

Ground State Energy of the Low Density Hubbard Model

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Abstract We derive a lower bound on the ground state energy of the Hubbard model for given value of the total spin. In combination with the upper bound derived previously by Giuliani (J. Math. Phys. 48:023302, 2007), our result proves that in the low density limit the leading order correction compared to the ground state energy of a non-interacting lattice Fermi gas is given by $8\pi a\varrho_u\varrho_d$, where $\varrho_{u(d)}$ denotes the density of the spin-up (down) particles, and a is the scattering length of the contact interaction potential. This result extends previous work on the corresponding continuum model to the lattice case.

Keywords Hubbard model · Scattering length · Ground state energy · Thermodynamic limit

1 Introduction

In recent years, much effort has been made to rigorously analyze the properties of dilute quantum gases at low temperature and low density. For repulsive pair interaction potentials, the leading order correction compared to the case of ideal quantum gases of the ground state energy and free energy of continuous quantum gases in the thermodynamic limit have been investigated in [2, 9–11, 14, 15, 17, 18].

In particular, in [9] it was proved that the ground state energy per unit volume of a low-density spin 1/2 Fermi gas with repulsive pair interaction is (in units where $\hbar = 2m = 1$) given by

$$\frac{3}{5}(6\pi^2)^{2/3}(\varrho_u^{5/3} + \varrho_d^{5/3}) + 8\pi a\varrho_u\varrho_d + o(\varrho^2). \quad (1.1)$$

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Here, $\rho_{u(d)}$ denotes the density of the spin-up (down) particles, and $a > 0$ is the scattering length of the interaction potential. The total density of the system equals $\rho = \rho_u + \rho_d$, and $(\rho_u - \rho_d)/(2\rho)$ is the average spin per particle. We remark that as long as the higher order terms can be neglected, the formula (1.1) leads to the conclusion that there is no net magnetization for small enough $a^3\rho$, while there is spontaneous magnetization for larger values [5].

The goal of this paper is to extend the analysis in [9] from the continuum to the lattice case. We restrict our attention to the case of a simple cubic, three-dimensional lattice. Without loss of generality, we choose units such that the spacing between two neighboring lattice sites is one; i.e., the configuration space for one (spinless) particle is \mathbb{Z}^3 .

For simplicity, we consider the case where the interaction potential between the particles has zero range, i.e., only particles on the same lattice site interact. This is the simplest version of the *Hubbard model*, which was originally introduced as a highly simplified model for fermions with repulsive (Coulomb) interaction. For a review of the history, rigorous results and open problems, we refer to [8, 19].

An upper bound to the ground state energy of the desired form was already derived in [3], hence we concentrate here on the lower bound. Our main result is given in Theorem 1 below. In combination, the two bounds show that the ground state energy per unit volume of the Hubbard model at low density $\rho = \rho_u + \rho_d$ and at given spin polarization $(\rho_u - \rho_d)/(2\rho)$ is given by

$$e_0(\rho_u, \rho_d) + 8\pi a\rho_u\rho_d + o(\rho^2),$$

where, as before, a denotes the (appropriately defined) scattering length of the interaction potential, and $e_0(\rho_u, \rho_d)$ is the ground state energy per unit volume of the ideal lattice Fermi gas.

1.1 Model and Main Result

We consider particles hopping on the simple cubic lattice \mathbb{Z}^3 . For N spinless fermions, the appropriate Hilbert space $\mathcal{H}(N)$ is the subspace of totally antisymmetric functions in $L^2(\mathbb{Z}^{3N})$, with norm

$$\|\psi\|_2 = \sqrt{\sum_{x_1 \in \mathbb{Z}^3} \cdots \sum_{x_N \in \mathbb{Z}^3} |\psi(x_1, \dots, x_N)|^2}.$$

We define $\mathcal{H}(N_u, N_d) \subset L^2(\mathbb{Z}^{3N_u+3N_d})$ as

$$\mathcal{H}(N_u, N_d) = \mathcal{H}(N_u) \otimes \mathcal{H}(N_d). \tag{1.2}$$

Elements of $\mathcal{H}(N_u, N_d)$ are thus functions of $N_u + N_d$ variables that are antisymmetric both in the first N_u and the last N_d variables. In appropriate units, the Hubbard Hamiltonian for N_u spin-up particles and N_d spin-down fermions in a box $[0, L]^3$ is given by

$$H = - \sum_{i=1}^{N_u} \Delta_{x_i} - \sum_{i=1}^{N_d} \Delta_{y_i} + g \sum_{i=1}^{N_u} \sum_{j=1}^{N_d} \delta_{x_i, y_j}, \tag{1.3}$$

where x_1, \dots, x_{N_u} and y_1, \dots, y_{N_d} are the coordinates of the spin-up and spin-down particles, respectively. The usual lattice Laplacian is denoted by Δ ; it acts as $(\Delta f)(x) = \sum_{y, |x-y|=1} (f(y) - f(x))$. We consider *Dirichlet boundary conditions* on $[0, L]$, i.e., we

restrict H to functions that vanish outside the cube $[1, L - 1]^3$. The thermodynamic limit corresponds to taking $L \rightarrow \infty$, $N_u \rightarrow \infty$ and $N_d \rightarrow \infty$ in such a way that

$$\varrho_u = \lim \frac{N_u}{L^3} \quad \text{and} \quad \varrho_d = \lim \frac{N_d}{L^3}.$$

Note that necessarily $0 \leq \varrho_{u(d)} \leq 1$ because of the antisymmetry of the wavefunctions.

We remark that instead of considering two species of spinless fermions with particle numbers N_u and N_d , as we do here, one can equivalently consider just one species of $N_u + N_d$ fermions with spin $1/2$, and restrict to the subspace where the z -component of the total spin equals $S_z = (N_u - N_d)/2$. We will use the former formulation for convenience.

The coupling constant g is assumed to be nonnegative and is allowed to take the value $+\infty$. The scattering length a of the interaction potential $g\delta_{0,x}$ is given by (cf. [3, (1.6)])

$$a = \frac{g}{8\pi(g\gamma + 1)}, \quad \gamma = \int_{[-\pi,\pi]^3} \frac{1}{4 \sum_{i=1}^3 (1 - \cos k^i)} \frac{dk}{(2\pi)^3}, \tag{1.4}$$

where $k = (k^1, k^2, k^3) \in \mathbb{R}^3$. We refer to Sect. 2.2 for details.

Our main result of this paper is the following.

Theorem 1 *Let $E_0(N_u, N_d, L)$ be the ground state energy of H in (1.3). If $L \rightarrow \infty$, $N_u \rightarrow \infty$, $N_d \rightarrow \infty$ with $\varrho_u = \lim_{L \rightarrow \infty} N_u/L^3$ and $\varrho_d = \lim_{L \rightarrow \infty} N_d/L^3$, then*

$$\liminf_{L \rightarrow \infty} \frac{1}{L^3} E_0(N_u, N_d, L) \geq e_0(\varrho_u, \varrho_d) + 8\pi a \varrho_u \varrho_d (1 - o(1)), \tag{1.5}$$

with $o(1) \leq C(a\varrho^{1/3})^{1/15}$ for some constant $C > 0$. Here $e_0(\varrho_u, \varrho_d)$ is the ground state energy per unit volume of the ideal lattice Fermi gas, and $\varrho = \varrho_u + \varrho_d$.

As already pointed out in the introduction, an upper bound of the desired form (1.5) was proved by Giuliani in [3], extending the method used in [9]. This shows that (1.5) actually holds as an equality.

It is easy to see that

$$e_0(\varrho_u, \varrho_d) = \frac{3}{5} (6\pi^2)^{2/3} (\varrho_u^{5/3} + \varrho_d^{5/3}) + O(\varrho^{7/3}) \tag{1.6}$$

for small ϱ . Hence, at fixed a , the expression for the ground state energy of the continuous Fermi gas (1.1) and the one for the lattice Fermi gas coincide up to terms of order $o(\varrho^2)$. Theorem 1 is slightly stronger, however, since the error term is $o(a\varrho^2)$, not $o(\varrho^2)$. Hence (1.5) should be viewed as a result for small $a\varrho^{1/3}$, which could be achieved either by making ϱ small or by making a small. We point out, however, that the case of small a is much simpler than the case of small ϱ , since the correct result can be obtained via first order perturbation theory in this case, while this is not possible for fixed a and small ϱ . For small a and fixed ϱ , the Hartree-Fock approximation becomes exact, as was shown in [1].

We state and prove Theorem 1 for the simple cubic lattice and zero-range interaction, for simplicity, but the method can be used in more general cases. For instance, different lattice structures could be considered, or longer-ranged hopping. Interactions of longer range could also be included, as long as they are non-negative and have a finite scattering length; and particles with more than two spin states could be considered, as in [9]. In combination with

the methods developed in [17], our technique can also be applied at non-zero temperature to estimate the pressure or the free energy.

The proof of Theorem 1 follows closely the corresponding continuum result in [9], with several important and non-trivial modifications, however. One of the main ingredients is the generalized Dyson Lemma, stated in Lemma 1 below, which allows for the replacement of the hard interaction potential $g\delta_{xy}$ by a softer and longer ranged potential, at the expense of the high momentum part of the kinetic energy. The proof of the corresponding Lemma 4 in [9] uses rotational invariance of \mathbb{R}^3 in an essential way, and hence does not extend to the lattice case of \mathbb{Z}^3 , where such a symmetry is absent. (See also the discussion in [3].) Our new Lemma 1 does not rely on this symmetry, however.

Another important estimate in [9] that does not carry over to the lattice case is a bound on the average number of particles that are close to their nearest neighbor. The estimate in [9, Lemma 6] uses an inequality by Lieb and Yau [13, Theorem 5] whose proof also relies on the rotational invariance of \mathbb{R}^3 . In Lemma 4 below we will present a weaker version of this inequality which is equally valid in the lattice case.

The strategy of the proof of Theorem 1 is similar to the proof in [9]. First, we separate the Hamiltonian H into two parts, the low momentum part of the kinetic energy on the one hand, and the high momentum part of the kinetic energy together with the interaction energy on the other hand. The first part is larger than $e_0(Q_u, Q_d)$, while the second part can be bounded from below by a softer interaction potential; this is the content of Lemma 1. In Lemma 2, we shall show that at low density the one particle density matrix of the ground state of the Hubbard model is close to a projection, namely the projection onto the Fermi sea. This information will then be used to prove that the expectation value of the softer interaction potential is given by $8\pi a Q_u Q_d$ to leading order. To bound some of the error terms, we need a bound on the expected number of particles whose distance to the nearest neighbor is small. This will be accomplished in Lemma 3.

In the next section, we shall state some preliminaries and introduce the notation used throughout the proof. Section 3 contains the main three lemmas, which we have already referred to above. Finally, in Sect. 4 the proof of Theorem 1 will be given.

2 Preliminaries

2.1 Notation

We start by introducing some notation that will be used throughout the proof. First, the gradient operator $\nabla = (\nabla^1, \nabla^2, \nabla^3)$ on $L^2(\mathbb{Z}^3)$ is defined as usual as

$$(\nabla^i f)(x) = f(x + e^i) - f(x),$$

with e^i denoting the unit vector in the i 'th coordinate direction. Its adjoint is given by $(\nabla^{i\dagger} f)(x) = f(x - e^i) - f(x)$. The Laplacian can then be expressed in terms of the gradient as

$$-\Delta = \nabla^\dagger \cdot \nabla = \nabla \cdot \nabla^\dagger.$$

For any subset $A \subset \mathbb{Z}^3$, we denote by θ_A its characteristic function. It will be convenient to introduce the notation

$$[\nabla^\dagger \theta_A \nabla]_s \equiv \frac{1}{2}(\nabla^\dagger \cdot \theta_A \nabla + \nabla \cdot \theta_A \nabla^\dagger).$$

Note that this is a nonnegative operator which plays the role of the (Neumann) Laplacian on A . For $A \subset \mathbb{Z}^3$ bounded, we denote by P_A the projection onto the normalized constant function on A ,

$$P_A \equiv \frac{|\theta_A\rangle\langle\theta_A|}{\|\theta_A\|_2^2}.$$

For $h \in L^1(\mathbb{Z}^3)$, we define the convolution operator C_h as

$$(C_h \psi)(x) = h * \psi(x) = \sum_{y \in \mathbb{Z}^3} h(x - y)\psi(y).$$

Its adjoint is given by $(C_h^\dagger \psi)(x) = \sum_{y \in \mathbb{Z}^3} \overline{h(y - x)}\psi(y)$.

We recall also the natural definition of the Fourier transform, mapping $L^2(\mathbb{Z}^3)$ to $L^2([-\pi, \pi]^3)$. For $p = (p^1, p^2, p^3) \in \mathbb{R}^3$, $|p^i| \leq \pi$,

$$\widehat{\psi}(p) = \sum_{x \in \mathbb{Z}^3} e^{-ip \cdot x} \psi(x).$$

Its inverse is given by

$$\psi(x) = \frac{1}{(2\pi)^3} \int_{[-\pi, \pi]^3} e^{ip \cdot x} \widehat{\psi}(p) dp.$$

Using the above definitions, the following properties are easily verified:

$$\begin{aligned} \widehat{\delta_{x,0}}(p) &= 1, \\ \widehat{h * \psi}(p) &= \widehat{h}(p)\widehat{\psi}(p), \\ \|\psi\|_2^2 &= \int_{[-\pi, \pi]^3} |\widehat{\psi}(p)|^2 \frac{dp}{(2\pi)^3}, \\ -\langle \psi | \Delta | \psi \rangle &= \sum_{j=1}^3 \int_{[-\pi, \pi]^3} (2 - 2 \cos p^j) |\widehat{\psi}(p)|^2 \frac{dp}{(2\pi)^3}. \end{aligned} \tag{2.1}$$

In particular, if M and M' are two functions satisfying

$$|\widehat{M}(p)|^2 + |\widehat{M'}(p)|^2 = 1 \quad \text{for all } p \in [-\pi, \pi]^3,$$

we can decompose the Laplacian Δ as

$$\Delta = C_M^\dagger \Delta C_M + C_{M'}^\dagger \Delta C_{M'}. \tag{2.2}$$

We will use this decomposition in the proof of Theorem 1 in order to separate the kinetic energy into the high momentum and the low momentum parts.

Finally, it will be convenient to introduce the operator

$$\Xi_A \equiv [\nabla^\dagger \cdot \theta_A \nabla]_s + \theta_A \Delta. \tag{2.3}$$

It has the property that

$$\langle f | \Xi_A | g \rangle = \frac{1}{2} \sum_{\substack{x \in A, y \notin A \\ |x-y|=1}} [f(x) + f(y)][g(y) - g(x)]. \tag{2.4}$$

2.2 Scattering Length

We denote by φ the solution of the zero-energy scattering equation

$$-\Delta\varphi(x) + \frac{1}{2}g\delta_{0,x}\varphi(x) = 0 \tag{2.5}$$

with boundary condition $\lim_{|x|\rightarrow\infty} \varphi(x) = 1$. It is given by [3, (1.5)]

$$\varphi(x) = 1 - 4\pi a \int_{[-\pi,\pi]^3} \frac{e^{ip\cdot x}}{2\sum_{j=1}^3(1-\cos p^j)} \frac{dp}{(2\pi)^3}, \tag{2.6}$$

where a is the scattering length (1.4). It can be shown [16] that there is a constant $C > 0$ such that

$$\left| \varphi(x) - 1 + \frac{a}{|x|} \right| \leq C \frac{a}{|x|^3}. \tag{2.7}$$

Note that, in particular, $a = \lim_{|x|\rightarrow\infty} (\varphi(x) - 1)|x|$. It can be readily checked that

$$-\sum_{x\in\mathbb{Z}^3} \Delta\varphi(x) = \frac{1}{2}g\varphi(0) = 4\pi a. \tag{2.8}$$

Another property of φ we will need is [3, (1.7)]

$$\sum_{\substack{x\in A, y\notin A \\ |x-y|=1}} (\varphi(y) - \varphi(x)) = 4\pi a \tag{2.9}$$

for any simply connected domain A containing the origin.

2.3 Non-interacting Fermions

We recall here briefly the ground state energy of non-interacting (spinless) fermions on the lattice \mathbb{Z}^3 . For $p \in [-\pi, \pi]^3$, the dispersion relation will be denoted by

$$E(p) = 2 \sum_{i=1}^3 (1 - \cos p^i).$$

For given density $0 \leq \varrho \leq 1$, the Fermi energy $E_f(\varrho)$ is determined by

$$(2\pi)^{-3} \int_{E(p)\leq E_f(\varrho)} dp = \varrho. \tag{2.10}$$

The ground state energy per unit volume in the thermodynamic limit is then

$$e(\varrho) = (2\pi)^{-3} \int_{E(p)\leq E_f(\varrho)} E(p) dp.$$

For spin 1/2 particles with spin-up density ϱ_u and spin-down density ϱ_d , the ground state energy is thus $e_0(\varrho_u, \varrho_d) = e(\varrho_u) + e(\varrho_d)$.

3 Auxiliary Lemmas

3.1 Lemma One

As mentioned in the Introduction, Lemma 1 is the main tool of this paper. It is similar to Lemma 4 in [9]. This lemma allows for bounding the hard interaction $g\delta_{0,x}$ from below by a softer interaction at the expense of the high momentum part of the kinetic energy and some error terms.

Lemma 1 For $r \in \mathbb{N}$, let $A(r)$ denote the cube $A(r) = [-r, r]^3 \cap \mathbb{Z}^3$. For any function $h \in L^1(\mathbb{Z}^3)$ satisfying $1 \geq \widehat{h}(p) \geq 0$, let

$$f_r(x) = \max_{y \in x+A(r)} |h'(y) - h'(x)|, \quad \text{where } \widehat{h}'(p) = 1 - \widehat{h}(p). \tag{3.1}$$

For $R \in \mathbb{N}$, let U, W and V denote the nonnegative operators

$$U = (2R + 1)^{-3} \theta_{A(R)}, \tag{3.2}$$

$$W = 16\pi f_R \sum_{x \in \mathbb{Z}^3} f_R(x) \tag{3.3}$$

and

$$V = (2R + 1)^{-3} [\theta_{A(R)} - P_{A(R)}]. \tag{3.4}$$

There exists a constant $C > 0$ such that for any $R \geq C$ and $0 < \varepsilon < 1, 0 < \eta < 1$,

$$C_h^\dagger [\nabla^\dagger \cdot \theta_{A(R)} \nabla]_s C_h + \frac{g}{2} \delta_{x,0} \geq 4\pi a \left[(1 - \varepsilon)(1 - \eta)U - \frac{W}{\varepsilon} - \frac{CV}{\eta} \right]. \tag{3.5}$$

Compared with the result in [9, Lemma 4], there is an additional error term V on the right side of (3.5). There is no restriction that U has to vanish at the origin, however, which was necessary in [9]. We note that the norm of U is given by $\|U\| = (2R + 1)^{-3}$, which is much smaller than the norm of $(g/2)\delta_{x,0}$ (which is $g/2$) for our choice of $R \gg 1$ below.

Proof We are actually going to prove the stronger statement that

$$\left\langle C_h^\dagger [\nabla^\dagger \cdot \Theta \nabla]_s C_h + \frac{g}{2} \delta_{x,0} \right\rangle_\psi \geq 4\pi a \left\langle (1 - \varepsilon)(1 - \eta)U - \frac{W}{\varepsilon} - \frac{CV}{\eta} \right\rangle_\psi \tag{3.6}$$

for any $\psi \in L^2(\mathbb{Z}^3)$. Here and in the following, we use the shorthand notation $\langle \cdot \rangle_\psi = \langle \psi | \cdot | \psi \rangle$. The non-negative function Θ is defined by

$$\Theta = \frac{1}{R - \widetilde{R}} \sum_{r=\widetilde{R}}^{R-1} \theta_{A(r)},$$

where we denote by \widetilde{R} the largest integer less than $R/2$. Since $\Theta \leq \theta_{A(R)}$, (3.6) implies (3.5).

To prove (3.6), we first define B_R as

$$B_R = \langle \psi | C_h^\dagger [\nabla^\dagger \cdot \Theta \nabla]_s | \varphi \rangle + \langle \psi | \frac{g}{2} \delta_{x,0} | \varphi \rangle.$$

Here, φ is given in (2.6). Using Schwarz’s inequality, it follows that $|B_R|^2$ is bounded from above as

$$|B_R|^2 \leq \left\langle C_h^\dagger [\nabla^\dagger \cdot \Theta \nabla]_s C_h + \frac{g}{2} \delta_{x,0} \right\rangle_\psi \left\langle [\nabla^\dagger \cdot \Theta \nabla]_s + \frac{g}{2} \delta_{x,0} \right\rangle_\varphi. \tag{3.7}$$

By the definition of φ , $\langle [\nabla^\dagger \cdot \Theta \nabla]_s + \frac{g}{2} \delta_{x,0} \rangle_\varphi \leq \langle -\Delta + \frac{g}{2} \delta_{x,0} \rangle_\varphi = 4\pi a$. Hence we see that the left side of (3.6) can be bounded from below as

$$\left\langle C_h^\dagger [\nabla^\dagger \cdot \Theta \nabla]_s C_h + \frac{g}{2} \delta_{x,0} \right\rangle_\psi \geq \frac{|B_R|^2}{4\pi a}. \tag{3.8}$$

Define $\chi \in L^2(\mathbb{Z}^3)$ via

$$|\chi\rangle = [\nabla^\dagger \cdot \Theta \nabla]_s |\varphi\rangle + \Delta |\varphi\rangle = [\nabla^\dagger \cdot \Theta \nabla]_s |\varphi\rangle + \frac{g}{2} \delta_{x,0} |\varphi\rangle.$$

Alternatively, using (2.3), $|\chi\rangle = (R - \tilde{R})^{-1} \sum_{r=\tilde{R}}^{R-1} \Xi_{A(r)} |\varphi\rangle$. Hence χ is supported in $A(R) \setminus A(\tilde{R} - 2)$. Moreover, $\chi(x)$ is a non-negative function for R large enough, as can be seen from (2.4) and the asymptotic behavior of φ in (2.7).

Let also $|\alpha\rangle = [\nabla^\dagger \cdot \Theta \nabla]_s |\varphi\rangle$. Since $\alpha(x) = \chi(x) - (g/2)\delta_{x,0}\varphi(0)$, also α is supported on $A(R)$. Moreover, $\sum_x \alpha(x) = 0$ because of (2.8) and (2.9). Since $C_h + C_{h'} = 1$,

$$B_R = \langle \psi | \chi \rangle - \langle \psi | C_{h'}^\dagger | \alpha \rangle.$$

Recall that $\sum_x \alpha(x) = 0$, and α is supported on $A(R)$. Hence

$$|(C_{h'}^\dagger \alpha)(x)| = \left| \sum_y (\overline{h'(y-x)} - \overline{h'(x)}) \alpha(y) \right| \leq f_R(x) \sum_y |\alpha(y)| = 8\pi a f_R(x),$$

with f_R defined in (3.1). Here we used the fact that $\chi(x)$ is non-negative and supported away from the origin, hence $\sum_x |\alpha(x)| = \sum_x \chi(x) + g\varphi(0)/2 = g\varphi(0) = 8\pi a$.

In particular, we conclude that

$$|B_R| \geq |\langle \psi | \chi \rangle| - 8\pi a \sum_{x \in \mathbb{Z}^3} |\psi(x)| f_R(x).$$

Using Schwarz’s inequality and the definition of W in (3.3), we thus obtain

$$|B_R|^2 \geq (1 - \varepsilon) \langle \psi | \chi \rangle \langle \chi | \psi \rangle - \frac{4\pi a^2}{\varepsilon} \sum_{x \in \mathbb{Z}^3} |\psi(x)|^2 W(x). \tag{3.9}$$

To get a lower bound on $|\chi\rangle \langle \chi|$, we use again Schwarz’s inequality, as well as the fact that χ is supported on $A(R)$. We obtain, for $0 < \eta < 1$,

$$\begin{aligned} |\chi\rangle \langle \chi| &\geq (1 - \eta) P_{A(R)} |\chi\rangle \langle \chi| P_{A(R)} + (1 - \eta^{-1}) (\theta_{A(R)} - P_{A(R)}) |\chi\rangle \langle \chi| (\theta_{A(R)} - P_{A(R)}) \\ &\geq (1 - \eta) (4\pi a)^2 \frac{P_{A(R)}}{(2R + 1)^3} + \|\chi\|_2^2 (1 - \eta^{-1}) (\theta_{A(R)} - P_{A(R)}). \end{aligned} \tag{3.10}$$

Here, we have again used the fact that $\sum_x \chi(x) = 4\pi a$.

To conclude the proof, we have to show that $\|\chi\|_2^2 \leq \text{const.} a^2/R^3$ for large R . This follows from the fact that

$$\chi(x) \leq \frac{2}{R - \tilde{R}} \sup_{|x| \geq \tilde{R}, |e|=1} |\varphi(x) - \varphi(x + e)| \leq Ca/R^3$$

for large R , as can be seen from the asymptotic behavior (2.7). Inserting the inequalities (3.10) and (3.9) into (3.8), we arrive at the desired result (3.6). □

If $|y_1 - y_2| > 2\sqrt{3}R$, the cubes of side length $2R$ centered at y_1 and y_2 , respectively, are disjoint. Hence we can obtain the following corollary of Lemma 1.

Corollary 1 *Let U, W and V be as in Lemma 1, and let $U_y = T_y U T_y^\dagger, W_y = T_y U T_y^\dagger$ and $V_y = T_y V T_y^\dagger$, where T_y is the translation operator $(T_y \psi)(x) = \psi(x - y)$. If y_1, \dots, y_n satisfy $|y_i - y_j| > 2\sqrt{3}R$ for all $i \neq j$, then*

$$-C_h^\dagger \Delta C_h + \frac{g}{2} \sum_{i=1}^n \delta_{x, y_i} \geq 4\pi a \sum_{i=1}^n \left[(1 - \varepsilon)(1 - \eta) U_{y_i} - \frac{W_{y_i}}{\varepsilon} - \frac{C V_{y_i}}{\eta} \right]. \tag{3.11}$$

3.2 Lemma Two

Recall that the Hilbert space $\mathcal{H}(N_u, N_d)$ is the subspace of $L^2(\mathbb{Z}^{3(N_u+N_d)})$ of functions that are separately antisymmetric in the N_u spin-up variables and the N_d spin-down variables. For $\Phi \in \mathcal{H}(N_u, N_d)$, let γ_u and γ_d denote the reduced one-particle density matrices of Φ for the spin-up and spin-down particles, respectively, with $\text{Tr } \gamma_u = N_u$ and $\text{Tr } \gamma_d = N_d$.

For $m \in \mathbb{Z}^3$, we define the functions $f_m(x) \in L^2(\mathbb{Z}^3)$ as

$$f_m(x) = (L + 1)^{-3/2} \exp(2\pi i m \cdot x (L + 1)^{-1}) \theta_{[0, L]^3}(x). \tag{3.12}$$

Note that the f_m 's are orthonormal functions. For any function ψ supported on $[1, L - 1]^3$, the expectation value $\langle \psi | -\Delta | \psi \rangle$ can be expressed as

$$\langle \psi | -\Delta | \psi \rangle = \sum_{m \in [-L/2, (L+1)/2]^3} E(2\pi m / (L + 1)) |\langle \psi | f_m \rangle|^2. \tag{3.13}$$

For $M \in \mathbb{N}$, let $\xi(M)$ denote the projection

$$\xi(M) = \sum_{E(2\pi m / (L+1)) \leq E_f(M / (L+1)^3)} |f_m\rangle \langle f_m|. \tag{3.14}$$

It is easy to see that

$$\lim_{M \rightarrow \infty, L \rightarrow \infty} M^{-1} \text{Tr } \xi(M) = 1 \tag{3.15}$$

in the thermodynamic limit $L \rightarrow \infty, M \rightarrow \infty$ with $M/L^3 \rightarrow \varrho$ for some $0 < \varrho \leq 1$.

Let $\xi(N_u) = \xi_u$ and $\xi(N_d) = \xi_d$ for simplicity. As mentioned in the introduction, we shall show in Lemma 2 that the reduced one particle density matrix $\gamma_{u(d)}$ of a ground state Φ of H is close to $\xi_{u(d)}$ in an appropriate sense.

Lemma 2 Let $\Phi \in \mathcal{H}_{N_u, N_d}$. Assume that, in the thermodynamic limit $N_{u(d)} \rightarrow \infty, L \rightarrow \infty$ with $\varrho_{u(d)} = N_{u(d)}/L^3$ fixed,

$$\limsup_{L \rightarrow \infty} \frac{1}{L^3} \langle \Phi | - \sum_{i=1}^{N_u} \Delta_{x_i} - \sum_{i=1}^{N_d} \Delta_{y_i} | \Phi \rangle \leq e_0(\varrho_u, \varrho_d) + Ca\varrho^2 \tag{3.16}$$

for some $C > 0$ independent of a and ϱ . Then

$$\limsup_{L \rightarrow \infty} \frac{1}{L^3} \text{Tr}[\gamma_{u(d)}(1 - \xi_{u(d)})] \leq \text{const. } \varrho \sqrt{a\varrho^{1/3}}. \tag{3.17}$$

Proof The proof is parallel to the proof of Lemma 5 in [9], following an argument in [4]. \square

3.3 Lemma Three

For given points $y_1, \dots, y_{N_d} \in \mathbb{Z}^3$, let $I_R(y_1, \dots, y_{N_d})$ denote the number of y_i 's whose distance to the nearest neighbor is less or equal to $2\sqrt{3}R$. Because Corollary 1 can be applied only to those y_i 's that stay away a distance larger than $2\sqrt{3}R$ from all the other particles, we will need an upper bound on the expectation value of I_R in the ground state of the Hubbard Hamiltonian. This will be accomplished in Lemma 3 below. It states that as long as R is much less than the average particle distance $\varrho^{-1/3}$, the expectation value of I_R in the ground state of H is small compared to the total number of particles N .

Lemma 3 Let $\Phi \in \mathcal{H}(N_u, N_d)$. Assume that for some constant $C > 0$, independent of ϱ_u and ϱ_d ,

$$\frac{1}{N} \langle \Phi | - \sum_{i=1}^{N_d} \Delta_i | \Phi \rangle \leq C\varrho^{2/3}. \tag{3.18}$$

Then

$$\langle \Phi | I_R(y_1, \dots, y_{N_d}) | \Phi \rangle \leq \text{const. } N((R + 1)^3 \varrho)^{2/5}. \tag{3.19}$$

Proof With D_i denoting the distance of y_i to the nearest neighbor among the y_k with $k \neq i$, we can write

$$I_R(y_1, \dots, y_{N_d}) = \sum_{i=1}^{N_d} \theta_{[0, 2\sqrt{3}R]}(D_i).$$

Here, $\theta_{[0, 2\sqrt{3}R]}$ denotes the characteristic function of $[0, 2\sqrt{3}R]$. It follows from Lemma 4 below that

$$\sum_{i=1}^{N_d} \theta_{[0, 2\sqrt{3}R]}(D_i) \leq -b \sum_{i=1}^{N_d} \Delta_{y_i} + b^{-3/2} \frac{2^{11/2}}{15\pi^2} N_d \sum_{x \in \mathbb{Z}^3} \theta_{[0, 2\sqrt{3}R]}(|x|) \tag{3.20}$$

for any $b > 0$. Using the assumption (3.18) and optimizing over the choice of b , we arrive at the result. \square

It remains to prove the bound (3.20), which is a special case of the following Lemma. Its proof uses a similar decomposition method as in [12].

Lemma 4 *Let f be nonnegative, with $\sum_{x \in \mathbb{Z}^3} f(|x|) < \infty$, and let D_i denote the distance of x_i to the nearest neighbor among all points x_j with $j \neq i$. On the subspace of antisymmetric N -particle wavefunctions in $L^2(\mathbb{Z}^{3N})$,*

$$\sum_{i=1}^N (-\Delta_i - f(D_i)) \geq -\frac{2^{11/2}}{15\pi^2} N \sum_{x \in \mathbb{Z}^3} f(|x|)^{5/2}. \tag{3.21}$$

Proof Let N_1 be the largest integer less or equal to $N/2$, and let $N_2 = N - N_1$. Consider a partition $P = (\pi_1, \pi_2)$ of the integers $1, \dots, N$ into two disjoint subsets with N_1 integers in π_1 and N_2 integers in π_2 . For a given P and $i \in \pi_1$, we define

$$D_i^P = \min\{|x_i - x_j|, j \in \pi_2\}.$$

It is easy to see that

$$\sum_{i=1}^N f(D_i) \leq 4 \binom{N}{N_1}^{-1} \sum_P \sum_{i \in \pi_1} f(D_i^P),$$

where the sum runs over all $\binom{N}{N_1}$ partitions of $\{1, \dots, N\}$. This follows from the fact that for given i and j , the probability that a partition P has the property that $i \in \pi_1$ and $j \in \pi_2$ equals $N_1 N_2 / (N(N - 1)) > 1/4$.

In particular, we see that

$$\sum_{i=1}^N (-\Delta_i - f(D_i)) \geq \binom{N}{N_1}^{-1} \sum_P \sum_{i \in \pi_1} \left(-\frac{N}{N_1} \Delta_i - 4f(D_i^P)\right).$$

For fixed $x_j, j \in \pi_2$, we can use the Lieb-Thirring estimate [6, Theorem 5.3] to conclude that

$$\sum_{i \in \pi_1} \left(-\frac{N}{N_1} \Delta_i - 4f(D_i^P)\right) \geq -\frac{8}{15\pi^2} \left(\frac{N_1}{N}\right)^{3/2} 4^{5/2} \sum_{x_1 \in \mathbb{Z}^3} f(D_1^P)^{5/2}.$$

Note that the antisymmetry of the wavefunctions is essential here. We can estimate

$$\sum_{x_1 \in \mathbb{Z}^3} f(D_1^P)^{5/2} \leq N_2 \sum_{x \in \mathbb{Z}^3} f(|x|)^{5/2}.$$

Using in addition that $N_1^{3/2} N_2 \leq N/2^{5/2}$, we arrive at the statement. □

4 Proof of Theorem 1

We write the Hamiltonian H in (1.3) as

$$H = \left(-\sum_{i=1}^{N_u} \Delta_{x_i} + \frac{1}{2}g \sum_{i=1}^{N_u} \sum_{j=1}^{N_d} \delta_{x_i, y_j}\right) + \left(-\sum_{i=1}^{N_d} \Delta_{y_i} + \frac{1}{2}g \sum_{i=1}^{N_u} \sum_{j=1}^{N_d} \delta_{x_i, y_j}\right). \tag{4.1}$$

Recall that we restrict H to functions that are antisymmetric both in the x and the y variables, and are supported on the cube $[1, L - 1]^{3(N_u + N_d)}$. In the following, we are going to

derive a lower bound only on the first term. The lower bound on the second term can be obtained in the same way by simply exchanging the role of x and y . Our bound is not a bound on the ground state energy of this first term, however, but rather estimates the expectation value of this term in the ground state of the full Hamiltonian H .

First, as mentioned in the Introduction, we decompose the kinetic energy $-\Delta$ into a high and a low momentum part. Let again $E_f(\varrho)$ denote the Fermi energy of an ideal gas of spinless fermions at density ϱ , defined in (2.10), and let

$$\widehat{M}(p) = \sqrt{\left[1 - \frac{E_f(\varrho_u)}{E(p)}\right]_+}.$$

Here, $[\cdot]_+ = \max\{\cdot, 0\}$ denotes the positive part. Moreover, let $\widehat{M}'(p) = \sqrt{1 - \widehat{M}(p)^2}$. As pointed out in (2.2), we can decompose the Laplacian as

$$\Delta = C_{M'}^\dagger \Delta C_{M'} + C_M^\dagger \Delta C_M.$$

We first claim that

$$\lim_{L \rightarrow \infty} \frac{1}{L^3} \inf \text{spec} \left[- \sum_{i=1}^{N_u} (C_{M'}^\dagger \Delta C_{M'})_i \right] \geq e(\varrho_u). \tag{4.2}$$

The proof follows in exactly the same way as the proof of (64) in [9], using an argument in [7].

We proceed with the high-momentum part. Let $l : \mathbb{R}^3 \rightarrow \mathbb{R}_+$ be a smooth, radial, positive function, with $l(p) = 0$ for $|p| \leq 1$, $l(p) = 1$ for $|p| \geq 2$, and $0 \leq l(p) \leq 1$ in-between. As in [9], we choose $\widehat{h}_s(p)$ as

$$\widehat{h}_s(p) = l(sp). \tag{4.3}$$

Since $h_s(p) = 0$ for $|p| \leq 1/s$, we can estimate

$$\widehat{M}(p)^2 = \left[1 - \frac{E_f(\varrho_u)}{E(p)}\right]_+ \geq \left[1 - \frac{E_f(\varrho_u)}{\min_{|p| \geq 1/s} E(p)}\right]_+ \widehat{h}_s(p)^2. \tag{4.4}$$

(Here, the minimum is taken over $p \in [-\pi, \pi]^3$, $|p| \geq 1/s$.) In particular, this implies that

$$-C_M^\dagger \Delta C_M \geq \left[1 - \frac{E_f(\varrho_u)}{\min_{|p| \geq 1/s} E(p)}\right]_+ (-C_{h_s}^\dagger \Delta C_{h_s}). \tag{4.5}$$

Since $E(p) \sim |p|^2$ for small $|p|$, and $E_f(\varrho_u) \leq \text{const.} \varrho_u^{2/3}$, we obtain

$$\left[1 - \frac{E_f(\varrho_u)}{\min_{|p| \geq 1/s} E(p)}\right]_+ \geq 1 - \text{const.} s^2 \varrho_u^{2/3} \tag{4.6}$$

as long as $s \gg 1$.

We note that with this choice of $\widehat{h}_s(p)$ the corresponding $\widehat{h}'_s(p) = 1 - \widehat{h}_s(p)$ is a smooth function that is supported in $|p| \leq 2s^{-1}$. As in [9], we conclude that the corresponding potential $W(x)$ defined in Lemma 1 satisfies (for $1 \leq R \leq \text{const.} s$)

$$W(x) \leq \text{const.} \frac{R^2}{s^5} \quad \text{and} \quad \sum_{x \in \mathbb{Z}^3} W(x) \leq \text{const.} \frac{R^2}{s^2} \tag{4.7}$$

for some constants depending only on the choice of l . Moreover, if $|y_i - y_j| > 2\sqrt{3}R$ for all $i \neq j$, then

$$\sum_{i=1}^{N_d} W_R(x - y_i) \leq \text{const.} \frac{1}{R^5} \tag{4.8}$$

independent of x and N_d .

We will now use Corollary 1 to get a lower bound on the sum of the high momentum part of the kinetic energy and the interaction energy. In order to be able to apply this corollary, we have to neglect the interaction of the x particles with those y particles that are *not* at least a distance $2\sqrt{3}R$ from the other y particles. Let us denote $Y = (y_1, \dots, y_{N_d})$, and let Y' be the subset of Y containing those y_i whose distance to all the other y_j 's is larger than $2\sqrt{3}R$. Note that, by definition, the cardinality of Y' is $|Y'| = N_d - I_R(y_1, \dots, y_{N_d})$, with I_R defined in Sect. 3.3. Moreover, let $Y'' \subset Y'$ be the set of $y_j \in Y'$ whose distance to the boundary of $[0, L]^3$ is at least $R + 1$. As argued in [9], $|Y''| \geq |Y'| - \text{const.} (L/R)^2$ and hence, in particular,

$$\lim_{L \rightarrow \infty} L^{-3} \langle \Phi | (|Y'| - |Y''|) | \Phi \rangle = 0 \tag{4.9}$$

in the ground state Φ of H .

Applying Corollary 1, together with (4.5), we obtain that for a given configuration of Y ,

$$-\sum_{i=1}^{N_u} [C_M^\dagger \Delta C_M]_i + \frac{g}{2} \sum_{i,j} \delta_{x_i, y_j} \geq \left[1 - \frac{E_f(Q_u)}{\min_{|p| \geq 1/s} E(p)} \right]_+ \sum_{i=1}^{N_u} [w_Y]_i, \tag{4.10}$$

with w_Y defined as

$$w_Y = \sum_{\{j: y_j \in Y''\}} 4\pi a \left((1 - \varepsilon)(1 - \eta) U_{y_j} - \frac{W_{y_j}}{\varepsilon} - \frac{C V_{y_j}}{\eta} \right). \tag{4.11}$$

For any $\Phi \in \mathcal{H}(N_u, N_d)$, we can express the expectation value of $\sum_i [w_Y]_i$ as

$$\langle \Phi | \sum_{i=1}^{N_u} [w_Y]_i | \Phi \rangle = \sum_Y \varrho_Y \text{Tr}[\gamma_Y w_Y], \tag{4.12}$$

where we denote by ϱ_Y the distribution function of $Y = (y_1 \dots y_{N_d})$, that is,

$$\varrho_Y = \langle \Phi | \delta_{Y=\{y_1 \dots y_{N_d}\}} | \Phi \rangle$$

and γ_Y denotes the one-particle density matrix of Φ for *fixed* Y , i.e.,

$$\gamma_Y(x, x') = \frac{N_u}{\varrho_Y} \sum_{x_2, \dots, x_{N_u}} \Phi(x, x_2, \dots, x_{N_u}, Y) \Phi(x', x_2, \dots, x_{N_u}, Y)^*.$$

Note that $0 \leq \gamma_Y \leq 1$ and $\text{Tr} \gamma_Y = N_u$. Moreover, $\sum_Y \varrho_Y = 1$ and $\sum_Y \varrho_Y \gamma_Y = \gamma_u$, which is the one-particle density matrix for the spin-up particles introduced earlier in Sect. 3.2.

From now on, we will consider Φ to be a ground state of H . The assumptions of Lemmas 2 and 3 are clearly satisfied for this Φ , as the upper bound derived in [3] shows.

Recall that ξ_u denotes the projection $\xi(N_u)$ defined in (3.14). We write $w_Y = w_{Y,+} + w_{Y,-}$, where $w_{Y,+} \geq 0$ stands for the part of w_Y in (4.11) containing U , whereas $w_{Y,-} \geq 0$ is the part of w_Y containing W and V . As proved in [9, Sect. V.C] we have, for any $\delta > 0$,

$$\begin{aligned} \text{Tr}[\gamma_Y w_Y] &\geq \text{Tr}[\xi_u w_{Y,+}](1 - \delta) - \text{Tr}[\xi_u w_{Y,-}](1 + \delta) \\ &\quad - (1 + \delta^{-1})(\|w_{Y,+}\| + \|w_{Y,-}\|) \text{Tr}[\gamma_Y(1 - \xi_u)] - \|w_Y\| \text{Tr}[\xi_u(1 - \gamma_Y)]. \end{aligned} \tag{4.13}$$

We are now going to bound the various terms on the right side of (4.13). First, using $\sum_{x \in \mathbb{Z}^3} U(x) = 1$ and the fact that ξ_u has a constant density, we have

$$\text{Tr}[\xi_u w_{Y,+}] = \frac{\text{Tr}[\xi_u]}{(L + 1)^3} (1 - \varepsilon)(1 - \eta)4\pi a|Y''|.$$

To estimate $\lim_{L \rightarrow \infty} L^{-3} \sum_Y \varrho_Y \text{Tr}[\xi_u w_{Y,+}]$, we can use (4.9), $|Y'| = N_d - I_R(Y)$ and Lemma 3 to conclude that

$$\lim_{L \rightarrow \infty} L^{-3} \sum_Y \varrho_Y \text{Tr}[\xi_u w_{Y,+}] \geq (1 - \varepsilon)(1 - \eta)4\pi a \varrho_u \varrho_d - \text{const.} a \varrho^2 ((R + 1)^3 \varrho)^{2/5}.$$

Here, we have also used that $\lim_{L \rightarrow \infty} L^{-3} \text{Tr}[\xi_u] = \varrho_u$, which follows from (3.15).

Analogously, using (4.7) and the fact that for any ψ and fixed y ,

$$\langle \psi | V_y | \psi \rangle = \frac{1}{2(2R + 1)^6} \sum_{(x,x') \in Y+A(R)} |\psi(x) - \psi(x')|^2 \leq \frac{1}{2} \max_{(x,x') \in Y+A(R)} |\psi(x) - \psi(x')|^2,$$

it is easy to get the upper bound

$$\lim_{L \rightarrow \infty} L^{-3} \sum_Y \varrho_Y \text{Tr}[\xi_u w_{Y,-}] \leq \text{const.} a \varrho_u \varrho_d \left(\frac{R^2}{\varepsilon s^2} + \frac{R^2 \varrho^{2/3}}{\eta} \right).$$

Moreover, using (4.8) and the fact that the distance between two $y_j \in Y''$ is at least $2\sqrt{3}R$, as well as $\eta \leq 1$, we find that,

$$\|w_Y\| \leq \|w_{Y,+}\| + \|w_{Y,-}\| \leq \text{const.} a \left(\frac{1}{\varepsilon s^2 R} + \frac{1}{\eta R^3} \right). \tag{4.14}$$

The bound in Lemma 2 implies that

$$\lim_{L \rightarrow \infty} L^{-3} \sum_Y \varrho_Y \text{Tr}[\gamma_Y(1 - \xi_u)] = \lim_{L \rightarrow \infty} L^{-3} \text{Tr}[\gamma_u(1 - \xi_u)] \leq \text{const.} \varrho(a^3 \varrho)^{1/6}.$$

Finally, the last term in (4.13) can be bounded as

$$\lim_{L \rightarrow \infty} L^{-3} \sum_Y \varrho_Y \|w_Y\| \text{Tr}[\xi_u(1 - \gamma_Y)] \leq \text{const.} a \left(\frac{1}{\varepsilon s^2 R} + \frac{1}{\eta R^3} \right) \varrho(a^3 \varrho)^{1/6},$$

where we have used (4.14) as well as the fact that $\text{Tr}[\xi_u(1 - \gamma_Y)] = \text{Tr}[\gamma_Y(1 - \xi_u)] + \text{Tr}[\xi_u - \gamma_Y]$. The last term, when averaged over Y , is $o(N)$ in the thermodynamic limit, i.e., $\sum_Y \varrho_Y \text{Tr}[\xi_u - \gamma_Y] = o(N)$.

Collecting all the bounds, and applying the same arguments also to the second term in (4.1), we arrive at the lower bound

$$\begin{aligned} & \lim_{L \rightarrow \infty} \frac{1}{L^3} E_0(N_u, N_d, L) \\ & \geq e_0(\varrho_u, \varrho_d) + 8\pi a \varrho_u \varrho_d \left[1 - \varepsilon - \eta - \delta - \text{const.} \left(s^2 \varrho^{2/3} + \frac{R^2}{\varepsilon s^2} + \frac{R^2 \varrho^{2/3}}{\eta} \right) \right. \\ & \quad \left. - \text{const.} \left((R^3 \varrho)^{2/5} + \frac{(a^3 \varrho)^{1/6}}{\delta} \left(\frac{1}{\eta R^3 \varrho} + \frac{1}{\varepsilon s^2 R \varrho} \right) \right) \right]. \end{aligned}$$

Here, we have assumed that $R \geq 1$ and that $s \gg 1$ in order to be able to apply the estimate (4.6). If we choose

$$R = \varrho^{-1/3} (a^3 \varrho)^{1/30}, \quad s = \varrho^{-1/3} (a^3 \varrho)^{1/90}, \quad \varepsilon = \delta = \eta = (a^3 \varrho)^{1/45} \tag{4.15}$$

this implies that

$$\lim_{L \rightarrow \infty} \frac{1}{L^3} E_0(N_u, N_d, L) \geq e_0(\varrho_u, \varrho_d) + 8\pi a \varrho_u \varrho_d (1 - \text{const.} (a \varrho^{1/3})^{1/15}),$$

which is the result stated in (1.5).

Recall that in order to be able to apply Lemma 1, it is necessary that $R \geq C$ for some constant $C > 0$, which for our choice of R in (4.15) is the case if

$$(a \varrho^{1/3})^{1/10} \geq C \varrho^{1/3}. \tag{4.16}$$

Under this assumption, also $s \gg 1$ is satisfied for small $a^3 \varrho$. For fixed a , (4.16) holds for small enough ϱ . However, if a is very small, (4.16) is violated. In this case, one can obtain our main result (1.5) actually much easier. One simply omits the use of Lemma 1 altogether, and applies our perturbative estimate (4.13) directly to the interaction potential $(g/2)\delta_{xy}$. Notice that for small a , $g \sim 8\pi a$ is also small. The resulting bound is

$$\lim_{L \rightarrow \infty} \frac{1}{L^3} E_0(N_u, N_d, L) \geq e_0(\varrho_u, \varrho_d) + g \varrho_u \varrho_d \left[1 - \delta - \text{const.} \frac{(a^3 \varrho)^{1/6}}{\delta \varrho} \right]. \tag{4.17}$$

Choosing $\delta = \varrho^{-1/2} (a^3 \varrho)^{1/12}$ and noting that $g \geq 8\pi a$ and $\varrho \geq \text{const.} (a^3 \varrho)^{1/10}$ in the parameter regime we are interested in here, this yields (1.5) in case (4.16) is violated.

This finishes the proof of Theorem 1.

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