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A weak KAM approach to the periodic stationary Hartree equation

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Abstract. We present, through weak KAM theory, an investigation of the stationary Hartree equation in the periodic setting. More in details, we study the Mean Field asymptotics of quantum many body operators thanks to various integral identities providing the energy of the ground state and the minimum value of the Hartree functional. Finally, the ground state of the multiple-well case is studied in the semiclassical asymptotics thanks to the Agmon metric.

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1. Introduction

1.1. Motivations

Let \mathbb{T}^n be the flat torus, we consider the many body operator \widehat{H} for $N\geq 2$ interacting particles

$$\widehat{H} := -\frac{\varepsilon^2}{2} \Delta_x + \sum_{1 \le i \le N} V_{ext}(x_i) + \frac{1}{N-1} \sum_{1 \le i < j \le N} V_{int}(x_i - x_j) = -\frac{\varepsilon^2}{2} \Delta_x + W(x)$$
(1.1)

with $x \in \mathbb{T}^n$, $x = (x_1, x_2, \ldots, x_N)$, $x_i \in \mathbb{T}^d$, $n := N \cdot d$, $V_{ext}, V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ and such that V_{int} has real and nonnegative toroidal Fourier components $\langle e_k, V_{int} \rangle_{L^2} \geq 0 \ \forall k \in \mathbb{Z}^d$. In this setting, \hat{H} can be regarded as a periodic Schrödinger operator with potential $W \in C^{\infty}(\mathbb{T}^n; \mathbb{R}_+)$. The eigenvalue equation for the ground state, namely for the lowest eigenvalue E_0 of \hat{H} with the unique positive eigenfunction $\psi_0 = e^{S/\varepsilon}$,

$$\widehat{H}\,\psi_0 = E_0\,\psi_0,\tag{1.2}$$

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is directly related the following viscous Hamilton–Jacobi equation for S,

$$\frac{1}{2}|\nabla_x S(x)|^2 - W(x) + \frac{\varepsilon}{2}\Delta S(x) = c(\varepsilon), \quad x \in \mathbb{T}^n.$$
(1.3)

The viscosity solutions theory for this Hamilton–Jacobi equation ensures a unique real value $c(\varepsilon)$, the Mañé critical value, such that (1.3) admits a unique $C^2(\mathbb{T}^n)$ —solution (see [2,17] and references therein). Thus, E_0 is related to $c(\varepsilon)$ and the eigenvalue Eq. (1.2) for the ground state is equivalent to (1.3) by the relations

$$\psi_0 = e^{S/\varepsilon}, \quad E_0 = -c(\varepsilon).$$
 (1.4)

This link between the many body operator \widehat{H} in (1.1) and the Hamilton– Jacobi equation (1.3) suggests us to apply some results of weak KAM theory and viscosity solutions theory (see for example [5,7,10–15,38] and references therein) in order to investigate around Mean Field limits as $N \to +\infty$ for \widehat{H} , here in the periodic setting and inside the stationary case. Indeed, in the present paper we show that Weak KAM theory provides additional tools for investigation of the Mean Field regime in the quantum many body theory and related Hartree equation. We recall that the original idea to apply these techniques of PDE's into the framework of quantum mechanics goes back to L.C. Evans in the papers [11,12] aimed to the study of certain semiclassical approximation problems of Schrödinger eigenfunctions as $\varepsilon \to 0$.

We will discuss about the role of the semiclassical parameter $\varepsilon > 0$, the number of particles N and their link within the main results of the paper, summarized by Theorems 1.1, 1.2, 1.3 and 3.2.

1.2. Outline of the results

First, we notice that thanks to the toroidal setting and in view of the C^2 —regularity of S solving (1.3) it follows the integral equality

$$\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \left(\frac{|\nabla_x S(x)|^2}{2} - W(x) \right) \, dx = c(\varepsilon), \quad x \in \mathbb{T}^n, \quad n = N \cdot d, \tag{1.5}$$

where W is given in (1.1). Thus, the asymptotics for $N \to +\infty$ furnishes an integral with increasing dimension, with normalization factor $1/(2\pi)^n$.

Second, we introduce the stationary Hartree equation related to many body operator (1.1), (see for example [18, 24-31, 39, 40] and references therein) here for L^2 - normalized $\varphi \in C^{\infty}(\mathbb{T}^d; \mathbb{C})$, i.e. $\|\varphi\|_{L^2(\mathbb{T}^d)} = 1$,

$$-\frac{\varepsilon^2}{2}\Delta_x\varphi + V_{ext}\varphi + \left(V_{int}\star|\varphi|^2\right)\varphi = \lambda\varphi, \qquad (1.6)$$

where \star denotes convolution. Here we are interested in any solution $\varphi_0 \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ realizing the minimum value of the Hartree energy functional

$$\mathcal{E}(\varphi) := \int_{\mathbb{T}^d} \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta + \frac{1}{2} \int_{\mathbb{T}^{2d}} |\varphi(\theta)|^2 V_{int}(\theta - \alpha) |\varphi(\alpha)|^2 d\alpha d\theta.$$
(1.7)

In this setting and without additional assumptions on the potentials, the minimum point φ_0 is not necessarily unique but it can be taken to be real positive function (see Sect. 2).

A standard result of Mean Field many body theory is the limit of the ground state energy: more precisely, the energy value $E_0 = E_0(N)$ fulfills (in the next we underline the dependence from N)

$$\lim_{N \to +\infty} \frac{E_0(N)}{N} = \mathcal{E}(\varphi_0).$$

In our work we propose (when $\varepsilon > 0$ is fixed) a proof of this result directly in the toroidal setting adapting some well known techniques of many body theory working on \mathbb{R}^n . More in details, we prove (see Proposition 4.2)

$$\mathcal{E}(\varphi_0) - \frac{\|V_{int}\|_{\infty}}{2(N-1)} \le \frac{E_0(N)}{N} \le \mathcal{E}(\varphi_0), \quad \forall N \ge 2.$$
(1.8)

We underline that both $\mathcal{E}(\varphi_0)$ and $E_0(N)$ are depending from $\varepsilon > 0$.

The next step is to rewrite the Hartree equation (1.6) at $\lambda = \mathcal{E}(\varphi_0)$ by using the form of a minimum $\varphi_0(\theta) = e^{\sigma(\theta)/\varepsilon}$, where $\sigma \in C^{\infty}(\mathbb{T}^d; \mathbb{R})$, so that (see Sect. 2.2)

$$-\frac{\varepsilon}{2}\Delta\sigma(\theta) - \frac{1}{2}|\nabla\sigma(\theta)|^2 + V_{ext}(\theta) + \left(V_{int} \star |e^{\sigma(\theta)/\varepsilon}|^2\right)(\theta) = \mathcal{E}(\varphi_0), \quad \theta \in \mathbb{T}^d.$$
(1.9)

Some simple arguments (see Lemma 4.1) give

$$\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - V_{ext}(\theta) - V_{int}(\theta) \right) \, d\theta = -\mathcal{E}(\varphi_0). \tag{1.10}$$

Notice the similarities between (1.10) and (1.5), both Hamilton–Jacobi equations written in a integral form, with potentials directly related to V_{ext} , V_{int} . This connection allows to prove the first result of the paper, given by the following

Theorem 1.1. Let $\overline{V} := (2\pi)^{-d} \int_{\mathbb{T}^d} V(\theta) d\theta$, $n = N \cdot d$, $S \in C^2(\mathbb{T}^n)$ be the solution of the H–J equation (1.3), and let $\sigma \in C^{\infty}(\mathbb{T}^d; \mathbb{R})$ be a solution of (1.9). Then, we have the equalities

$$E_0(N) = -\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} \, dx + N \cdot \left(\overline{V}_{ext} + \frac{\overline{V}_{int}}{2}\right), \qquad (1.11)$$

$$\mathcal{E}(\varphi_0) = -\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma(\theta)|^2}{2} d\theta + \overline{V}_{ext} + \overline{V}_{int}.$$
 (1.12)

Moreover, for any fixed $0 < \varepsilon \leq 1$ the following statements are equivalent:

(i)
$$\lim_{N \to +\infty} \frac{E_0(N)}{N} = \mathcal{E}(\varphi_0),$$

(ii)
$$\lim_{n \to +\infty} \frac{1}{n(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} dx = \frac{1}{d(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2}\right) d\theta.$$

We stress that the equality (ii) in Thm. 1.1 is a bridge between a family of integrals on \mathbb{T}^n , with increasing dimension, and the integral on \mathbb{T}^d with fixed dimension where the Hartree equation does hold. The above equivalence result, together with the inequalities in (1.8), ensure the limit (ii).

In the non-interacting case, namely for $V_{int} = 0$, since $\psi_0(x) = \prod_{i=1}^N \varphi_0(x_i)$ it is clear that the above limits (i) - (ii) become identities

$$\begin{split} \frac{E_0(N)}{N} &= \mathcal{E}(\varphi_0),\\ \frac{1}{n(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} \, dx = \frac{1}{d(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma(\theta)|^2}{2} \, d\theta. \end{split}$$

We now focus our attention to the direct application of weak KAM theory to stationary Hartree equation and Mean Field asymptotics.

Let $u \in C^{0,1}(\mathbb{T}^n; \mathbb{R})$ be a viscosity solution (see [7,12,15,32] and references therein) of the Hamilton–Jacobi equation with potential W given in (1.1),

$$\frac{1}{2}|\nabla u(x)|^2 - W(x) = \max_{y \in \mathbb{T}^n} - W(y) =: c(0), \quad x \in \mathbb{T}^n.$$
(1.13)

Here c(0) is the Mañé critical value, which turns out in the classical mechanical case to be the maximum of the potential energy (-W), in the above formula). It is the unique value such that there exists some global viscosity solution for the equation (1.13), $c(0) = \max_{x \in \mathbb{T}^n} -W(y) = -\min_{y \in \mathbb{T}^n} W(y)$. We also remind the $C_{\text{loc}}^{1,1}$ —regularity on an open dense subset of \mathbb{T}^n for all the viscosity solutions, see [38]. Among all the possible solutions of (1.13), one can pick up the so-called 'physical' viscosity solution ensuring that (see Lemma 2 in [2])

$$\lim_{\varepsilon_j \to 0^+} \|S - u\|_{C^0(\mathbb{T}^n)} = 0$$
 (1.14)

along some subsequence $\varepsilon_j \to 0^+$. Such a solution u becomes unique under some further assumptions on the Aubry set (see [2]). However (when n is fixed) we always have the limit

$$\lim_{\varepsilon \to 0^+} c(\varepsilon) = c(0). \tag{1.15}$$

Since $E_0(N) = -c(\varepsilon)$ and $c(0) = -\min_{y \in \mathbb{T}^n} W(y)$, this is equivalent to

$$\lim_{\varepsilon \to 0^+} E_0(N) = \min_{y \in \mathbb{T}^n} W(y) \tag{1.16}$$

restoring the well known semiclassical asymptotics, as $\varepsilon \to 0^+$, of the ground state energy to the minimum of the classical energy $\min_{(x,p)} \frac{1}{2}|p|^2 + W(x) = \min_y W(y)$. Thus, for every fixed $n \in \mathbb{N}$ and $\nu > 0$, there exists $\delta = \delta(n, \nu) > 0$ such that

$$c(\varepsilon) - c(0)| < \nu, \quad \forall \ 0 < \varepsilon < \delta(n, \nu).$$
(1.17)

The target to get more informations on $\delta(n, \nu)$ is a nontrivial spectral problem since one need to exhibit the dependence of first eigenvalue E_0 both from ε than from the dimension $n = N \cdot d$. For example, select the most simple case where d = 1, $V_{int} = 0$ and $\min_{\theta \in \mathbb{T}} V_{ext}(\theta) = 0$ with nondegenerate local minima, i.e. $V''_{ext} > 0$ on these points. Then, c(0) = 0 and $c(\varepsilon) \simeq N \cdot \varepsilon$ so that $\delta(n, \nu) \simeq \nu/n$. This can be proved through the application of the Weyl law which gives the asymptotics of the number of eigenvalues on a fixed interval for operators on manifolds (like \mathbb{T}^n), see [20] and references therein. A general study requires less restrictive assumptions on V_{ext}, V_{int} and more refined arguments of spectral theory in the periodic setting, which is not the target of the present paper. We stress however that the difference $c(\varepsilon) - c(0)$ and the function $\delta(n,\nu)$ both play a crucial role in the next two results.

In view of the above observations, we now focus again our attention to integral identities, for which we have a nice control on dependence from the parameters ε and n. This will be the content of the second result of the paper, where we do not need to apply a selection for the viscosity u solving (1.13).

Theorem 1.2. Let u be any viscosity solution of (1.13), let S and $c(\varepsilon)$ given in (1.4). Let σ be as in (1.9). Then, $\forall 0 < \varepsilon \leq 1$

$$\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla u(x)|^2 \ dx = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla S(x)|^2 \ dx + c(0) - c(\varepsilon).$$
(1.18)

Moreover, for $0 < \varepsilon < \delta(n, \nu)$ with δ as in (1.17) we have

(iii)
$$\left| \frac{1}{n(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla u(x)|^2}{2} dx - \frac{1}{d(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2} \right) d\theta \right|$$

$$\leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)} .$$

By the assumption $0 < \varepsilon < \delta(n, \nu)$ we make a link between the semiclassical parameter ε and $n = N \cdot d$ where N is the number of particles. This kind of link can also be found (for other targets) in the literature of Mean Field regime for certain quantum systems, see for example [16] and references therein.

A direct consequence of Theorems 1.1 and 1.2 is that any viscosity solution u of the Hamilton–Jacobi equation (1.13) can be used to approximate the minimum value of the Hartree functional [and also $E_0(N)/N$ thanks to (1.8)]. Indeed, a direct consequence is the quantitative estimate

$$\left|\mathcal{E}(\varphi_0) - \left(\overline{V}_{ext} + \frac{\overline{V}_{int}}{2} - \frac{d}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} |\nabla u(x)|^2 dx\right)\right| \le \frac{\|V_{int}\|_{\infty}}{2(N-1)} + \frac{d\nu}{n}.$$
 (1.19)

In order to improve the statement (iii), we now consider the operator

$$\widehat{H}_{\alpha} := -\frac{\varepsilon^2}{2} \Delta_x + \sum_{1 \le i \le N} V_{ext}(x_i) + \frac{1}{(N-1)^{\alpha}} \sum_{1 \le i < j \le N} V_{int}(x_i - x_j) \quad (1.20)$$

with the exponent $\alpha \geq 1$. In the case $\alpha > 1$ now the interaction part of the potential works as a 'perturbative' term in the framework of the above Mean Field limit as $N \to +\infty$. Indeed, this is equivalent to take \hat{H} as in (1.1) with the rescaled function $V_{int}/(N-1)^{\alpha-1}$.

The third result of the paper provides a Mean Field asymptotics linked to a simplified setting with respect to Hartree equation.

Theorem 1.3. Let u be any viscosity solution of (1.13). Then, for \hat{H}_{α} as in (1.20) with $\alpha > 1$, any fixed $\nu > 0$ and $0 < \varepsilon < \delta(n, \nu)$ we have

$$(\mathbf{iv}) \quad \left|\frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla u(x)|^2}{2} \, dx - \frac{1}{d} \cdot \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma_0(\theta)|^2}{2} d\theta\right|$$

$$\leq rac{
u}{n} + rac{5\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha-1}}$$

where $\sigma_0 \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ is the unique (up to constants) solution of

$$-\frac{\varepsilon^2}{2}\Delta\sigma_0(\theta) - \frac{1}{2}|\nabla\sigma_0(\theta)|^2 + V_{ext}(\theta) = \lambda_0, \quad \theta \in \mathbb{T}^d,$$
(1.21)

and $\lambda_0 := \inf_{\|\varphi\|=1} \int_{\mathbb{T}^d} \frac{1}{2} \varepsilon^2 |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta.$

The above result shows that, in the asymptotics of large N, the Hartree energy is reduced to the functional without the interaction potential, and the Hartree equation is reduced to the ε -viscous Hamilton–Jacobi equation written on \mathbb{T}^d . Notice that for d = 1 one can recover informations about the solution of (1.21), since $e^{\sigma/\varepsilon}$ is now the eigenfunction of the lowest eigenvalue of the one dimensional Schrödinger operator $-\frac{1}{2}\varepsilon^2\frac{d^2}{d\theta^2} + V_{ext}(\theta)$, see [37]. However, despite the simplified setting of Theorem 1.3 where $\alpha > 1$ and V_{int} does not play a role in the equation for σ_0 , we have that for $d \ge 2$ the equation (1.21) is (in general) nontrivial since cannot be reduced to the sum of one-dimensional problems. See Sect. 3 for the link with the Agmon distance and multiple-well case.

To conclude, we recall that the application of KAM theory or weak KAM theory into the semiclassical Analysis of Schrödinger operators can be given for various problems: like the study of WKB quasimodes, Wigner measures or the asymptotics of the spectrum (see [3,4,6,8,21,23,34-36,43] and references therein). For the use of Fourier Integral Operators and solutions of Hamilton–Jacobi equation to represent the unitary operator solving the quantum dynamics we address to [19,22] and references therein.

2. Settings and preliminaries

2.1. The class of potentials

The class of potentials are nonnegative and satisfy the regularity $V_{ext}, V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$. In addition, we require that V_{int} has real and nonnegative Fourier components $\langle e_k, V_{int} \rangle_{L^2} := (2\pi)^{-d} \int_{\mathbb{T}^d} e^{-ik\cdot\theta} V_{int}(\theta) \, d\theta \ge 0 \, \forall k \in \mathbb{Z}^d$, and this assumption will be used in the proof of Proposition 4.2. We thus have

$$V_{int}(\theta) = \sum_{k \in \mathbb{Z}^d} c_k \, \cos\left(k \cdot \theta\right)$$

where $c_k \in \mathbb{Z}^d$, $c_k \geq 0$. In order to recover the C^{∞} —regularity one can assume for example that $c_k \sim e^{-|k|}$ as $|k| \to +\infty$. Moreover, thanks to the additional condition on the Fourier components $c_0 \geq -\sum_{|k|>0} c_k$ it follows $V_{int} \geq 0$.

About the external potential, we also require (only to prove Theorem 3.2) the additional condition to have a finite number of minimum points at $V_{ext} = 0$. This is realized for example by defining

$$V_{ext}(\theta) := \sum_{|k| \le R} b_k \cos(k \cdot \theta), \text{ for some } R > 1,$$

and where we can choose the Fourier components $b_k \in \mathbb{R}$ (in this case can be negative) in such a way that $V_{ext} \geq 0$ and $\min V_{ext} = 0$.

2.2. Some remarks on periodic Hartree equation

Under the above assumption $V_{ext}, V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ we have that Hartree functional $\varphi \mapsto \mathcal{E}(\varphi)$ given in (1.7) is weakly lower semicontinuous. Moreover, this Hartree functional is also coercive on $H^1(\mathbb{T}^d; \mathbb{C})$ since $\mathcal{E}(\varphi) \geq \frac{1}{2}\varepsilon^2 \|\nabla\varphi\|_{L^2}^2$ and Poincaré inequality on \mathbb{T}^d reads $\|\varphi\|_{L^2} \leq C \|\nabla\varphi\|_{L^2}$, hence $\|\varphi\|_{H^1} \to +\infty$ implies $\mathcal{E}(\varphi) \to +\infty$. Thus, it follows the existence of minimizers $\varphi_0 \in H^1(\mathbb{T}^d; \mathbb{C})$. The related Euler–Lagrange equation (tought in the distributional sense) at the value $\lambda_0 := \mathcal{E}(\varphi_0)$ reads

$$-\frac{\varepsilon^2}{2}\Delta\varphi_0 + V_{ext}\varphi_0 + (V_{int}\star|\varphi_0|^2)\varphi_0 = \lambda_0\varphi_0.$$
(2.1)

Moreover, since $V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ then $V_{int} \star |\varphi_0|^2$ belongs to $C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$. Hence, we can regard the equation (2.1) as a linear Schrödinger equation written with the potential $\Phi := V_{ext} + V_{int} \star |\varphi_0|^2 \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$. Furthermore, we remind that all the operators of type $-\frac{1}{2}\varepsilon^2\Delta + \Phi$ on \mathbb{T}^d with smooth potentials have finite dimensional eigenspaces with smooth eigenfunctions, and thus we deduce the inclusion $\varphi_0 \in C^{\infty}(\mathbb{T}^d; \mathbb{C})$. We also remark that φ_0 can be taken to be a real positive function, indeed by denoting $\varphi_0 = \rho e^{i\phi}$, with $\rho \in \mathbb{R}_+$ and $\phi \in \mathbb{R}$ we can write $|\varphi_0|^2 = \rho^2$ and $|\nabla \varphi_0|^2 = |\nabla \rho|^2 + \rho^2 |\nabla \phi|^2$ so that $\mathcal{E}(\varphi_0) \geq \mathcal{E}(\rho)$. We conclude that minimizers can take the form $\varphi_0 = e^{\sigma}$ with $\sigma \in C^{\infty}(\mathbb{T}^d; \mathbb{R})$ which allows to write equation (1.9).

3. Ground state of multiple-well problem

In this section we arrange the semiclassical study of the ground state for operators $\hat{H} := -\frac{1}{2}\varepsilon^2 \Delta + W$ with a potential energy $W(x) \ge 0$ assuming zero only in a finite number of wells, $W(a_\alpha) = 0$, $\alpha = 1, ..., k$. For example, referring to (1.1), this is occurring in the non-interacting case for $V_{int} = 0$ where $W(x) = \sum_{1 \le i \le N} V_{ext}(x_i)$ or in the framework of Theorem 1.3 to study equation (1.21). With respect to this target, the results shown by Simon [41,42] for the double-well case represent an important starting point.

The wave function of the ground state ψ_0 has the following form together the energy level E_0 (see 1.4): $\psi_0 = e^{S/\varepsilon}$, $E_0 = -c(\varepsilon)$, where (see 1.3)

$$\frac{1}{2}|\nabla_x S(x)|^2 - W(x) + \frac{\varepsilon}{2}\Delta S(x) = c(\varepsilon), \quad x \in \mathbb{T}^n$$

By considering the same arguments around the formulae (1.13) and (1.14), i.e. the 'physical solutions' by Gomes, we underline that the uniform limit of $S(x) = S_{\varepsilon}(x)$, along some subsequence $\varepsilon_j \to 0^+$, is running to a viscosity solution u, $\lim_{\varepsilon_j\to 0^+} ||S - u||_{C^0(\mathbb{T}^n)} = 0$, of the Hamilton-Jacobi equation

$$\frac{1}{2}|\nabla u(x)|^2 - W(x) = c(0), \qquad (3.1)$$

with c(0) = 0, which is the maximum of the *instanton* potential energy -W.

Before proceeding, it is necessary to recall an essential theorem that one can derive from the seminal paper [33] and here displayed in a form presented in [15].

Theorem 3.1. The function u is a viscosity solution of the Hamilton–Jacobi equation $H(x, \nabla u(x)) = c$ if and only if it solves the following fixed point problem: for all $x \in \mathbb{T}^n$ and for all $t \ge 0$,

$$u(x) = T_t^{-}u(x) + ct = \inf_{\gamma} \left\{ u(\gamma(0)) + \int_0^t L(\gamma(s), \dot{\gamma}(s)) ds \right\} + ct,$$

where the infimum is over all piecewise C^1 curves $\gamma : [0,t] \to \mathbb{T}^n$ such that $\gamma(t) = x$ and c = c(0) is the Mañé critical value.

In our case $L = \frac{1}{2}|\dot{x}|^2 + W(x)$ is the instanton Lagrangian function related to the Hamiltonian $H = \frac{1}{2}|\dot{x}|^2 - W(x)$ and c = 0. To gain the physical viscosity solution u(x) of the stationary equation (3.1), we are leaded to the fixed point problem:

$$u(x) = \inf_{\gamma} \left(u(\gamma(0)) + \int_0^t \frac{|\dot{\gamma}(s)|^2}{2} + W(\gamma(s))ds \right) \quad \forall t \ge 0$$
(3.2)

In what follows we will give an innovative interpretation to the fixed point Eq. (3.2). By Proposition 2 of Carmona and Simon's paper [9], one can achieve that

$$\hat{\rho}(x,y) = \inf_{\gamma,t \ge 0} \left\{ \int_0^t \frac{1}{2} |\dot{\gamma}(s)|^2 ds + W(\gamma(s)) ds \mid \gamma(0) = x, \, \gamma(t) = y \right\}$$

represents an alternative definition of the Agmon metric ρ (see [1]), $\hat{\rho}(x, y) = \rho(x, y)$,

$$\rho(x,y) := \inf_{\gamma} \int_0^1 \sqrt{2W(\gamma(\tau))} |\dot{\gamma}(\tau)| \, d\tau, \tag{3.3}$$

with $\gamma : [0,1] \to \mathbb{T}^n$ and $\gamma(0) = x$, $\gamma(1) = y$. Notice that under the integral (3.3) we see a positively 1-homogeneous function in the variable $\dot{\gamma}$, so it comes out invariant under reparametrization of the time:

$$[0,t] \longrightarrow [0,1], \quad s \longmapsto \tau(s) = s/t.$$
(3.4)

If in the points x or y the potential energy W vanishes, separating curves γ between x and y at the level E = c = 0 cannot be anymore reparametrized with a *finite* interval time [0, t], so that an opportune standard limit procedure is needed, see details at Section 1.3, after the proof of Prop. 2 of [9]. For the convenience of the reader we propose a version adapted to our aim of those calculations. From $0 \leq (|\dot{\gamma}(s)| - \sqrt{2W(\gamma(s))})^2$ we have

$$\sqrt{2W(\gamma(s))}|\dot{\gamma}(s)| \le \frac{|\dot{\gamma}(s)|^2}{2} + W(\gamma(s)).$$

By considering the integral for any u(x), we obtain:

$$u(\gamma(0)) + \int_0^t \sqrt{2W(\gamma(s))} |\dot{\gamma}(s)| ds \le u(\gamma(0)) + \int_0^t \frac{|\dot{\gamma}(s)|^2}{2} + W(\gamma(s)) ds \,. \tag{3.5}$$

The inequality is preserved passing to the infimum and the equality is achieved at the minimum energy level E = 0. Indeed, in this case we have:

$$\frac{|\dot{\gamma}(s)|^2}{2} - W(\gamma(s)) = 0, \text{ or } |\dot{\gamma}(s)| = \sqrt{2W(\gamma(s))}.$$

All these last considerations, are leading to rewrite the fixed point problem (3.2) in the following form:

$$u(x) = \inf_{\gamma} \left(u(\gamma(0)) + \int_0^1 \sqrt{2W(\gamma(\tau))} |\dot{\gamma}(\tau)| d\tau \right), \tag{3.6}$$

where the infimum is over all curves $\gamma : [0,1] \to \mathbb{T}^n$ such that $\gamma(1) = x$ at E = 0. We now give the following characterization for the multiple-well case, namely under the assumptions that there exists only a finite number of points of the torus \mathbb{T}^n in which the potential function W vanishes.

Theorem 3.2. Let $a_{\alpha} \in \mathbb{T}^n$, $\alpha = 1, \ldots, k$, $W(a_{\alpha}) = 0$ and $W(x) > 0, \forall x \in \mathbb{T}^n \setminus \{a_{\alpha}\}_{\alpha=1,\ldots,k}$. Let u be a viscosity solution of (3.1) satisfying $u(a_{\alpha}) = 0$ for all $\alpha = 1, \ldots, k$. Then u is given by

$$u(x) = \min \{\rho(a_1, x), \rho(a_2, x), \dots, \rho(a_k, x)\},$$
(3.7)

where ρ is the Agmon metric (3.3), solving the fixed point Eq. (3.6).

Proof. We suppose that in correspondence of a generic point x, the minimum of Eq. (3.7) is reached relatively to the well a_{α} . From the definition of the Agmon metric (3.3), we have that

$$\rho(a_{\alpha}, x) = \inf_{\gamma} \int_0^1 \sqrt{2W(\gamma(\tau))} |\dot{\gamma}(\tau)| d\tau$$
(3.8)

with $\gamma(0) = a_{\alpha}$ and $\gamma(1) = x$. To conclude the proof, we observe that $u(x) = \rho(a_{\alpha}, x)$ solves equation (3.6), with $u(\gamma(0)) = u(a_{\alpha}) = 0$.

Under the further assumption that W has non degenerate Hessian at the minimum points a_{α} , we know (by [2]) that the Aubry set consists in a finite number of hyperbolic periodic orbits of the Euler–Lagrange flow. This ensures that the physical Hamilton–Jacobi solution u(x) is unique. As a consequence, thanks to Theorem 3.2 and limit (1.14) we have thus proved that the function given in (3.7) is linked to the ground state $\psi_0 = e^{S/\varepsilon}$ of the operator $\hat{H} := -\frac{1}{2}\varepsilon^2\Delta + W$ by the following limit (upon passing by a converging subsequence, in C^0 —norm)

$$\lim_{\varepsilon_j \to 0} \varepsilon_j \ln \psi_0 = u. \tag{3.9}$$

This is the multiple-well version (on \mathbb{T}^n) of Theorem 2 shown by Simon [41] that works for the double well case on \mathbb{R}^n and makes use of large deviations methods. On the other hand, we also stress that Simon's result does not need to consider a suitable subsequence, namely the limit (3.9) works for $\varepsilon \to 0$.

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4. Proof of the results

We can now devote our attention to the proof of the results outlined in the Introduction.

Proof of Theorem 1.1. We begin by

$$\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \left(\frac{1}{2} |\nabla_x S(x)|^2 - W(x) \right) \, dx = c(\varepsilon), \tag{4.1}$$

where $c(\varepsilon) = -E_0$ and $n := N \cdot d$. In particular,

$$\int_{\mathbb{T}^n} W(x) \mathrm{d}x = \int_{\mathbb{T}^n} \left(\sum_{1 \le i \le N} V_{ext}(x_i) + \frac{1}{N-1} \sum_{1 \le i < j \le N} V_{int}(x_i - x_j) \right) \mathrm{d}x$$

which reads

$$\int_{\mathbb{T}^n} W(x) \, dx = \sum_{1 \le i \le N} \int_{\mathbb{T}^n} V_{ext}(x_i) \, dx + \frac{1}{N-1} \sum_{1 \le i < j \le N} \int_{\mathbb{T}^n} V_{int}(x_i - x_j) \, dx.$$

Recall the setting $\overline{V} := (2\pi)^{-d} \int_{\mathbb{T}^d} V(\theta) d\theta$, so that integrating the first term

$$\int_{\mathbb{T}^n} W(x) \, dx = N(2\pi)^{N \cdot d} \, \overline{V}_{ext} + \frac{1}{N-1} \sum_{1 \le i < j \le N} \int_{\mathbb{T}^n} V_{int}(x_i - x_j) \, dx.$$

Integrating the second term, we first observe that $\int_{\mathbb{T}^n} f(x-y)dx = \int_{\mathbb{T}^n} f(x)dx$ for all fixed $y \in \mathbb{T}^n$. We deduce

$$\int_{\mathbb{T}^n} W(x) \, dx = N(2\pi)^{N \cdot d} \, \overline{V}_{ext} + \frac{1}{N-1} \frac{N(N-1)}{2} (2\pi)^{N \cdot d} \, \overline{V}_{int},$$

and this implies

$$\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} W(x) \, dx = N \, \overline{V}_{ext} + \frac{1}{2} N \, \overline{V}_{int}$$

Thus, Eq. (4.1) can be rewritten as

$$E_0(N) = -\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla S(x)|^2 \, dx + N \cdot \left(\overline{V}_{ext} + \frac{1}{2}\overline{V}_{int}\right) \tag{4.2}$$

The second statement of the Theorem,

$$\mathcal{E}(\varphi_0) = -\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \frac{1}{2} |\nabla \sigma(\theta)|^2 d\theta + \overline{V}_{ext} + \overline{V}_{int}, \qquad (4.3)$$

follows directly from Lemma 4.1.

To conclude, in view of (4.2)–(4.3) and recalling that N = n/d we get that the difference

$$\Delta := \mathcal{E}(\varphi_0) - \frac{E_0(N)}{N} \tag{4.4}$$

equals

$$\Delta = \frac{d}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} \, dx - \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2} \right) d\theta.$$

Hence

$$\frac{\Delta}{d} = \frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} dx - \frac{1}{d} \cdot \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2}\right) d\theta.$$
(4.5)

This gives the equivalence between (i) and (ii) in the statement.

Lemma 4.1. Let σ be the solution of (1.9), then

$$\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - V_{ext}(\theta) - V_{int}(\theta) \right) \, d\theta = -\mathcal{E}(\varphi_0).$$

Proof. Pick the equation

$$-\frac{\varepsilon}{2}\Delta\sigma(\theta) - \frac{1}{2}|\nabla\sigma(\theta)|^2 + V_{ext}(\theta) + \left(V_{int} \star |e^{\sigma(\theta)/\varepsilon}|^2\right)(\theta) = \mathcal{E}(\varphi_0)$$

and integrate over \mathbb{T}^d so that

$$\int_{\mathbb{T}^d} -\frac{1}{2} |\nabla \sigma(\theta)|^2 + V_{ext}(\theta) d\theta + \int_{\mathbb{T}^d} \left(V_{int} \star |e^{\sigma(\theta)/\varepsilon}|^2 \right) (\theta) \, d\theta = (2\pi)^d \, \mathcal{E}(\varphi_0).$$

The lefthand side reads

$$\int_{\mathbb{T}^d} -\frac{1}{2} |\nabla \sigma(\theta)|^2 + V_{ext}(\theta) d\theta + \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\theta - \alpha) |e^{\sigma(\theta)/\varepsilon}|^2 d\alpha d\theta,$$

namely, since $\int_{\mathbb{T}^n} f(x-y) dx = \int_{\mathbb{T}^n} f(x) dx$ for all fixed $y \in \mathbb{T}^n$, we have

$$\int_{\mathbb{T}^d} -\frac{1}{2} |\nabla \sigma(\theta)|^2 + V_{ext}(\theta) d\theta + (2\pi)^d \,\overline{V}_{int} \int_{\mathbb{T}^d} |e^{\sigma(\theta)/\varepsilon}|^2 d\theta.$$

Since $\varphi_0(\theta) := e^{\sigma(\theta)/\varepsilon}$ is L^2 - normalized we obtain the equality

$$\int_{\mathbb{T}^d} -\frac{1}{2} |\nabla \sigma(\theta)|^2 + V_{ext}(\theta) + V_{int}(\theta) \ d\theta = (2\pi)^d \ \mathcal{E}(\varphi_0).$$

Proof of Theorem 1.2. The equality

$$\frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla u(x)|^2 \, dx = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla S(x)|^2 \, dx + c(0) - c(\varepsilon)$$

follows directly from the difference between (1.5) and the integral over \mathbb{T}^n of (1.13). As a consequence,

$$\frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla u(x)|^2 \, dx = \frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{1}{2} |\nabla S(x)|^2 \, dx + \frac{c(0) - c(\varepsilon)}{n}.$$

Moreover, recalling (4.4)–(4.5) together with Proposition 4.2 below, we have

$$\begin{split} & \left|\frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla S(x)|^2}{2} \, dx - \frac{1}{d} \cdot \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2}\right) d\theta \right| \\ & \leq \frac{\|V_{int}\|_{\infty}}{2d(N-1)}. \end{split}$$

Since $|c(\varepsilon) - c(0)| < \nu$ provided $0 < \varepsilon < \delta(n, \nu)$, we conclude

$$\begin{split} & \left| \frac{1}{n} \cdot \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla u(x)|^2}{2} \, dx - \frac{1}{d} \cdot \frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2} \right) d\theta \right| \\ & \leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)}. \end{split}$$

Proof of Theorem 1.3. Let $\sigma_0 \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ be the unique (up to constants) solution of

$$-\frac{\varepsilon}{2}\Delta\sigma_0(\theta) - \frac{1}{2}|\nabla\sigma_0(\theta)|^2 + V_{ext}(\theta) = \lambda_0, \quad \theta \in \mathbb{T}^d,$$

where $\lambda_0 := \inf_{\|\varphi\|_{L^2}=1} \int_{\mathbb{T}^d} \frac{1}{2} \varepsilon^2 |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta$. Thus,

$$\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma_0(\theta)|^2}{2} d\theta = \overline{V}_{ext} - \lambda_0.$$
(4.6)

We now use the inequality (iii) shown in Theorem 1.2, by replacing \overline{V}_{int} by $\overline{V}_{int}/(N-1)^{\alpha-1}$, $\alpha > 1$, so that

$$\begin{aligned} \left| \frac{1}{n(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla u(x)|^2}{2} \, dx - \frac{1}{d(2\pi)^d} \int_{\mathbb{T}^d} \left(\frac{|\nabla \sigma(\theta)|^2}{2} - \frac{\overline{V}_{int}}{2(N-1)^{\alpha-1}} \right) d\theta \right| \\ &\leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha}} \,, \end{aligned}$$

and thus

$$\begin{aligned} \left| \frac{1}{n(2\pi)^n} \int_{\mathbb{T}^n} \frac{|\nabla u(x)|^2}{2} \, dx - \frac{1}{d(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma(\theta)|^2}{2} d\theta \\ &\leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha}} + \frac{\overline{V}_{int}}{2d(N-1)^{\alpha-1}}. \end{aligned} \end{aligned}$$

Now Eq. (1.10) is modified with the rescaled V_{int} ,

$$\frac{1}{(2\pi)^d} \int_{\mathbb{T}^d} \frac{|\nabla \sigma(\theta)|^2}{2} \ d\theta = \overline{V}_{ext} + \frac{\overline{V}_{int}}{(N-1)^{\alpha-1}} - \mathcal{E}(\varphi_0).$$
(4.7)

In view of (4.6)–(4.7), we need to get an estimate for $D := \mathcal{E}(\varphi_0) - \lambda_0 \ge 0$

$$D = \inf_{\varphi} \left\{ \int_{\mathbb{T}^d} \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta + \frac{1}{2} \int_{\mathbb{T}^{2d}} |\varphi(\theta)|^2 \frac{V_{int}(\theta - \alpha)}{(N - 1)^{\alpha - 1}} |\varphi(\alpha)|^2 d\alpha d\theta \right\}$$
$$- \inf_{\varphi} \int_{\mathbb{T}^d} \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta.$$

Notice that for $\|\varphi\| = 1$ we have

$$\frac{1}{2} \int_{\mathbb{T}^{2d}} |\varphi(\theta)|^2 \frac{V_{int}(\theta - \alpha)}{(N-1)^{\alpha - 1}} |\varphi(\alpha)|^2 d\alpha d\theta \le \frac{\|V_{int}\|_{\infty}}{2(N-1)^{\alpha - 1}}$$

and thus we have the following upper bound for ${\cal D}$

$$D \leq \inf_{\varphi} \int_{\mathbb{T}^d} \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta + \frac{\|V_{int}\|_{\infty}}{2(N-1)^{\alpha-1}} - \inf_{\varphi} \int_{\mathbb{T}^d} \frac{\varepsilon^2}{2} |\nabla \varphi|^2 + V_{ext}(\theta) |\varphi(\theta)|^2 d\theta = \frac{\|V_{int}\|_{\infty}}{2(N-1)^{\alpha-1}}.$$

We conclude

$$\left|\frac{1}{n(2\pi)^n}\int_{\mathbb{T}^n}\frac{|\nabla u(x)|^2}{2}\ dx - \frac{1}{d(2\pi)^d}\int_{\mathbb{T}^d}\frac{|\nabla \sigma_0(\theta)|^2}{2}d\theta\right|$$

$$\leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha}} + \frac{\overline{V}_{int}}{2d(N-1)^{\alpha-1}} + \frac{\overline{V}_{int}}{d(N-1)^{\alpha-1}} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha-1}},$$

but since $\overline{V}_{int} \leq ||V_{int}||_{\infty}$ the final upper bound can be written by

$$\leq \frac{\nu}{n} + \frac{\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha}} + \frac{2\|V_{int}\|_{\infty}}{d(N-1)^{\alpha-1}} \leq \frac{\nu}{n} + \frac{5\|V_{int}\|_{\infty}}{2d(N-1)^{\alpha-1}}.$$

In the next result we mainly follow the same arguments shown in section 3 of [25], here adapted for the toroidal case.

Proposition 4.2. Let $\mathcal{E}(\varphi_0)$ be the minimum value of the Hartree functional and let E_0 be the lowest eigenvalue of \hat{H} . Then,

$$\mathcal{E}(\varphi_0) - \frac{\|V_{int}\|_{\infty}}{2(N-1)} \le \frac{E_0(N)}{N} \le \mathcal{E}(\varphi_0), \quad \forall N \ge 2.$$

Proof. We rewrite the operator $\hat{H} = -\frac{1}{2}\varepsilon^2 \Delta_x + W(x)$ as

$$\widehat{H} = \sum_{1 \le i \le N} \widehat{h}_i + \frac{1}{N-1} \sum_{1 \le i < j \le N} V_{int}(x_i - x_j)$$

where $V_{ext}, V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ and $\hat{h}_i := -\frac{1}{2}\varepsilon^2 \partial_{x_i}^2 + V_{ext}(x_i)$. Let φ_0 be a minimizer of $\mathcal{E}(\varphi)$ and define $\xi_0(x) := \prod_{i=1}^N \varphi_0(x_i)$, then

$$\langle \xi_0, \widehat{H}\xi_0 \rangle = N\mathcal{E}(\varphi_0)$$

Hence, the upper bound is directly obtained by

$$E_0 := \langle \psi_0, \widehat{H}\psi_0 \rangle = \inf_{\|\psi\|=1} \langle \psi, \widehat{H}\psi \rangle \le \langle \xi_0, \widehat{H}\xi_0 \rangle = N\mathcal{E}(\varphi_0).$$

Conversely, we first observe that the ground state $\psi_0 = \psi_0(x_1, x_2, \ldots, x_N)$ is symmetric with respect to exchange of variables. Indeed, let us denote \hat{P}_{ij} as the exchange (selfadjoint) operator on $L^2(\mathbb{T}^n)$ that works as

$$(\widehat{P}_{ij}\psi)(x_1,\ldots,x_i,x_j,\ldots,x_N) := \psi(x_1,\ldots,x_j,x_i,\ldots,x_N)$$

where $x_i \in \mathbb{T}^d$ and $n = N \cdot d$. Now easily notice the commutation property $[\hat{H}, \hat{P}_{ij}] = 0$ since $[W, \hat{P}_{ij}] = 0$. We thus have that \hat{H} and \hat{P}_{ij} have a common base of eigenfunctions (symmetric or anti-symmetric). As a consequence, the strictly positive eigenfunction $\psi_0 > 0$ (associated to the nondegenerate eigenvalue E_0) cannot be an antisymmetric function. We deduce that ψ_0 is symmetric and that we can restrict the variational problem $\inf_{\|\psi\|=1} \langle \psi, \hat{H}\psi \rangle$ to $\psi \in L^2_s(\mathbb{T}^n)$ here defined as the functions in $L^2(\mathbb{T}^n)$ such that $\hat{P}_{ij}\psi = \hat{P}_{ji}\psi$. Now we can apply Hoffmann–Ostenhof inequality for $L^2_s(\mathbb{T}^n)$

$$\left\langle \psi_0, \sum_{i=1}^N \widehat{h}_i \psi_0 \right\rangle \ge N \left\langle \sqrt{\rho_{\psi_0}}, \widehat{h} \sqrt{\rho_{\psi_0}} \right\rangle$$
(4.8)

where $\rho_{\psi_0}(\theta) := \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} \dots \int_{\mathbb{T}^d} |\psi_0(\theta, x_2, x_3, \dots, x_N)|^2 dx_2 dx_3, \dots, dx_N$. The proof of (4.8) can be found in Lemma 3.2 of [25] written for symmetric functions in $L^2(\mathbb{R}^n)$, but working also on $L^2_s(\mathbb{T}^n)$.

As for interaction part, pick an arbitrary $\eta \in L^1(\mathbb{T}^d; \mathbb{R})$ and use the inequality shown in our Lemma 4.3,

$$\sum_{1 \le i < j \le N} V_{int}(x_i - x_j) \ge \sum_{1 \le i \le N} (V_{int} \star \eta)(x_i) -\frac{1}{2} \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) \eta(\alpha) \eta(\theta) d\alpha d\theta - \frac{N}{2} \|V_{int}\|_{\infty}.$$

Now integrate with the normalized ψ_0 and use the lower bound with $\eta := N\rho_{\psi_0}$, so that for $g_0 := \sqrt{\rho_{\psi_0}}$ we have

$$\int_{\mathbb{T}^{n}} \psi_{0}(x) \frac{1}{N-1} \sum_{1 \leq i < j \leq N} V_{int}(x_{i} - x_{j}) \psi_{0}(x) dx \\
\geq \frac{N^{2}}{2(N-1)} \int_{\mathbb{T}^{2d}} |g_{0}(\theta)|^{2} V_{int}(\theta - \alpha) |g_{0}(\alpha)|^{2} d\alpha d\theta - \frac{N \|V_{int}\|_{\infty}}{2(N-1)} \\
\geq \frac{N}{2} \int_{\mathbb{T}^{2d}} |g_{0}(\theta)|^{2} V_{int}(\theta - \alpha) |g_{0}(\alpha)|^{2} d\alpha d\theta - \frac{N \|V_{int}\|_{\infty}}{2(N-1)}.$$
(4.9)

In view of (4.8)–(4.9) and recalling that φ_0 is a minimizer of $\mathcal{E}(\varphi)$ we conclude

$$\mathcal{E}(\varphi_0) - \frac{\|V_{int}\|_{\infty}}{2(N-1)} \le \mathcal{E}(g_0) - \frac{\|V_{int}\|_{\infty}}{2(N-1)} \le \frac{E_0(N)}{N}.$$

Lemma 4.3. Let $V_{int} \in C^{\infty}(\mathbb{T}^d; \mathbb{R}_+)$ be as in Sect. 2.1. Then, $\forall \eta \in L^1(\mathbb{T}^d; \mathbb{R})$

$$\sum_{1 \le i < j \le N} V_{int}(x_i - x_j) \ge \sum_{1 \le i \le N} (V_{int} \star \eta)(x_i)$$
$$-\frac{1}{2} \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) \eta(\alpha) \eta(\theta) d\alpha d\theta - \frac{N}{2} \|V_{int}\|_{\infty}.$$

Proof. Define $f(x, \alpha) := \eta(\alpha) - \sum_{1 \le i \le N} \delta(\alpha - x_i)$ and observe that

$$\frac{1}{2} \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) f(x, \alpha) f(x, \theta) d\alpha d\theta$$

$$= -\sum_{1 \le i \le N} (V_{int} \star \eta)(x_i) + \frac{1}{2} \int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) \eta(\alpha) \eta(\theta) d\alpha d\theta$$

$$+ \sum_{1 \le i < j \le N} V_{int}(x_i - x_j) + \frac{N}{2} V_{int}(0).$$
(4.10)

Notice in particular that $0 \leq V_{int}(0) \leq ||V_{int}||_{\infty}$.

By the use of toroidal Fourier transform $\widehat{V}_{int}(k) := (2\pi)^{-d} \int_{\mathbb{T}^d} V_{int}(y) e^{-ik \cdot y} dy$ (which gives in fact the Fourier components) and related standard properties as unitary operator from $L^2(\mathbb{T}^d)$ into square integrable functions on \mathbb{Z}^d with $\ell^2(\mathbb{Z}^d)$ scalar product, we get

$$\int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) f(x, \alpha) f(x, \theta) d\alpha d\theta$$

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$$= \int_{\mathbb{T}^d} \sum_{k \in \mathbb{Z}^d} \widehat{V}_{int}(k-\theta) \widehat{f}(x,k) f(x,\theta) d\theta$$

where $\widehat{f}(x,k) = \widehat{\eta}(k) - (2\pi)^{-d} \sum_{1 \le i \le N} e^{ik \cdot x_i}$ and $\widehat{V}_{int}(k-\theta) = \widehat{V}_{int}(k)e^{ik\cdot\theta}$. Thus,

$$\begin{split} &\int_{\mathbb{T}^d} \int_{\mathbb{T}^d} V_{int}(\alpha - \theta) f(x, \alpha) f(x, \theta) d\alpha d\theta \\ &= \sum_{k \in \mathbb{Z}^d} \widehat{V}_{int}(k) \widehat{f}(x, k) \int_{\mathbb{T}^d} e^{ik \cdot \theta} f(x, \theta) d\theta \\ &= (2\pi)^d \sum_{k \in \mathbb{Z}^d} \widehat{V}_{int}(k) \widehat{f}(x, k) \widehat{f^*}(x, k) \\ &= (2\pi)^d \sum_{k \in \mathbb{Z}^d} \widehat{V}_{int}(k) |\widehat{f}(x, k)|^2 \ge 0 \end{split}$$
(4.11)

where the last inequality is ensured thanks to the assumption $\widehat{V}_{int}(k) \geq 0$. To conclude, combining (4.11) with (4.10) we get the statement.

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