.3) squeezes the angular momentum fluctuations in one direction while increasing them in the perpendicular direction, and the unitary  $e^{-i\phi_N J_x}$  rotates the state on the Bloch sphere around the  $x$ -axis, in such a way that the squeezing direction be along the  $z$ -axis. In fact, choosing  $\theta_N = N^{-\alpha-1/2}$  and  $\phi_N$  given by  $\tan \phi_N = N^{\alpha-1/2}$  with an exponent  $\alpha \in (1/6, 1/2)$ , a lengthy calculation gives in the limit  $N \gg 1$

$$\langle (\Delta J_z)^2 \rangle_{\text{sq}} = \langle (\Delta \mathcal{N}_-)^2 \rangle_{\text{sq}} \approx \frac{N^{2\alpha}}{4} \ll \frac{N}{4}, \quad \langle (\Delta J_y)^2 \rangle_{\text{sq}} \approx \frac{N^{2(1-\alpha)}}{4} \gg \frac{N}{4} \quad (\text{C.4})$$

and

$$\langle \Psi_{\text{sq}} | J_x | \Psi_{\text{sq}} \rangle = \langle u_{\text{H}\mp}, \gamma_{\Psi_{\text{sq}}}^{(1)} u_{\text{H}\pm} \rangle \approx \frac{N}{2} - \frac{N^{1-2\alpha}}{4}, \quad (\text{C.5})$$

so that  $\Psi_{\text{sq}}$  satisfies the minimal spin uncertainty condition (C.2) to leading order in  $N$ .

The energy of the squeezed state (C.3) is

$$\langle \Psi_{\text{sq}} | H_{\text{BH}} | \Psi_{\text{sq}} \rangle \approx T_N N \left( 1 - \frac{1}{2} N^{-2\alpha} \right) + U_N \frac{N^{2\alpha}}{4}$$

with error terms of order  $(|T_N| + U_N)N^{1-4\alpha}$ . Comparing with the energy of the coherent state,

$$\langle \Psi_{\text{dloc}} | H_{\text{BH}} | \Psi_{\text{dloc}} \rangle = T_N N + U_N \frac{N}{4},$$

we find that  $\Psi_{\text{sq}}$  has a lower energy than  $\Psi_{\text{dloc}}$  when  $|T_N|/U_N < N^{2\alpha}/2$ . Since the exponent  $\alpha$  can be chosen arbitrary close to  $1/2$  and  $U_N = O(N^{-1})$ , we may expect a transition between a delocalized regime where the ground state of  $H_{\text{BH}}$  is close to  $\Psi_{\text{dloc}}$  (Rabi regime) to a localized regime where it is close to a spin squeezed state (Josephson regime) occurring for  $|T_N| \sim 1$ , as reported in Table 1.

According to (2.23) and (C.5), the one-body density matrix of  $\Psi_{\text{sq}}$  is almost equal to the density matrix (2.11) of the delocalized state, up to corrections of order  $N^{1-2\alpha}$  in the off-diagonal elements. Thus one can conjecture that in the Josephson regime  $N^{-2} \ll |T_N| \ll 1$ , the one-body density matrix  $\gamma_{\Psi_{\text{sq}}}^{(1)}$  of the ground state is close to  $\gamma_{\text{dloc}}^{(1)}$  and has only one macroscopic eigenvalue. This conjecture and the localization properties of the ground state reported in Table 1 are supported by numerical simulations (see e.g. [20]).

Finally, we note that the state  $\Psi$  with Gaussian components (2.26) considered in Section 2.3 has properties similar to  $\Psi_{\text{sq}}$  in the large  $N$  limit. In fact, choosing  $\sigma_N = N^\alpha$ , simple calculations

show that  $\Psi$  and  $\Psi_{\text{sq}}$  have to leading order in  $N$  the same variances of  $J_z$  and  $J_y$  and expectation of  $J_x$ , given by (C.4) and (C.5).

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UNIVERSITÉ GRENOBLE ALPES & CNRS, LPMMC, F-38000 GRENOBLE, FRANCE  
*E-mail address:* nicolas.rougerie@lpmmc.cnrs.fr

UNIVERSITÉ GRENOBLE ALPES & CNRS, INSTITUT FOURIER & LPMMC, F-38000 GRENOBLE, FRANCE,  
 PRESENT ADDRESS: DEPARTAMENTO DE INGENIERÍA MATEMÁTICA, UNIVERSIDAD DE CONCEPCIÓN, CHILE  
*E-mail address:* dspehner@ing-mat.udec.cl