

# Universal diagonal estimates for minimizers of the Levy–Lieb functional

S. Di Marino<sup>1</sup> · A. Gerolin<sup>2,3</sup> · L. Nenna<sup>4</sup>

Received: 1 March 2023 / Revised: 31 August 2023 / Accepted: 8 September 2023 / Published online: 7 October 2023 © The Author(s), under exclusive licence to Springer Nature B.V. 2023

### Abstract

Given a wave-function minimizing the Levy–Lieb functional, the intent of this short note is to give an estimate of the probability of the particles being in positions  $(x_1, \ldots, x_N)$  in the  $\delta$ -close regime  $D_{\delta} = \bigcup_{i \neq j} \{|x_i - x_j| \le \delta\}$ .

Keywords Multimarginal optimal transportation  $\cdot$  Levy-Lieb  $\cdot$  Diagonal estimates  $\cdot$  DFT

 $\textbf{MSC Codes} \ 49S05 \cdot 49Q22$ 

## Contents

1	Introduction	2
2	Notation	4
3	Estimate for the kinetic energy	5
4	New trial state: swapping particles and estimate for the potential	8
5	Diagonal estimates for the wave-function	10
Re	eferences	15

L. Nenna luca.nenna@universite-paris-saclay.fr

> S. Di Marino simone.dimarino@unige.it

A. Gerolin agerolin@uottawa.ca

- <sup>1</sup> MaLGA, Università degli Studi di Genova (DIMA), Genoa, Italy
- <sup>2</sup> Department of Mathematics and Statistics, University of Ottawa, Ottawa, Canada
- <sup>3</sup> Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, Canada
- <sup>4</sup> Laboratoire de mathématiques d'Orsay, CNRS, Université Paris-Saclay, 91405 Orsay, France

#### **1** Introduction

Density functional theory attempts to describe all the relevant information about a many-body quantum system at ground state in terms of the one electron density  $\rho$ . Following Levy and Lieb's approach [29, 32], the ground state energy can be rephrased as the following variational principle involving only the electron density

$$\mathcal{E}_0[v] = \inf_{\substack{\rho \in \mathcal{A}^N \\ \int_{\mathbb{R}^3} v(x) \, d\rho < +\infty}} \left\{ F_{LL,\varepsilon}[\rho] + \int_{\mathbb{R}^3} v(x) \, d\rho \right\},\,$$

where  $\mathcal{A}^N = \{\rho \in L^1(\mathbb{R}^3) : \rho \ge 0, \sqrt{\rho} \in H^1, \rho(\mathbb{R}^3) = N\}$  is the set of admissible densities, v is an external potential and the Levy–Lieb functional  $F_{LL,\varepsilon}$  is defined as

$$F_{LL,\varepsilon}[\rho] := \min_{\substack{\psi \in \mathcal{W} \\ \psi \mapsto \rho}} \left\{ \int_{\mathbb{R}^{3N}} \varepsilon |\nabla \psi|^2(x) + v_{ee}(x) |\psi|^2(x) \, dx \right\},\tag{1}$$

where  $v_{ee}(x_1, \ldots, x_N) = \sum_{i < j} \frac{1}{|x_i - x_j|}$  is the Coulomb interaction potential between the *N* electrons,  $\mathcal{W} \subset H^1(\mathbb{R}^{3N}) \cap \{||\psi||_{L^2} = 1\}$ , with an additional constraint on the symmetry of the wavefunction which we will discuss later, and  $\psi \mapsto \rho$  means that the one-body density of  $\psi$  is  $\rho$ , that is  $\rho = N \int_{\mathbb{R}^{3(N-1)}} |\psi|^2$ . The Levy–Lieb functional is indeed the lowest possible (kinetic plus interaction) energy of a quantum system having the prescribed density  $\rho$ . This universal functional is the central object of density functional theory, since knowing it would allow one to compute the ground state energy of a system with any external potential v. For a complete review on it we refer the reader to [31].

The vector space  $\mathcal{W}$  in (1) is the search space of wavefunctions: the natural choice would be to consider  $\mathcal{H}^N = \bigwedge_{i=1}^N H^1(\mathbb{R}^3; \mathbb{C})$ , that is the fermionic space of anti-symmetric wavefunctions, however we will use  $S^N = \bigotimes_{S,i=1}^N H^1(\mathbb{R}^3; \mathbb{C})$ , the bosonic space of *symmetric* wavefunctions, that is

$$\psi(x_{\sigma(1)},\ldots,x_{\sigma(N)}) = \psi(x_1,\ldots,x_N), \quad \forall \sigma \in S$$

Then the vector space W for the bosonic case can be defined as

$$\mathcal{W} := \{ \psi \in S^N \text{ and } ||\psi||_{L^2} = 1 \}.$$
(2)

In fact, although the electrons are *fermions*, also *bosonic* wave-functions can be of interest, and they can be mathematically more treatable: for example we can assume that bosonic minimizers  $\psi$  for (1) are positive, which will guarantee that  $|\psi|^2$  is a minimizer for (11), which is the functional we will actually treat. Notice that the ground-state energy of *fermionic* systems are generally higher than *bosonic* ones. In our analysis, however, the *bosonic* case is not very restrictive since we are looking at the regime  $\varepsilon$  small.

Our approach interprets the Levy–Lieb functional as a (Fisher-information regularized) multi-marginal optimal transport problem.

Connection with optimal transportation theory It has been recently shown that the limit functional as  $\varepsilon \to 0$  corresponds to a multi-marginal optimal transport problem [2, 12, 13, 30] (see also the seminal works in the physics and chemistry literature [5, 36–39]): rather than wave-functions, one has now enlarged the constrained search in (1) to minimize among probability measures on  $\mathbb{R}^{3N}$  having  $\rho$  as marginal, that is

$$F_0[\rho] := \inf_{\mathbb{P}\in\Pi_N(\rho)} \left\{ \int_{\mathbb{R}^{3N}} v_{ee}(x_1,\ldots,x_N) \, d\mathbb{P}(x_1,\ldots,x_N) \right\},\tag{3}$$

where  $\Pi_N(\rho)$  denotes the set of probability measures on  $\mathbb{R}^{3N}$  having  $\rho/N$  as marginals.

The multi-marginal optimal transport with Coulomb cost (3) has garnered attention in the mathematics, physics and chemistry communities and the literature on the subject is growing considerably. Recent developments include results on the existence and non-existence of Monge-type solutions minimizing (3) (e.g., [3, 5, 7, 8, 11, 12, 19, 21]), structural properties of Kantorovich potentials (e.g., [4, 9, 18, 25]), grandcanonical optimal transport [20], efficient computational algorithms (e.g., [1, 14, 17, 23, 26]) and the design of new density functionals (e.g., [6, 24, 28, 34]). The first order expansion around the limit  $\varepsilon \rightarrow 0$  of the Levy–Lieb functional was obtained in [10].

We refer to the surveys (and references therein) [18, 22] for a self-contained presentation on multi-marginal optimal transport approach in Density Functional Theory as well as the review article [40] for a the recent developments from a chemistry standpoint.

*Main result of this paper* In [4, 9, 16] it is shown that the support supp( $\mathbb{P}^*$ ) of a solution  $\mathbb{P}^*$  of the limiting problem (3) is uniformly bounded away of the diagonal, i.e. one has always  $|x_i - x_j| \ge \delta > 0$  for any  $x_i, x_j \in \text{supp}(\mathbb{P}^*)$ . In other words, the electrons are always at a certain distance away from each other, which is the expected behaviour since we are in a *classical* framework.

In the sequel we will denote with  $D_{\delta}$  the enlarged diagonal

$$D_{\delta} = \{ (x_1, \dots, x_N) \in \mathbb{R}^{3N} : \exists i \neq j \text{ s.t. } |x_i - x_j| \le \delta \}.$$

In particular the result in [4, 9] can be rephrased saying that the solution to the multimarginal optimal transport problem is concentrated on the complement of  $D_{\delta}$  for some  $\delta$ . An important feature of the results is that  $\delta$  depends only on concentration properties of  $\rho$ . In fact defining

$$\kappa(\rho, r) := \sup_{x \in \mathbb{R}^3} \rho(B(x, r))/N, \tag{4}$$

the authors in [9] prove that if  $\kappa(\rho, \beta) < \frac{1}{2(N-1)}$  then one can choose  $\delta = \frac{\beta}{2N}$ . Our main result is to extend this property also for  $\varepsilon > 0$  small. In particular we do not expect to have  $\psi_{\varepsilon} = 0$  on  $D_{\delta}$  but we show that the probability of having the electrons in position  $x \in D_{\delta}$  is very small (5).

**Theorem 1.1** (Exponential off-diagonal localization for Coulomb) Let  $\rho \in \mathcal{A}^N$  and let  $\psi_{\varepsilon}$  be a minimizer for (1) in the bosonic case, that is  $\psi_{\varepsilon} \in \mathcal{W}$  with  $\mathcal{W}$  as defined in (2), where  $v_{ee}(x_1, \ldots, x_N) = \sum_{i < j} \frac{1}{|x_i - x_j|}$ . Let us consider  $\beta$  such that  $\kappa(\rho, \beta) \leq \frac{1}{4(N-1)}$  then, let  $\alpha \leq \frac{\beta}{32N}$ , and suppose  $\varepsilon N^2 \ll \alpha$ . Then, for  $\mathbb{P}_{\varepsilon}(x) = |\psi_{\varepsilon}|^2(x)$  we have

$$\int_{D_{\alpha/2}} \mathbb{P}_{\varepsilon}(x) \, dx \le e^{-\frac{1}{24}\sqrt{\frac{\alpha}{\varepsilon}}}.$$
(5)

In the proof we actually work with a general repulsive pairwise potential  $v_{ee}$ , which satisfies the hypothesis (7), stated in the next section. The result in general is the following one:

**Theorem 1.2** (Exponential off-diagonal localization for general interaction cost) Let  $\rho \in A_N$  and let  $\psi_{\varepsilon}$  be a minimizer for (1) in the bosonic case where  $v_{ee}$  satisfies (7) for some  $\theta, \Theta : (0, \infty) \to [0, \infty)$  decreasing such that  $\lim_{t\to 0^+} \theta(t) = +\infty$ . Let  $\beta$  be such that  $\kappa(\rho, \beta) \leq \frac{1}{4(N-1)}$  and let  $\alpha$  such that  $\theta(2\alpha) \leq 8(N-1)\Theta(\beta/2)$ , and suppose  $\varepsilon N^2 \ll \alpha^2 \theta(2\alpha)$ . Then, for  $\mathbb{P}_{\varepsilon}(x) = |\psi_{\varepsilon}|^2(x)$  we have

$$\left| \int_{D_{\alpha/2}} \mathbb{P}_{\varepsilon}(x) \, dx \le e^{-\frac{1}{12}\sqrt{\frac{\alpha^2 \theta(2\alpha)}{2\varepsilon}}}. \right|$$
(6)

Notice that in [9] the diagonal estimate is proven also in the weaker (and sharper) hypotesis  $\kappa(\rho, \beta) < \frac{1}{N}$ : while we believe that also in that case a similar generalization in the case  $\varepsilon > 0$  holds true, the proof will be more technical and not so trasparent. For the same reason the inequality  $\kappa(\rho, \beta) \le \frac{1}{4(N-1)}$  is used instead of  $\kappa(\rho, \beta) < \frac{1}{2(N-1)}$  in order to have more transparent estimates in the end.

*Organization of the paper* In Sect. 2 we introduce the notations we are going to use throughout all the paper. In Sect. 3 we give the estimates concerning kinetic energy term in the Levy–Lieb functional. Section 4 is then devoted to the construction of a competitor for the Levy–Lieb functional; finally in Sect. 5 we derive the diagonal estimates for the wave-function and, thus, prove Theorems 1.1 and 1.2 via the iteration of a decay estimate.

#### 2 Notation

Consider a subset  $I \subseteq \{1, ..., N\}$ , with cardinality k = |I|, defined as  $I = \{i_1, ..., i_k\}$ , with  $1 \le i_1 < i_2 < \cdots < i_k$ . Then, the *I*-projection is defined by

$$\pi_I : \mathbb{R}^{3N} \to \mathbb{R}^{3k}, \quad \pi_I((x_1, \dots, x_N)) = (x_{i_1}, x_{i_2}, \dots, x_{i_k}).$$

Sometimes we will denote  $x_I = \pi_I(x)$  and if  $I = J^c$ , then  $x = (x_I, x_J)$ . With a slight abuse of notation, for a function  $\mathbb{P} \in L^1(\mathbb{R}^{3N})$ ,  $I \subseteq \{1, ..., N\}$  and  $J = I^c$  we denote

$$(\pi_I)_{\sharp}(\mathbb{P})(x_I) = \int \mathbb{P}(x_I, x_J) \, dx_J,$$

which on density of measures act precisely as the push-forward through the projection function  $\pi_I$ .

As we have already mentioned above, we denote by  $\Pi_N(\rho)$  the set of probability measures on  $\mathbb{R}^{3N}$  having the *N* one body marginals equal to  $\rho/N$ .

In the following we will consider an electron–electron pair interaction repulsion potential,  $v_{ee}$ , with the following form:

$$v_{ee}(x_1, \dots, x_N) = \sum_{i < j} c(x_i, x_j), \quad \text{where}$$
  

$$\theta(|x - y|) \le c(x, y) \le \Theta(|x - y|) \quad \forall x, y \in \mathbb{R}^3$$
  
for some  $\theta, \Theta : (0, \infty) \to [0, \infty)$  decreasing such that  $\lim_{t \to 0^+} \theta(t) = +\infty.$ 
(7)

Moreover, with a slight abuse of notation, we will denote by

$$\mathbb{P} \in \mathcal{P}(\mathbb{R}^{3N}) \mapsto v_{ee}(\mathbb{P}) := \int_{\mathbb{R}^{3N}} v_{ee}(x_1, \dots, x_N) \, d\mathbb{P}(x_1, \dots, x_N). \tag{8}$$

Notice that we will often identify a measure  $\mathbb{P}$  with its density.

Finally, given an open set  $\Omega \subseteq \mathbb{R}^{3N}$ , for every r > 0 we denote with  $\Omega_{-r}$  its *r*-thinning, that is the set of points inside  $\Omega$  whose distance from  $\partial \Omega$  is greater or equal than *r*. In particular

$$\Omega_{-r} := \{ x \in \mathbb{R}^{3N} : B(x, r) \subseteq \Omega \}.$$
(9)

#### 3 Estimate for the kinetic energy

In this section we give some preliminary estimates for the kinetic energy term of the Levy-Lieb functional. Denoting  $L^1_+$  the cone of positive  $L^1$  functions, we define  $\mathcal{E}_{kin} : L^1_+(\mathbb{R}^{3N}) \to \mathbb{R}$  the Kinetic energy associated to some absolutely continuos *N*-probability measure *h* 

$$\mathcal{E}_{kin}(h) := \begin{cases} \int_{\mathbb{R}^{3N}} \frac{\sum_{i=1}^{N} |\nabla_i h(x_1, \dots, x_N)|^2}{h(x_1, \dots, x_N)} \, dx_1, \dots, dx_N & \text{if } \sqrt{h} \in H^1(\mathbb{R}^{3N}) \\ +\infty & \text{otherwise} \end{cases}$$
(10)

When it will be clear from the context we will also abbreviate  $\mathcal{E}_{kin}(h) = \int \frac{|\nabla h|^2}{h} dx$ . Notice that the kinetic energy functional is also known as the Fisher information. Moreover if  $\psi \in H^1(\mathbb{R}^{3N}; \mathbb{R})$ , then

$$4\int |\nabla\psi|^2 dx = \mathcal{E}_{\rm kin}(|\psi|^2) = \mathcal{E}_{\rm kin}(\mathbb{P}_{\psi}),$$

where  $\mathbb{P}_{\psi} = |\psi|^2$  is the joint probability associated to the wave-function  $\psi$ . The string of equalities above is thus true when  $\psi$  is a minimizer for the bosonic case. The following Lemma summarises some results concerning the homogeneity, sub-additivity (which is a consequence of theorem 7.8 in [33]) and the decomposability under projection of the kinetic energy (a similar result also appears in [27, 35]).

**Lemma 3.1** Let  $\mathcal{E}_{kin}$  defined as in (10). Then

- (i)  $\mathcal{E}_{kin}$  is 1-homogeneous, that is  $\mathcal{E}_{kin}(\lambda \mathbb{P}) = \lambda \mathcal{E}_{kin}(\mathbb{P})$  for every  $\lambda > 0$ ;
- (ii) given  $\mathbb{P}_1, \ldots, \mathbb{P}_k \in L^1(\mathbb{R}^{3N})$ , we have

$$\mathcal{E}_{kin}(\mathbb{P}_1 + \dots + \mathbb{P}_k) \leq \mathcal{E}_{kin}(\mathbb{P}_1) + \mathcal{E}_{kin}(\mathbb{P}_2) + \dots + \mathcal{E}_{kin}(\mathbb{P}_k)$$

(iii) Let  $\mathbb{P} \in L^1_+(\mathbb{R}^{3N})$ . Given  $I, J \subseteq \{1, ..., N\}$  two nonempty disjoint sets such that  $I = J^c$ , we denote by  $\mathbb{P}_I = (\pi_I)_{\sharp}\mathbb{P}$  and  $\mathbb{P}_J = (\pi_J)_{\sharp}\mathbb{P}$ . Then we have (here  $N_I = \sharp I$  and  $N_J = \sharp J$ )

$$\mathcal{E}_{\mathrm{kin}}^{N}(\mathbb{P}) \geq \mathcal{E}_{\mathrm{kin}}^{N_{I}}(\mathbb{P}_{I}) + \mathcal{E}_{\mathrm{kin}}^{N_{J}}(\mathbb{P}_{J}),$$

where the equality holds if and only if  $\mathbb{P}(x) = \mathbb{P}_I(x_I)\mathbb{P}_J(x_J)/\lambda$ , where  $\lambda = \int \mathbb{P}$ . In particular if  $\mathbb{P}$  is the density of a probability measure, we have that the equality happens if and only if  $x_I$  and  $x_J$  are independent under the probability  $\mathbb{P}$ .

**Proof** (i) The 1-homogeneity is obvious.

(ii) For the subadditivity it is sufficient to prove it for k = 2; then for every x, by Cauchy–Schwarz inequality we have

$$(\mathbb{P}_{1}(x) + \mathbb{P}_{2}(x)) \left( \frac{|\nabla \mathbb{P}_{1}(x)|^{2}}{\mathbb{P}_{1}(x)} + \frac{|\nabla \mathbb{P}_{2}(x)|^{2}}{\mathbb{P}_{2}(x)} \right) \ge (|\nabla \mathbb{P}_{1}(x)| + |\nabla \mathbb{P}_{2}(x)|)^{2},$$

which, after using the triangular inequality and dividing by  $\mathbb{P}_1 + \mathbb{P}_2$  can be rewritten as

$$\frac{|\nabla(\mathbb{P}_1 + \mathbb{P}_2)|^2}{\mathbb{P}_1 + \mathbb{P}_2} \le \frac{|\nabla\mathbb{P}_1|^2}{\mathbb{P}_1} + \frac{|\nabla\mathbb{P}_2|^2}{\mathbb{P}_2},$$

which integrated gives us the conclusion.

(iii) As for the last point we fix  $x_J$  and we use the Cauchy–Schwarz inequality with respect to the measure  $dx_I$ :

$$\left(\int \mathbb{P}(x_I, x_J) dx_I\right) \cdot \left(\int \frac{|\nabla_J \mathbb{P}(x_I, x_J)|^2}{\mathbb{P}(x_I, x_J)} dx_I\right) \ge \left(\int |\nabla_J \mathbb{P}(x_I, x_J)| dx_I\right)^2$$

🖉 Springer

$$\geq \left|\nabla_J \left(\int \mathbb{P}(x_I, x_J) dx_I\right)\right|^2,$$

where in the last passage we used the triangular inequality and we took the derivative out of the integral. Now we recognize  $\mathbb{P}_J(x_J) = \int \mathbb{P}(x_I, x_J) dx_I$  and so we can write this as

$$\int \frac{|\nabla_J \mathbb{P}(x_I, x_J)|^2}{\mathbb{P}(x_I, x_J)} dx_I \ge \frac{|\nabla_J \mathbb{P}_J(x_J)|^2}{\mathbb{P}_J(x_J)}.$$

Integrating this with respect to  $dx_J$  and doing a similar computation for  $x_I$ , we obtain the conclusion, that is

$$\iint \frac{|\nabla \mathbb{P}(x_I, x_J)|^2}{\mathbb{P}(x_I, x_J)} dx_I dx_J \ge \int \frac{|\nabla_J \mathbb{P}_J(x_J)|^2}{\mathbb{P}_J(x_J)} dx_J + \int \frac{|\nabla_I \mathbb{P}_I(x_I)|^2}{\mathbb{P}_I(x_I)} dx_I$$

From the equality cases in C–S and triangular inequality combined we get  $\nabla_J \mathbb{P}(x_I, x_J) = v(x_J)\mathbb{P}(x_I, x_J)$  for some vector field v; by a simple integration we actually get  $v = \nabla(\mathbb{P}_J)/\mathbb{P}_J$ ; this can be seen as  $\nabla_J \log(\mathbb{P}) = \nabla_J \log \mathbb{P}_J$ ; similarly we can get  $\nabla_I \log(\mathbb{P}) = \nabla_I \log \mathbb{P}_I$ . Summing up this two equalities we get  $\nabla(\mathbb{P}(x)/\mathbb{P}_I(x_I)\mathbb{P}_J(x_J)) = 0$ .

The following lemma is a straightforward adaptation of Theorem 3.2 in [15] giving the IMS localization formula; we have added a short proof for sake of completeness.

**Lemma 3.2** Let  $\eta_1, \eta_2, \eta_3 : \mathbb{R}^{3N} \to [0, 1]$  be  $C^1$  functions such that  $\eta_1 + \eta_2 + \eta_3 \equiv 1$ . Then, for every function  $\mathbb{P} \in L^1_+(\mathbb{R}^{3N})$  we have

$$\begin{aligned} & \mathcal{E}_{\mathrm{kin}}(\mathbb{P}\eta_1) + \mathcal{E}_{\mathrm{kin}}(\mathbb{P}\eta_2) + \mathcal{E}_{\mathrm{kin}}(\mathbb{P}\eta_3) \\ &= \mathcal{E}_{\mathrm{kin}}(\mathbb{P}) + \int \left( \frac{|\nabla \eta_1|^2}{\eta_1} + \frac{|\nabla \eta_2|^2}{\eta_2} + \frac{|\nabla \eta_3|^2}{\eta_3} \right) \mathbb{P} \, dx. \end{aligned}$$

**Proof** For every i = 1, 2, 3 pointwisely we have:

$$\frac{|\nabla(\mathbb{P}\eta_i)|^2}{\mathbb{P}\eta_i} = \frac{|\eta_i \nabla \mathbb{P} + \mathbb{P}\nabla \eta_i|^2}{\mathbb{P}\eta_i} = \frac{\eta_i^2 |\nabla \mathbb{P}|^2 + 2\eta_i \mathbb{P}\nabla \mathbb{P} \cdot \nabla \eta_i + \mathbb{P}^2 |\nabla \eta_i|^2}{\mathbb{P}\eta_i}$$
$$= \eta_i \frac{|\nabla \mathbb{P}|^2}{\mathbb{P}} + 2\nabla \mathbb{P} \cdot \nabla \eta_i + \mathbb{P}\frac{|\nabla \eta_i|^2}{\eta_i}$$

Adding them up and using that  $\sum \eta_i = 1$  and  $\sum \nabla \eta_i = 0$ , we get

$$\sum_{i} \frac{|\nabla(\mathbb{P}\eta_i)|^2}{\mathbb{P}\eta_i} = \frac{|\nabla\mathbb{P}|^2}{\mathbb{P}} + \mathbb{P}\sum_{i} \frac{|\nabla\eta_i|^2}{\eta_i},$$

which integrated, gives us the desired identity.

#### 4 New trial state: swapping particles and estimate for the potential

The scope of this subsection is to create a competitor for the minimization of the functional

$$\mathcal{F}_{LL,\varepsilon}(\mathbb{P}) := \begin{cases} \frac{\varepsilon}{4} \mathcal{E}_{kin}(\mathbb{P}) + v_{ee}(\mathbb{P}) & \text{if } \mathbb{P} \in \Pi_N(\rho) \\ +\infty & \text{otherwise,} \end{cases}$$
(11)

where  $\mathcal{E}_{kin}$  is defined in (10),  $v_{ee}$  satisfies (7) and  $\Pi_N(\rho)$  denotes the set of probability measures on  $\mathbb{R}^{3N}$  having  $\rho/N$  as marginals. The idea is to try to mimic what it is done in [4, 9, 16], in the semiclassical case  $\varepsilon = 0$ : in that case we take two points  $y, z \in \mathbb{R}^{3N}$ and substitute them with  $\tilde{y}, \tilde{z}$  where we have interchanged their first compenent, that is  $\tilde{y} = (z_1, y_2, \dots, y_n)$  and  $\tilde{z} = (y_1, z_2, \dots, z_n)$ .

In order to do so for the *N*-particle distribution  $\mathbb{P}$ , we will consider two small bumps centered around *y* and *z* 

$$\eta_1(x) = \lambda_1 \eta \left( \frac{x - y}{r_1} \right)$$
 and  $\eta_2(x) = \lambda_2 \eta \left( \frac{x - z}{r_2} \right)$ , (12)

for some  $\lambda_1, \lambda_2, r_1, r_2$  to be chosen later and some  $\eta \in C_c^1(B(0, 1)), \eta \ge 0$ . First of all we assume that  $\operatorname{supp}(\eta_1) \cap \operatorname{supp}(\eta_2) = \emptyset$ , which can be granted as long as

$$r_1 + r_2 < |y - z|, \tag{13}$$

and then we assume  $\int \eta_1 \mathbb{P} = \int \eta_2 \mathbb{P} = m$  which can be accomplished again by choosing the appropriate  $\lambda_i, r_i$ . Let us then define

$$\rho_1^i(x_1) = (\pi_{\{1\}})_{\sharp}(\eta_i \mathbb{P}), \qquad \rho_1^i(x_2, x_3, \dots, x_N) = (\pi_{\{1\}^c})_{\sharp}(\eta_i \mathbb{P}), \tag{14}$$

$$\mathbb{P}_{1} = \frac{1}{m} \rho_{1}^{2} \rho_{\hat{1}}^{1}, \qquad \mathbb{P}_{2} = \frac{1}{m} \rho_{1}^{1} \rho_{\hat{1}}^{2}, \qquad (15)$$

where  $\rho_1^i$  and  $\rho_1^i$  are the marginals of  $\eta_i \mathbb{P}$  and  $\mathbb{P}_1$  and  $\mathbb{P}_2$  are densities concentrated around  $\tilde{y} = (z_1, y_2, \dots, y_n)$  and  $\tilde{z} = (y_1, z_2, \dots, z_n)$  respectively. We then finally consider

$$\mathbb{P} := \mathbb{P} - \mathbb{P}\eta_1 - \mathbb{P}\eta_2 + \mathbb{P}_1 + \mathbb{P}_2, \tag{16}$$

which will be the competitor for a minimizer  $\mathbb{P}$  of the functional  $\mathcal{F}_{LL,\varepsilon}$ .

**Remark 4.1** Given  $y, z, r_1, r_2$  that satisfy (13), the only condition that remains to be checked is whether  $\overline{\mathbb{P}}$  is a competitor: we will prove that this is the case for every  $\lambda_1$  and  $\lambda_2$  small enough.

In fact we have to check that  $\overline{\mathbb{P}} \geq 0$  and that it has the correct marginals. For the positivity, notice that for  $\lambda_1$  and  $\lambda_2$  small enough, we have  $\eta_1 + \eta_2 \leq 1$  and so  $\mathbb{P} - \eta_1 \mathbb{P} - \eta_2 \mathbb{P} \geq 0$ , which will guarantee that  $\overline{\mathbb{P}} \geq 0$ .

For the marginal constraint, notice that by (14) and (15) we have that  $\eta_1 \mathbb{P} + \eta_2 \mathbb{P}$  and  $\mathbb{P}_1 + \mathbb{P}_2$  have the same marginals, in particular also  $\mathbb{P}$  and  $\overline{\mathbb{P}}$  share the same marginals.

**Lemma 4.1** Let  $\mathbb{P}$  be such  $\mathcal{F}_{LL,\varepsilon}(\mathbb{P}) < +\infty$ . Given  $y, z \in \mathbb{R}^{3N}$ , let  $\eta_1, \eta_2, \mathbb{P}_1, \mathbb{P}_2, \overline{\mathbb{P}}$  defined by (12),(13), (14), (15) and (16). Then

$$\mathcal{E}_{\mathrm{kin}}(\bar{\mathbb{P}}) \leq \mathcal{E}_{\mathrm{kin}}(\mathbb{P}) + \int \mathbb{P}(x) \left( \frac{|\nabla \eta_1|^2}{\eta_1} + \frac{|\nabla \eta_2|^2}{\eta_2} + \frac{|\nabla \eta_1 + \nabla \eta_2|^2}{1 - \eta_1 - \eta_2} \right) dx;$$
$$v_{ee}(\bar{\mathbb{P}}) = v_{ee}(\mathbb{P}) - \int \mathbb{P}(\eta_1 + \eta_2) \sum_{i>1} c(x_1, x_i) dx + \int (\mathbb{P}_1 + \mathbb{P}_2) \sum_{i>1} c(x_1, x_i) dx.$$

**Proof** Let us consider  $\eta_3 = 1 - \eta_1 - \eta_2$ . Then we have  $\overline{\mathbb{P}} = \eta_3 \mathbb{P} + \mathbb{P}_1 + \mathbb{P}_2$ . Using Lemma 3.1, in particular the subadditivity and the exact energy split in case of independent variables for  $\mathcal{E}_{kin}$ , we get (by (15))

$$\begin{aligned} \varepsilon_{\mathrm{kin}}(\mathbb{P}) &\leq \varepsilon_{\mathrm{kin}}(\eta_{3}\mathbb{P}) + \varepsilon_{\mathrm{kin}}(\mathbb{P}_{1}) + \varepsilon_{\mathrm{kin}}(\mathbb{P}_{2}) \\ &= \varepsilon_{\mathrm{kin}}(\eta_{3}\mathbb{P}) + \varepsilon_{\mathrm{kin}}(\rho_{1}^{2}) + \varepsilon_{\mathrm{kin}}\left(\rho_{1}^{1}\right) + \varepsilon_{\mathrm{kin}}\left(\rho_{1}^{1}\right) + \varepsilon_{\mathrm{kin}}\left(\rho_{1}^{2}\right); \end{aligned}$$

$$\tag{17}$$

we then recall (14) and the inequality for the split energy (Lemma 3.1 (iii)) to get

$$\mathcal{E}_{\mathrm{kin}}(\rho_{1}^{i}) + \mathcal{E}_{\mathrm{kin}}\left(\rho_{1}^{i}\right) \leq \mathcal{E}_{\mathrm{kin}}(\eta_{i}\mathbb{P})$$
(18)

and so we conclude using (17), (18) and then Lemma 3.2.

For the estimate with the potential, it is clear that

$$v_{ee}(\bar{\mathbb{P}}) = v_{ee}(\mathbb{P}) - \int \mathbb{P}(\eta_1 + \eta_2) v_{ee}(x) dx + \int (\mathbb{P}_1 + \mathbb{P}_2) v_{ee}(x) dx;$$

Since  $v_{ee}(x) = \sum_{i < j} c(x_i, x_j)$  we just need to show that the contribution due to  $c(x_i, x_j)$  whenever 1 < i < j cancels out in the last two integrals. In fact in both integrals we can integrate out the first variable: denoting  $I = \{1\}$  and  $J = I^c$  for example we have

$$\int \mathbb{P}\eta_1 c(x_i, x_j) \, dx_I dx_J = \int c(x_i, x_j) \left( \int \mathbb{P}\eta_1 \, dx_I \right) \, dx_J$$
$$= \int c(x_i, x_j) \rho_1^1(x_J) \, dx_J$$
$$= \int c(x_i, x_j) \rho_1^1(x_J) \left( \int \frac{\rho_2^1(x_I)}{m} \, dx_I \right) \, dx_J$$
$$= \int c(x_i, x_j) \mathbb{P}_1 \, dx.$$

Deringer

In a similar way we can show that  $\int \mathbb{P}\eta_2 c(x_i, x_j) dx = \int \mathbb{P}_2 c(x_i, x_j) dx$ . Now by definition of  $\mathbb{P}_1$  and  $\mathbb{P}_2$ , this implies that

$$-\int \mathbb{P}(\eta_1 + \eta_2) \left(\sum_{1 < i < j} c(x_i, x_j)\right) dx + \int (\mathbb{P}_1 + \mathbb{P}_2) \left(\sum_{1 < i < j} c(x_i, x_j)\right) dx$$
$$= -\int (\mathbb{P}_1 + \mathbb{P}_2) \left(\sum_{1 < i < j} c(x_i, x_j)\right) dx + \int (\mathbb{P}_1 + \mathbb{P}_2) \left(\sum_{1 < i < j} c(x_i, x_j)\right) dx = 0,$$

which yields to the desired result.

#### 5 Diagonal estimates for the wave-function

We devote this last section to derive the diagonal estimates for the bosonic wave-function which minimizes the Levy–Lieb functional proving in particular Theorems 1.1 and 1.2. In the sequel we will denote  $C_1(x) = \sum_{i=2}^{N} c(x_1, x_i)$ 

**Lemma 5.1** Let  $\rho$  be an one body marginal distribution with  $\rho(\mathbb{R}^3) = N$  and let  $\beta > 0$  be such that  $\kappa(\rho, \beta) \leq \frac{1}{4(N-1)}$ , where  $\kappa$  is defined as in (4). Then, for every  $\mathbb{P} \in \prod_N(\rho)$  and  $y \in \mathbb{R}^{3N}$ , for every  $r_1, r_2$  such that  $r_1 + 2r_2 < \beta$  and  $\delta > 0$ , there exists  $z \in \mathbb{R}^{3N}$  such that, defining  $\eta_1, \eta_2, \mathbb{P}_1, \mathbb{P}_2, m$  as in (12), (14) and (15)

(i)  $\int C_1(x)(\mathbb{P}_1 + \mathbb{P}_2)dx \le 2(N-1)\Theta(\beta - r_1 - 2r_2)m;$ (ii) z is a  $(1 + \delta, 1/2)$ -doubling point at scale  $r_2$  for  $\mathbb{P}$ , that is

$$\int_{B(z,r_2)} \mathbb{P} dx \le 2(1+\delta)^{3N} \int_{B(z,r_2/(1+\delta))} \mathbb{P} dx.$$

**Proof** For  $\gamma > 0$ , let us consider the set

$$\Omega = \left\{ z \in \mathbb{R}^{3N} : |z_1 - y_i| \ge \gamma - r_2 \text{ and } |y_1 - z_i| \ge \gamma - r_2, \forall i = 2, \dots, N \right\}.$$

We know that if  $z \in \Omega$  we will have of course

...

$$C_1(y'_1, z'_2, \dots, z'_N) + C_1(z'_1, y'_2, \dots, y'_N)$$
  
<  $2(N-1)\Theta(\gamma - r_1 - 2r_2) \ \forall y' \in B(y, r_1), z' \in B(z, r_2).$ 

which in particular implies  $\int C_1(x)(\mathbb{P}_1 + \mathbb{P}_2) dx \le 2(N-1)\Theta(\gamma - r_1 - 2r_2)m$ . Now we want to see that there exists a 1/2 doubling point in  $\Omega$ ; in order to do that, it is easy to see that

$$\Omega_{-r_2} \subseteq \{ y' \in \mathbb{R}^{3N} : |y'_1 - y_i| \ge \gamma \text{ and } |y_1 - y'_i| \ge \gamma, \forall i = 2, \dots, N \}$$

And now a similar computation to what is done in [4, Lemma 2.3] and in [9, proof of Theorem 1.3 (i)] will give us

$$\int_{\Omega_{-r_2}} \mathbb{P}(x) \, dx \ge 1 - 2(N-1)\kappa(\rho, \gamma).$$

Now if we consider  $\gamma = \beta$  we have  $\kappa(\rho, \beta) \le \frac{1}{4(N-1)}$ , and so we can apply Lemma 5.2 with  $r = \frac{r_2}{1+\delta}$  get the existence of a  $(1 + \delta, 1/2)$ -doubling point at scale  $r_2$  in  $\Omega$ .  $\Box$ 

**Lemma 5.2** (Existence of doubling points) Let  $\mathbb{P} \in L^1_+(\mathbb{R}^{3N})$  be the density of a probability measure and let r > 0. Let us consider an open set  $\Omega \subseteq \mathbb{R}^{3N}$ ; we denote  $M_r := \int_{\Omega_{-r}} \mathbb{P}(x) dx$ , where  $\Omega_{-r}$  is the *r*-thinning of the set  $\Omega$ , defined as in (9). Then, whenever  $M_r > 0$ , for every  $\delta > 0$  there exists  $y \in \Omega$ , such that

$$\int_{B(y,(1+\delta)r)} \mathbb{P}(x) \, dx \leq \frac{(1+\delta)^{3N}}{M_r} \int_{B(y,r)} \mathbb{P}(x) \, dx,$$

that is, the measure  $\mathbb{P}(x) dx$  is doubling at the point y at scale r, with doubling constant  $\frac{(1+\delta)^{3N}}{M_r}$ .

**Proof** Suppose on the contrary that for every  $y \in \Omega$  the reversed inequality holds

$$\int_{B(y,(1+\delta)r)} \mathbb{P}(x) \, dx > \frac{(1+\delta)^{3N}}{M_r} \int_{B(y,r)} \mathbb{P}(x) \, dx.$$

Then we can integrate this inequality on the whole  $\Omega$ 

$$\int_{\Omega} \int_{B(y,(1+\delta)r)} \mathbb{P}(x) \, dx \, dy > \frac{(1+\delta)^{3N}}{M_r} \int_{\Omega} \int_{B(y,r)} \mathbb{P}(x) \, dx \, dy.$$

Let  $\omega_{3N}$  be the volume of the unit ball in  $\mathbb{R}^{3N}$ . Using Fubini we get

$$\begin{split} \omega_{3N} \cdot \left( (1+\delta)r \right)^{3N} &= \int_{\mathbb{R}^{3N}} \int_{B(y,(1+\delta)r)} \mathbb{P}(x) \, dx \, dy \geq \int_{\Omega} \int_{B(y,(1+\delta)r)} \mathbb{P}(x) \, dx \, dy \\ M_r \omega_{3N} \cdot r^{3N} &= \int_{\Omega_{-r}} \mathbb{P}(x) |B(x,r)| \, dz = \int_{\Omega_{-r}} \int_{|x-y| < r} \mathbb{P}(x) \, dy \, dx \\ &= \int_{\Omega} \int_{B(y,r) \cap \Omega_{-r}} \mathbb{P}(x) \, dx \, dy \leq \int_{\Omega} \int_{B(y,r)} \mathbb{P}(x) \, dx \, dy, \end{split}$$

where we crucially used that if  $y \in B(x, r)$  and  $x \in \Omega_{-r}$  then  $y \in \Omega$ . We thus reached a contradiction.

**Proposition 5.1** (One step decay) Let us consider  $\rho$  and  $\beta$  such that  $\kappa(\rho, \beta) \leq \frac{1}{4(N-1)}$ . Then there exists  $\alpha_0 = \alpha(\beta, \varepsilon)$  such that if  $\mathbb{P}$  minimizes (11), we have that for every

🖄 Springer

 $y \in D_{\alpha}$  such that  $\alpha \leq \alpha_0$ , and every  $\tilde{r} \leq \alpha/2$ , we have

$$\int_{B(y,\tilde{r}/(1+\delta))} \mathbb{P}(x) \, dx \le \frac{1}{\delta^2 \tilde{r}^2 \frac{\theta(2\alpha)}{2(1+\delta)^2 \varepsilon} + 1} \int_{B(y,\tilde{r})} \mathbb{P}(x) \, dx, \tag{19}$$

whenever  $\delta > 0$  is such that  $\theta(2\alpha) > 256\varepsilon C(\delta)/\beta^2$ , where

$$C(\delta) := \frac{(1+\delta)^2 \cdot (2(1+\delta)^{3N} - 1)}{\delta^2}.$$
 (20)

An implicit choice for  $\alpha_0$  is for example  $\theta(2\alpha_0) > 8 \max\{(N-1)\Theta(\beta/2), 832\varepsilon N^2/\beta^2\}$ .

**Proof** Let  $y \in D_{\alpha}$  and without loss of generality we can assume that  $|y_1 - y_2| < \alpha$ ; let *z* given by Lemma 5.1. We then consider  $r_1, r_2, \eta_1, \eta_2, \lambda_1, \lambda_2, \mathbb{P}_1, \mathbb{P}_2, \mathbb{P}$  defined by (12),(13), (14), (15) and (16); being  $\mathbb{P} \in \Pi_N(\rho)$ , we get, by the minimality of  $\mathbb{P}$ ,

$$\mathcal{F}_{LL,\varepsilon}(\mathbb{P}) \geq \mathcal{F}_{LL,\varepsilon}(\mathbb{P}),$$
$$\frac{\varepsilon}{4}\mathcal{E}_{\mathrm{kin}}(\bar{\mathbb{P}}) + v_{ee}(\bar{\mathbb{P}}) \geq \frac{\varepsilon}{4}\mathcal{E}_{\mathrm{kin}}(\mathbb{P}) + v_{ee}(\mathbb{P});$$

now we can use the estimates in Lemma 4.1 in order to conclude that

$$\frac{\varepsilon}{4} \int \mathbb{P}\left(\frac{|\nabla\eta_1|^2}{\eta_1} + \frac{|\nabla\eta_2|^2}{\eta_2} + \frac{|\nabla\eta_1 + \nabla\eta_2|^2}{1 - \eta_1 - \eta_2}\right) dx$$
$$\geq \int \mathbb{P}(\eta_1 + \eta_2) C_1(x) dx - \int (\mathbb{P}_1 + \mathbb{P}_2) C_1(x) dx$$

Now we make the choice  $\eta(x) = \min\left\{\frac{(1+\delta)(1-|x|)_+}{\delta}, 1\right\}^2$ . In particular  $0 \le \eta \le 1$  and  $\eta \equiv 1$  if  $|x| < \frac{1}{1+\delta}$ , and moreover  $\frac{|\nabla \eta|^2}{\eta} = 4|\nabla \sqrt{\eta}|^2 \equiv 4\left(\frac{1+\delta}{\delta}\right)^2$  if  $\frac{1}{1+\delta} \le |x| \le 1$  and 0 otherwise. Notice that  $\eta_1$  and  $\eta_2$  are centred in y and z respectively, we thus have

$$\frac{1}{4} \int \mathbb{P} \frac{|\nabla \eta_1|^2}{\eta_1} = \frac{(1+\delta)^2}{\delta^2 r_1^2} \int_{B(y,r_1) \setminus B(y,r_1/(1+\delta))} \mathbb{P}\lambda_1 \, dx$$
$$= \frac{(1+\delta)^2}{\delta^2 r_1^2} \left( \int_{B(y,r_1)} \mathbb{P}\lambda_1 \, dx - \int_{B(y,r_1/(1+\delta))} \mathbb{P}\lambda_1 \, dx \right)$$

In a similar way we have

$$\begin{split} \frac{1}{4} \int \mathbb{P} \frac{|\nabla \eta_2|^2}{\eta_2} &= \frac{(1+\delta)^2}{\delta^2 r_2^2} \left( \int_{B(z,r_2)} \mathbb{P}\lambda_2 \, dx - \int_{B(z,r_2/(1+\delta))} \mathbb{P}\lambda_2 \, dx \right) \\ &\leq \frac{(1+\delta)^2 \cdot (2(1+\delta)^{3N}-1)}{\delta^2 r_2^2} \cdot \int_{B(z,r_2/(1+\delta))} \mathbb{P}\lambda_2 \, dx \leq \frac{C(\delta)}{r_2^2} \cdot m_2 \, dx \end{split}$$

🖉 Springer

where in the last steps we used Lemma 5.1 (ii) and the definition of  $C(\delta)$  (20). Notice then that in the regime  $\lambda_1, \lambda_2 \ll 1$  [we remind that  $\lambda_1, \lambda_2$  are two parameters in the definition of the bumps  $\eta_1$  and  $\eta_2$ , see (12)] we have that the last contribution for the localization error  $\int \frac{|\nabla \eta_1 + \nabla \eta_2|^2}{1 - \eta_1 - \eta_2} \mathbb{P}$  is of order  $O(\lambda_1^2)$ .

Now we use that  $\int C_1(x) \mathbb{P} \eta_1 dx \ge \theta(\alpha + 2r_1) \cdot m$ , the nonnegativity of  $C_1$  (notice that we do not have any other information on  $C_1$  on the support of  $\eta_2$ ) and the estimates we have for  $\int C_1(x) (\mathbb{P}_1 + \mathbb{P}_2) dx$  to get

$$\int \mathbb{P}(\eta_1 + \eta_2) C_1(x) dx - \int (\mathbb{P}_1 + \mathbb{P}_2) C_1(x) dx$$
  
 
$$\geq [\theta(\alpha + 2r_1) - 2(N - 1)\Theta(\beta - r_1 - 2r_2)] \cdot m.$$

Putting everything together we have

$$\varepsilon \frac{(1+\delta)^2}{\delta^2 r_1^2} \int_{B(y,r_1)} \mathbb{P}\lambda_1 \, dx \ge \left[ \theta(\alpha+2r_1) - 2(N-1)\Theta(\beta-r_1-2r_2) - \frac{\varepsilon C(\delta)}{r_2^2} \right] \cdot m + \varepsilon \frac{(1+\delta)^2}{\delta^2 r_1^2} \int_{B(y,r_1/(1+\delta))} \mathbb{P}\lambda_1 \, dx - O(\lambda_1^2)$$

$$(21)$$

Define

$$F(r_1, \varepsilon, \alpha) := \max \left\{ \theta(\alpha + 2r_1) - 2(N-1)\Theta(\beta - r_1 - 2r_2) - \frac{4\varepsilon C(\delta)}{r_2^2} : r_2 > 0 \right\}.$$

We can take  $r_1 = \tilde{r} \le \alpha/2 \le \beta/4$  and  $r_2 = \beta/8$ , and then choose  $\alpha < \alpha_0$  such that

$$\frac{\theta(2\alpha)}{2} - 2(N-1)\Theta(\beta/2) > \frac{\theta(2\alpha)}{4} \quad \text{and} \quad \frac{\theta(2\alpha)}{2} - \frac{\varepsilon C(\delta)}{r_2^2} > \frac{\theta(2\alpha)}{4}, \quad (22)$$

obtaining  $F(r_1, \varepsilon, \alpha) \ge \theta(2\alpha)/2$ .

We can now use  $m \ge \int_{B(y,r_1/(1+\delta))} \lambda_1 \mathbb{P}(x) dx$  and, dividing by  $\lambda_1$ , we can write the inequality (21) as

$$\int_{B(y,r_1/(1+\delta))} \mathbb{P}(x) \, dx \le \frac{1+O(\lambda_1)}{\frac{\delta^2 r_1^2 F(r_1,\varepsilon,\alpha)}{(1+\delta)^2 \varepsilon} + 1} \int_{B(y,r_1)} \mathbb{P}(x) \, dx, \tag{23}$$

Thanks to Remark 4.1, we can take the limit  $\lambda_1 \rightarrow 0$  to get rid of the term  $O(\lambda_1)$ : in fact it is the only term in (23) which depends on  $\lambda_1$  or  $\lambda_2$ . Using then the lower bound estimate  $F(r_1, \varepsilon, \alpha) \ge \theta(2\alpha)/2$  in (23) we get precisely

$$\int_{B(y,\tilde{r}/(1+\delta))} \mathbb{P}(x) \, dx \leq \frac{1}{\delta^2 \tilde{r}^2 \frac{\theta(2\alpha)}{2(1+\delta)^2 \varepsilon} + 1} \int_{B(y,\tilde{r})} \mathbb{P}(x) \, dx.$$

Deringer

In order to understand for which  $\alpha$  and  $\delta$  this inequality holds, we have to ensure that the two conditions (22) are satisfied, that is

$$\theta(2\alpha) \ge \max\left\{8(N-1)\Theta\left(\frac{\beta}{2}\right), 256\frac{\varepsilon C(\delta)}{\beta^2}\right\};$$
(24)

notice that  $\alpha_0$  can be characterized as the maximal  $\alpha$  for which there exists some  $\delta$  for which (24) is satisfied that is when  $C(\delta)$  as small as possible, which is approximately achieved for  $\delta = \frac{2}{3N}$ . With this choice we have  $C(2/(3N)) \le 26N^2$  and thus

$$\theta(2\alpha_0) \ge 8 \max\left\{ (N-1)\Theta\left(\frac{\beta}{2}\right), 832\frac{\varepsilon N^2}{\beta^2} \right\}.$$
(25)

We will now iterate the estimate in Proposition 5.1

**Theorem 5.1** Let us consider  $\rho$  and  $\beta$  such that  $\kappa(\rho, \beta) \leq \frac{1}{4(N-1)}$ . Then let us consider  $\alpha < \alpha_0$  (as in Proposition 5.1) and suppose  $A := \frac{\alpha^2 \theta(2\alpha)}{8\varepsilon} \gg N^2$ . Then if  $\mathbb{P}$  minimizes (11) we have that

$$\int_{D_{\alpha/2}} \mathbb{P}(x) \, dx \le e^{-\frac{1}{6}\sqrt{\frac{\alpha^2 \theta(2\alpha)}{8\varepsilon}}} \int_{D_{2\alpha}} \mathbb{P}(x) \, dx.$$

**Proof** Let us consider  $\delta$  such that  $\delta^2 A = e^2$ . By the hypothesis on A we have  $\delta \ll 1/N$ ; in particular, by (20) we can estimate  $C(\delta) \le \frac{2}{\delta^2}$ , and then it is easy to see that  $\theta(2\alpha) > 256\varepsilon C(\delta)/\beta^2$  and thus we can apply Proposition 5.1 with  $\tilde{r} = \alpha_k = \frac{\alpha}{2}(1+\delta)^{-k}$  to obtain for every  $y \in D_{\alpha}$ 

$$\int_{B(y,\alpha_{k+1})} \mathbb{P}(x) \, dx \leq \frac{1}{\delta^2 \alpha^2 \frac{\theta(2\alpha)}{8(1+\delta)^{2k+2}\varepsilon} + 1} \int_{B(z,\alpha_k)} \mathbb{P}(x) \, dx$$
$$\leq \frac{(1+\delta)^{2k+2}}{e^2} \int_{B(y,\alpha_k)} \mathbb{P}(x) \, dx. \tag{26}$$

We can now iterate the estimate for  $k = 0, ..., k_0$  where  $(1 + \delta)^{2k_0+2} \le e^2 \le (1 + \delta)^{2k_0+4}$ . At that point we have

$$\begin{split} \int_{B(y,\alpha/2e)} \mathbb{P}(x) \, dx &\leq \int_{B(y,\alpha_{k_0+1})} \mathbb{P}(x) \, dx \leq \frac{(1+\delta)^{(k_0+1)(k_0+2)}}{(e^2)^{k_0+1}} \int_{B(y,\alpha_0)} \mathbb{P}(x) \, dx \\ &\leq e^{-k_0} \int_{B(y,\alpha/2)} \mathbb{P}(x) \, dx. \end{split}$$

Integrating this inequality for  $y \in D_{\alpha}$  we get

$$\omega_{3N} \left(\frac{\alpha}{2e}\right)^{3N} \int_{D_{\alpha/2}} \mathbb{P}(y) \, dy \leq \int_{D_{\alpha}} \int_{B(y,\alpha/2e)} \mathbb{P}(x) \, dx \, dy$$

🖉 Springer

$$\leq e^{-k_0} \int_{D_{\alpha}} \int_{B(y,\alpha/2)} \mathbb{P}(x) \, dx \, dy$$
$$\leq e^{-k_0} \omega_{3N} \left(\frac{\alpha}{2}\right)^{3N} \int_{D_{2\alpha}} \mathbb{P}(y) \, dy.$$

Now we notice that  $k_0 + 2 \ge \frac{\ln(e^2)}{2\ln(1+\delta)} \ge \frac{2}{4\delta} = \frac{\sqrt{A}}{2e}$  and so  $e^{-k_0} \le 10e^{-\frac{\sqrt{A}}{2e}}$ . In particular

$$\int_{D_{\alpha/2}} \mathbb{P}(y) \, dy \le 10 e^{-\frac{\sqrt{A}}{2e} + 3N} \int_{D_{2\alpha}} \mathbb{P}(y) \, dy;$$

notice that since  $A \gg N^2$  we have  $\ln(10) + \frac{\sqrt{A}}{2e} - 3N \ge \frac{\sqrt{A}}{6}$ .

**Proof** (Theorems 1.1 and 1.2) First we notice that if  $\psi_{\varepsilon}$  is a minimizer for (1) in the bosonic case then  $\mathbb{P}_{\varepsilon} = |\psi_{\varepsilon}|^2$  is a minimizer for (11). Then we notice that if  $\theta(2\alpha) \leq 8(N-1)\Theta(\beta/2)$  and  $\varepsilon N^2 \ll \alpha^2 \theta(2\alpha)$ , we have also  $\alpha < \alpha_0$  and so we can apply Theorem 5.1. From that we finish using that  $\mathbb{P}_{\varepsilon}$  is a probability density and so  $\int_{D_{2\alpha}} \mathbb{P}_{\varepsilon}(y) dy \leq 1$ . The conclusions for Theorem 1.1 are then implied by using  $\theta(t) = \Theta(t) = 1/t$ .

**Acknowledgements** Part of this work has been developed during a Research in Pairs program where the authors were hosted at the MFO (Mathematisches Forschungsinstitut Oberwolfach) in January 2017. S.D.M. is a member of GNAMPA (INdAM) and acknowledges the support of the AFOSR project FA8655-22-1-7034. A.G. acknowledges partial support of his research by the Canada Research Chairs Program and Natural Sciences and Engineering Research Council of Canada. L.N. is partially on academic leave at Inria (team Matherials) for the year 2022–2023 and acknowledges the hospitality if this institution during this period. His work was supported by a public grant as part of the Investissement d'avenir project, reference ANR-11-LABX-0056-LMH, LabEx LMH and from H-Code, Université Paris-Saclay. The authors want to thank M. Lewin for comments (and references) on a preliminary draft of the paper. They are also indebted to two anonymous referees for their many insightful comments on an earlier draft of this work.

#### Declarations

**Conflict of interest** On behalf of all authors, the corresponding author states that there is no conflict of interest.

#### References

- Benamou, J.-D., Carlier, G., Nenna, L.: A numerical method to solve multi-marginal optimal transport problems with coulomb cost, pp. 577–601 (2016)
- Bindini, U., De Pascale, L.: Optimal transport with Coulomb cost and the semiclassical limit of density functional theory. J. Éc. polytech. Math. 4, 909–934 (2017)
- Bindini, U., De Pascale, L., Kausamo, A.: On Seidl-type maps for multi-marginal optimal transport with Coulomb cost (2020). arXiv preprint arXiv:2011.05063
- Buttazzo, G., Champion, T., De Pascale, L.: Continuity and estimates for multimarginal optimal transportation problems with singular costs. Appl. Math. Optim. 78, 185–200 (2017)
- Buttazzo, G., De Pascale, L., Gori-Giorgi, P.: Optimal-transport formulation of electronic densityfunctional theory. Phys. Rev. A 85, 062502 (2012)

- Chen, H., Friesecke, G.: Pair densities in density functional theory. Multiscale Model. Simul. 13(4), 1259–1289 (2015)
- Colombo, M., De Pascale, L., Di Marino, S.: Multimarginal optimal transport maps for one-dimensional repulsive costs. Can. J. Math. 67, 350–368 (2015)
- Colombo, M., Di Marino, S.: Equality between Monge and Kantorovich multimarginal problems with Coulomb cost. Ann. Mat. Pura Appl. (4) 194(2), 307–320 (2015)
- Colombo, M., Di Marino, S., Stra, F.: Continuity of multimarginal optimal transport with repulsive cost. SIAM J. Math. Anal. 51(4), 2903–2926 (2019)
- Colombo, M., Di Marino, S., Stra, F.: First order expansion in the semiclassical limit of the Levy–Lieb functional (2021). arXiv e-prints, page arXiv:2106.06282
- 11. Colombo, M., Stra, F.: Counterexamples in multimarginal optimal transport with coulomb cost and spherically symmetric data. Math. Models Methods Appl. Sci. 26(06), 1025–1049 (2016)
- Cotar, C., Friesecke, G., Klüppelberg, C.: Density functional theory and optimal transportation with Coulomb cost. Commun. Pure Appl. Math. 66(4), 548–599 (2013)
- Cotar, C., Friesecke, G., Klüppelberg, C.: Smoothing of transport plans with fixed marginals and rigorous semiclassical limit of the Hohenberg–Kohn functional. Arch. Ration. Mech. Anal. 228(3), 891–922 (2018)
- 14. Coyaud, R., Ehrlacher, V., Lombardi, D., et al.: Approximation of optimal transport problems with marginal moments constraints. Technical report (2019)
- Cycon, H.L., Froese, R.G., Kirsch, W., Simon, B.: Schrödinger Operators with Application to Quantum Mechanics and Global Geometry. Texts and Monographs in Physics, study Springer, Berlin (1987)
- De Pascale, L.: Optimal transport with Coulomb cost. Approximation and duality. ESAIM Math. Model. Numer. Anal. 49(6), 1643–1657 (2015)
- 17. Di Marino, S., Gerolin, A.: An optimal transport approach for the Schrödinger bridge problem and convergence of Sinkhorn algorithm (2019)
- Di Marino, S., Gerolin, A., Nenna, L.: Optimal Transportation Theory with Repulsive Costs, "Topological Optimization and Optimal Transport in the Applied Sciences" of Radon Series on Computational and Applied Mathematics, Chapter 9, pp. 204–256. De Gruyter (2017)
- 19. Di Marino, S., Gerolin, A., Nenna, L., Seidl, M., Gori-Giorgi, P.: in preparation
- Di Marino, S., Lewin, M., Nenna, L.: Grand-canonical optimal transport (2022). arXiv preprint arXiv:2201.06859
- Friesecke, G.: A simple counterexample to the Monge ansatz in multimarginal optimal transport, convex geometry of the set of Kantorovich plans, and the Frenkel–Kontorova model. SIAM J. Math. Anal. 51(6), 4332–4355 (2019)
- Friesecke, G., Gerolin, A., Gori-Giorgi, P.: The strong-interaction limit of density functional theory (2022). arXiv preprint arXiv:2202.09760
- Friesecke, G., Schulz, A.S., Vögler, D.: Genetic column generation: fast computation of highdimensional multi-marginal optimal transport problems. SIAM J. Sci. Comput. (2021). arXiv preprint: arXiv:2103.12624
- Gerolin, A., Grossi, J., Gori-Giorgi, P.: Kinetic correlation functionals from the entropic regularisation of the strictly-correlated electrons problem. J. Chem. Theory Comput. 16(1), 488–498 (2019)
- Gerolin, A., Kausamo, A., Rajala, T.: Duality theory for multi-marginal optimal transport with repulsive costs in metric spaces. ESAIM Control Optim. Calc. Var. 25, 62 (2019)
- Khoo, Y., Lin, L., Lindsey, M., Ying, L.: Semidefinite relaxation of multi-marginal optimal transport for strictly correlated electrons in second quantization (2019)
- Kiessling, M.K.-H.: The Hartree limit of Born's ensemble for the ground state of a bosonic atom or ion. J. Math. Phys. 53(9), 095223 (2012)
- Lani, G., Di Marino, S., Gerolin, A., van Leeuwen, R., Gori-Giorgi, P.: The adiabatic strictly-correlatedelectrons functional: kernel and exact properties. Phys. Chem. Chem. Phys. 18, 21092–21101 (2016)
- Levy, M.: Universal variational functionals of electron densities, first-order density matrices, and natural spin–orbitals and solution of the *v*-representability problem. Proc. Natl. Acad. Sci. U.S.A. 76(12), 6062–6065 (1979)
- Lewin, M.: Semi-classical limit of the Levy–Lieb functional in density functional theory. C. R. Math. Acad. Sci. Paris 356(4), 449–455 (2018)
- Lewin, M., Lieb, E.H., Seiringer, R.: Universal functionals in density functional theory (2019). arXiv preprint arXiv:1912.10424
- 32. Lieb, E.H.: Density functionals for Coulomb systems. Int. J. Quantum Chem. 24, 243–277 (1983)

- Lieb, E.H., Loss, M.: Analysis. Graduate Studies in Mathematics, vol. 14, 2nd edn. American Mathematical Society, Providence (2001)
- Mirtschink, A., Umrigar, C.J., Morgan, J.D., III., Gori-Giorgi, P.: Energy density functionals from the strong-coupling limit applied to the anions of the he isoelectronic series. J. Chem. Phys. 140(18), 18A532 (2014)
- Rougerie, N.: Théorèmes de de Finetti, limites de champ moyen et condensation de Bose-Einstein. Spartacus-idh, Paris (2016). Cours Peccot au Collège de France (2014)
- Seidl, M., Di Marino, S., Gerolin, A., Nenna, L., Giesbertz, K.J.H., Gori-Giorgi, P.: The strictlycorrelated electron functional for spherically symmetric systems revisited. ArXiv e-prints (2017)
- 37. Seidl, M.: Strong-interaction limit of density-functional theory. Phys. Rev. A 60, 4387-4395 (1999)
- Seidl, M., Gori-Giorgi, P., Savin, A.: Strictly correlated electrons in density-functional theory: a general formulation with applications to spherical densities. Phys. Rev. A 75, 042511 (2007)
- Seidl, M., Perdew, J.P., Levy, M.: Strictly correlated electrons in density-functional theory. Phys. Rev. A 59, 51–54 (1999)
- Vuckovic, S., Gerolin, A., Daas, T.J., Bahmann, H., Friesecke, G., Gori-Giorgi, P.: Density functionals based on the mathematical structure of the strong-interaction limit of DFT. Wiley Interdiscip. Rev. Comput. Mol. Sci. 13, e1634 (2022)

Publisher's Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

Springer Nature or its licensor (e.g. a society or other partner) holds exclusive rights to this article under a publishing agreement with the author(s) or other rightsholder(s); author self-archiving of the accepted manuscript version of this article is solely governed by the terms of such publishing agreement and applicable law.