Ground state energies of the Hubbard models and the Hartree Fock approximation

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Abstract

According to the ‘folk knowledge’, the Hartree-Fock (H-F) approximation applied to the Hubbard model becomes exact in the limit of small coupling $U$ (the smaller $|U|$, the better is the H-F approximation). In [1] Bach and Poelchau have substantiated a certain version of this assertion by providing a rigorous estimate of the difference between the true ground-state energy of the simplest version of the Hubbard model and the H-F approximation to this quantity. In this paper we extend their result in two directions: i) we relax the assumption about the strict translational invariance of the hopping matrix, ii) we prove an analogous estimate for a class of multiband Hubbard models.

Keywords: Hubbard model, Hartree-Fock approximation, correlation inequalities.

1 Introduction

The Hubbard model has been introduced almost 60 years ago [3, 4, 5], originally to explain ferromagnetism of transition metals. Although this attempt was not successful, the model and its multiband extensions play, since then, the role of a ‘minimal models’ for strongly correlated electron systems and is broadly used to model phenomena, which cannot be explained within the simple one-particle picture, provided e.g. by the band theory. It is believed that the Hubbard model (and/or its multiband extensions) qualitatively captures the essence of such phenomena as a variety of magnetic orderings (ferro- and antiferromagnetic as well as more complicated magnetic structures), metal–insulator transitions and the high-temperature superconductivity. More recently the fermion and boson versions of the Hubbard model have been successfully applied to model atomic gases in traps.

However, despite being only a simplified model of complex real physical systems, the Hubbard model is ‘notoriously difficult’ (Lieb, [6]): exact solutions or rigorous
results are rare even in the case of its simplest one-band variant. The same can be also said of reliable approximations to its solutions. The most frequently used one is the Hartree-Fock (H-F) approximation which introduces substantial simplifications but remains still non-trivial (see for instance [7] and [8]). There is a broad consensus that this approximation works well for small values of the Coulomb coupling constant $U$ of the interaction term of the Hubbard model Hamiltonian. An important step towards justifying this expectation has been made by Bach and Poelchau [1] (see also [2]) who have rigorously proved an inequality which provides an estimate of the difference between the true ground-state energy of the simplest version of the Hubbard model and the H-F approximation to this quantity.

The crucial element of the derivation of the estimate given in [1] is relating a certain constant appearing in one of the established inequalities to the density of states of the free system, i.e. of the Hubbard model with the coupling $U$ set to zero (a solvable system). In this way the constant in question gets expressed in terms of the density (in the context of the lattice models called also the degree of filling), i.e. the ratio of the number of fermions to the number of the lattice sites of the system and the coupling constant $U$. In this note after recalling the steps made by Bach and Poelchau we show that their general scheme of the derivation of the estimate can be almost straightforwardly generalized in two directions. Firstly, the adopted in [1] assumption about strict translational invariance of the hopping matrix can be relaxed; secondly, a class of multiband Hubbard models can be treated in the similar manner. The generalization essentially consists of modifying the solvable part of the problem, that is to consider the appropriate density of states and relating the mentioned constant to the characteristics of the considered version of the Hubbard model.

2 Generalities

We thus consider spin one-half particles living on a finite subset $\Lambda = [-L + 1, L]^d \cap \mathbb{Z}^d$ of the hypercubic lattice. Periodic boundary conditions in all directions will be assumed ($\Lambda$ becomes in this way a ‘discrete hypertorus’). The one-particle Hilbert space $\mathcal{H}$ is therefore the space of spinor-valued functions: $\mathcal{H} = \mathbb{C}^{2|\Lambda|}$ of (complex) dimension $2|\Lambda|$. The Hilbert space of the simplest version of the fermionic Hubbard model (considered in [1]) is built as a Fock space $\mathcal{F}(\mathcal{H})$ over the one-particle Hilbert space $\mathcal{H}$, that is as the direct sum

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{N=0}^{2|\Lambda|} \mathcal{F}_N,$$

of $N$-particle Hilbert spaces $\mathcal{F}_N \equiv \mathcal{F}_N(\mathcal{H})$ constructed as $N$-fold antisymmetrized tensor products of one-particle Hilbert spaces (since the $\mathcal{H}$ is $2|\Lambda|$-dimensional, maximal $N$ equals $2|\Lambda|$ and the dimension of the entire $\mathcal{F}(\mathcal{H})$ is $2^{2|\Lambda|} = 4^{|\Lambda|}$). The zero particle space is a one dimensional space spanned by the no-particle “vacuum” vector which we denote $|0\rangle$. In the considered case of spin 1/2 fermions the spaces $\mathcal{F}_N$ naturally split into direct sums of subspaces $\mathcal{F}_{N+}\mathcal{F}_{N-} \equiv \mathcal{F}_{N+}\mathcal{F}_{N-}$, where $N_{\pm}$ are numbers of fermions with spin up and down. As usually, with every one-particle state $|\psi\rangle \in \mathcal{H}$ one
can associate the creation and annihilation operators $c^\dagger(\psi), c(\psi)$ which act on $\mathcal{F}(\mathcal{H})$. The $N$-particle Hilbert space $\mathcal{F}_N$ can be then spanned by $\binom{2|\Lambda|}{N}$ vectors of the form

$$\left(\prod_{k=1}^{N} c^\dagger(f_{i_k})\right)|0\rangle,$$

where $(i_1, \ldots, i_N)$ are all possible $N$-element subsets of the set $2|\Lambda|$ indices $i$ labeling vectors $|f_i\rangle$ of an orthonormal basis of $\mathcal{H}$. One particular such basis is formed by vectors $|\mathbf{x}, \sigma\rangle$, where $\sigma = \pm$ and $\mathbf{x}$ runs over $|\Lambda|$ sites of the lattice $\Lambda$ (the state $|\mathbf{x}, \sigma\rangle$ represents the particle with the spin projection $\sigma$ localized at the site $\mathbf{x}$). The corresponding creation and annihilation operators denoted $c^\dagger_{\mathbf{x}, \sigma}, c_{\mathbf{x}, \sigma}$ create and annihilate a fermion with the spin projection $\sigma$ at the site $\mathbf{x}$. Obviously, if

$$|f_i\rangle = \sum_{\mathbf{x} \in \Lambda} \sum_{\sigma = \pm} |\mathbf{x}, \sigma\rangle f^\sigma_i(\mathbf{x}),$$

$(f^\sigma_i(\mathbf{x})$ is the lattice “wave function” of the fermion in the state $|f_i\rangle$), then

$$c^\dagger(f_i) = \sum_{\mathbf{x} \in \Lambda} \sum_{\sigma = \pm} c^\dagger_{\mathbf{x}, \sigma} f^\sigma_i(\mathbf{x}), \quad c(f_i) = \sum_{\mathbf{x} \in \Lambda} \sum_{\sigma = \pm} c_{\mathbf{x}, \sigma} (f^\sigma_i(\mathbf{x}))^*. \quad (2)$$

In the language of second quantization the Hamiltonian of the simplest version of the Hubbard model, written in terms of the operators $c^\dagger_{\mathbf{x}, \sigma}, c_{\mathbf{x}, \sigma}$, takes the form

$$\hat{H} = \hat{T} + \hat{V}, \quad (3)$$

with

$$\hat{T} = -\sum_{\langle \mathbf{x}, \mathbf{y} \rangle} \sum_{\sigma = \pm} t_{\mathbf{x}, \mathbf{y}} c^\dagger_{\mathbf{x}, \sigma} c_{\mathbf{y}, \sigma}, \quad (4)$$

and

$$\hat{V} = U \sum_{\mathbf{x}} n_{\mathbf{x}+} n_{\mathbf{x} -}. \quad (5)$$

Here $t_{\mathbf{x}, \mathbf{y}}$ is the hopping matrix, $U$ is the Coulomb coupling constant (we consider a repulsive interaction with $U > 0$) and $n_{\mathbf{x}, \sigma} = c^\dagger_{\mathbf{x}, \sigma} c_{\mathbf{x}, \sigma}$ are the operators of the numbers of particles with the spin projection $\sigma$ at the lattice site $\mathbf{x}$. The symbol $\sum_{\langle \mathbf{x}, \mathbf{y} \rangle}$ means summation over all possible pairs of lattice sites. In this Section, following Bach and Poelchau, we assume that the hoping matrix $t_{\mathbf{x}, \mathbf{y}}$ is translationally invariant that is, that $t_{\mathbf{x}, \mathbf{y}} = t_{\mathbf{x} - \mathbf{y}, 0} \equiv t(\mathbf{x} - \mathbf{y})$. (In the following this assumption will be modified by allowing for periods greater than the unit one).

It will be convenient to introduce also the operators

$$\hat{\mathbf{N}} = \sum_{\mathbf{x}} \sum_{\sigma = \pm} n_{\mathbf{x}, \sigma}, \quad \hat{n} = \frac{\hat{\mathbf{N}}}{|\Lambda|}, \quad (6)$$

of the total number of particles and of the total density, respectively

We first define the true ground state energy $E_{gs}(n)$ of the $N$-fermion system as the infimum of the expectation values of the Hamiltonian (3) in states belonging to $F_N$
that is, in states of the system of density $n = N/|\Lambda|$:

$$E_{gs}(n) = \inf \{ \langle \Psi | \hat{H} | \Psi \rangle : |\Psi\rangle \in F(\mathcal{H}), \quad \langle \Psi | \Psi \rangle = 1, \quad n|\Psi\rangle = n|\Psi\rangle \}.$$  
(7)

As the Hilbert space of the considered system is finite-dimensional, $E_{gs}(n)$ given by (7) is the same as the lowest eigenvalue in $F_N$ of the Hamiltonian $\hat{H}$, that is its eigenvalue on a (normalized) ground-state vector $|\Psi_{gs}\rangle \in F_N(\mathcal{H})$ such that $n|\Psi_{gs}\rangle = n|\Psi_{gs}\rangle$ and $\hat{H}|\Psi_{gs}\rangle = E_{gs}|\Psi_{gs}\rangle$. The formula (7) is, however, more convenient in further considerations than the eigenvalue equation.

The corresponding Hartree-Fock (H-F) ground state energy $E_{hf}(n)$ is defined as

$$E_{hf}(n) = \inf \{ \langle \Phi | \hat{H} | \Phi \rangle : |\Phi\rangle \in SD_N \}.$$  
(8)

$SD_N \subset F_N(\mathcal{H})$ denotes the set of $N$-particle vectors constructed as the Slater determinants that is, of vectors of the form

$$SD_N = \left\{ |\Phi\rangle = \prod_{j=1}^{N} c_{j}^{\dagger} (f_{j}) |0\rangle : |f_{1}\rangle, \ldots, |f_{N}\rangle \in \mathcal{H}, \quad \langle f_{i} | f_{j} \rangle = \delta_{ij} \right\}.$$  
(9)

A vector $|\Phi_{hf}\rangle \in SD_N$ such that $E_{hf} = \langle \Phi_{hf} | \hat{H} | \Phi_{hf} \rangle$ will be called the Hartree-Fock ground state of the Hamiltonian $\hat{H}$.

Both quantities, $E_{hf}(n)$ and $E_{gs}(n)$, are thus obtained by minimizing the expectation values of the same Hamiltonian $\hat{H}$ (3) but each one over a different set of vectors (belonging to $F_N$): $E_{gs}(n)$ is the minimum over the entire $N$-particle subspace $F_N$, that is over all possible vectors $|\Psi\rangle$ which in general have the form

$$|\Psi\rangle = \sum_{x_1, \ldots, x_N \in \Lambda} \sum_{\sigma_1, \ldots, \sigma_N} \Psi_{\sigma_1 \ldots \sigma_N} (x_1, \ldots, x_N) c_{x_1 \sigma_1}^{\dagger} \ldots c_{x_N \sigma_N}^{\dagger} |0\rangle,$$

while $E_{hf}(n)$ is the minimum over only the set of $N$-particle vectors having the factorizable form, that is (cf. the formula (2)) such that

$$\Psi_{\sigma_1 \ldots \sigma_N} (x_1, \ldots, x_N) = f_{1}^{\sigma_1} (x_1) \ldots f_{N}^{\sigma_N} (x_N).$$

The standard Ritz variational principle implies therefore the inequality

$$E_{gs}(n) \leq E_{hf}(n) \quad \text{i.e.} \quad \Delta E(n) \equiv E_{gs}(n) - E_{hf}(n) \leq 0.$$  
(10)

In other words, $\Delta E(n)$ is by construction bounded from from above.

In [1] a lower bound on $\Delta E(n)$ has been obtained in the form of the following

**Theorem [1].** Let $\hat{t}$ be a translationally invariant hopping matrix with a finite support, such that in the thermodynamic (TD) limit its Fourier transform $\hat{t} \equiv \epsilon$ (that is, the

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1The antisymmetrization which is implied by the name “Slater determinant” is, of course, ensured by the properties of the operators $c_{x,\sigma}^{\dagger}$. 

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dispersion function), $\epsilon : [-\pi, \pi]^d \to \mathbb{R}$, is a Morse function (i.e. a function the critical points of which are non-degenerate), and let $\Lambda$ be a sufficiently large lattice such that $\text{supp}(t) \subset \Lambda$. Finally, let $n = N/\Lambda$ be the density. Then:

- if the dimension of the lattice $\Lambda$ is $d = 2$, 
  \[ 0 \geq \Delta E(n) \geq -\text{const.} \left( n^{2/3}U^{4/3}(1 + |\ln U|) + n^{1/2}U|\Lambda|^{-1/4} \right) , \]  
  \[ (11) \]

- if the dimension of the lattice $\Lambda$ is $d \geq 3$, 
  \[ 0 \geq \Delta E(n) \geq -\text{const.} \left( n^{2/3}U^{4/3} + n^{1/2}U|\Lambda|^{-1/2d} \right) . \]  
  \[ (12) \]

This theorem has been proved by using the correlation inequalities. We present main points of this proof below. After that, we present our extensions of this result.

### 3 Sketch of the proof

To present the sketch of the proof some additional definitions must be given. We first introduce the family of projection operators

\[ \hat{X}_x = \sum_{\sigma} \langle x, \sigma | x, \sigma \rangle , \]  
\[ (13) \]

acting on $\mathcal{H}$ and such that ($\hat{1}_1$ is the unit operator acting on $\mathcal{H}$)

\[ \sum_x \hat{X}_x = \hat{1}_1 . \]  
\[ (14) \]

The interaction operator (5) restricted to the two-particle space $\mathcal{F}_2$ and extended to act on the entire $\mathcal{H} \otimes \mathcal{H}$ (denoted therefore $\hat{V}_2$) can be expressed in terms of $\hat{X}_x$ as:

\[ \hat{V}_2 = U \sum_x \hat{X}_x \otimes \hat{X}_x , \]  
\[ (15) \]

Similarly, the kinetic energy operator (4) restricted to the one-particle space $\mathcal{F}_1 \equiv \mathcal{H}$ (and denoted therefore $\hat{T}_1$) can be written as

\[ \hat{T}_1 = \sum_{(x,y)} \sum_{\sigma} t_{x,y} \langle x, \sigma | y, \sigma \rangle . \]  
\[ (16) \]

Needed will be also the density operators which can be defined as follows. Let the set of vectors $\{|\phi_1\rangle, \ldots, |\phi_{2|\Lambda|}\rangle\}$ form an orthonormal basis of $\mathcal{H}$ and let $|\Psi\rangle$ be some normalized vector of $\mathcal{F}(\mathcal{H})$. The associated operators: the one-particle density operator (1-pdo) $\hat{\gamma}_\Psi$ acting on $\mathcal{H}$, and the two-particle density operator (2-pdo) $\hat{\Gamma}_\Psi$ acting on $\mathcal{H} \otimes \mathcal{H}$ are then defined by the formulae

\[ \hat{\gamma}_\Psi = \sum_{k,l} |\phi_k\rangle \langle \Psi | c^\dagger(\phi_k)c(\phi_l)|\Psi\rangle \langle \phi_k| , \]  
\[ (17) \]

\[ \hat{\Gamma}_\Psi = \sum_{k,l,m,n} |\phi_m\rangle \otimes |\phi_n\rangle \langle \Psi | c^\dagger(\phi_k)c^\dagger(\phi_l)c(\phi_m)c(\phi_n)|\Psi\rangle \langle \phi_k| \otimes \langle \phi_l| . \]  
\[ (18) \]

(Higher-particle densities can be defined analogously, but will not be needed in our considerations). The operators $\hat{\gamma}_\Psi$ and $\hat{\Gamma}_\Psi$ have the following, easy to check, properties:
• They are independent of the choice of the orthonormal basis $|\phi_i\rangle$ of $\mathcal{H}$

• They are both positive Hermitian operators such that:

$$0 \leq \hat{\gamma}_\Psi = \hat{\gamma}_\Psi^\dagger \leq \hat{1}_1, \quad \text{Tr}_1(\hat{\gamma}_\Psi) = \langle \Psi | \hat{N} | \Psi \rangle = N,$$

$$0 \leq \hat{\Gamma}_\Psi = \hat{\Gamma}_\Psi^\dagger \leq \hat{1}_2 \text{Tr}_2(\hat{\Gamma}_\Psi),$$

(19)

(Tr$_1$ and Tr$_2$ denote traces of operators acting on $\mathcal{H}$ and $\mathcal{H} \otimes \mathcal{H}$, respectively and $\hat{1}_1$ and $\hat{1}_2$ are the unit operators on these subspaces).

• If $|\Phi\rangle \in SD_N$, i.e. if the state $|\Phi\rangle$ is constructed as a Slater determinant, then $\hat{\gamma}_\Phi = \hat{\gamma}_\Phi^2$ and, moreover, $\hat{\gamma}_\Phi$ is an orthogonal projection onto the $N$ dimensional subspace of $\mathcal{H}$ spanned by the vectors used to construct $|\Phi\rangle$.

• The 2-pdo associated with $|\Phi\rangle \in SD_N$ takes the form $\hat{\Gamma}_\Phi = \hat{\Gamma}_\Phi^\dagger = \hat{A}_2(\hat{\gamma}_\Phi \otimes \hat{\gamma}_\Phi)$, where $\hat{A}_2$ is the antisymmetrization operator acting on $\mathcal{H} \otimes \mathcal{H}$: $\hat{A}_2|f\rangle \otimes |g\rangle = |f\rangle \otimes |g\rangle - |g\rangle \otimes |f\rangle$ (in the notation of [1] $\hat{A}_2 = \hat{1}_2 - \hat{E}x$, where $\hat{E}x$ is the exchange operator).

Let now $\hat{\gamma}_{gs}$ and $\hat{\Gamma}_{gs}$ be the 1- and 2-pdo’s, respectively, corresponding to the true ground state $|\Psi_{gs}\rangle$ of the Hubbard model Hamiltonian (3). The ground state energy $E_{gs}$ can be then written as

$$E_{gs}(n) = \text{Tr}_1(\hat{T}_1 \hat{\gamma}_{gs}) + \frac{1}{2} \text{Tr}_2(\hat{V}_2 \hat{\gamma}_{gs}).$$

(20)

where $\hat{T}_1$ and $\hat{V}_2$ have been defined above. In the analogous manner the H-F ground state energy can be written as

$$E_{hf}(n) = \inf \{ E_{HF}[\gamma_\Psi], \ |\Phi\rangle \in SD_N \},$$

(21)

where

$$E_{HF}[\gamma_\Psi] \equiv \text{Tr}_1(\hat{T}_1 \gamma_\Psi) + \frac{1}{2} \text{Tr}_2[\hat{V}_2 \hat{A}_2(\gamma_\Psi \otimes \gamma_\Psi)],$$

is the the Hartree-Fock energy functional.

The lower bound on $\Delta E(n)$ defined in (10) is now obtained as follows. Let $\hat{\gamma}_0$ be the 1-pdo associated with the ground state $|\Phi_0\rangle$ of the free Hamiltonian, i.e. of $\hat{T}_1$ (4). Obviously $|\Phi_0\rangle$ has the form of a Slater determinant. One expects that $\hat{\gamma}_{gs}(U) \rightarrow \hat{\gamma}_0$ for $U \rightarrow 0$. The rigorous proof of this fact in the form of a lower bound on $\Delta E(n)$ has been given in [1]. The bound, being a function of the coupling $U$, assesses the rate of this convergence. The proof consists of the following points: i) write an estimate of $\Delta E(n)$ using $\Gamma_{gs}$ (Lemma 1); ii) using the appropriate correlation inequality, go over from $\Gamma_{gs}$ to $\hat{\gamma}_{gs}$ (reduction of the two-body problem to a one-body one) (Lemma 2); iii) put a bound on $\hat{\gamma}_{gs}$ to obtain the final estimate of $\Delta E(n)$ in terms of $U$, $n$ and $|\Lambda|$ only (Lemmas 3 and 4). More explicitly we have [1]:

**Lemma 1.**

$$\Delta E(n) \geq \frac{U}{2} \sum_{x \in \Lambda} \text{Tr}_2 \left[ (\hat{X}_x \otimes \hat{X}_x) \left( \hat{\Gamma}_{gs} - \hat{A}_2(\hat{\gamma}_0 \otimes \hat{\gamma}_0) \right) \right].$$

(22)
Lemma 2. (**) \( \hat{X} \) stands for a bounded Hermitian projection operator acting on \( \mathcal{H} \)

\[
\frac{1}{2} \text{Tr}_2((\hat{X} \otimes \hat{X}) \hat{\Gamma}_{gs}) - \text{Tr}_1[\hat{X} \hat{\gamma}_0] \text{Tr}_1[\hat{X} \hat{\gamma}_gs] + \frac{1}{2} \left( \text{Tr}_1[\hat{X} \hat{\gamma}_0] \right)^2 + \frac{1}{2} \text{Tr}_1[\hat{X} \hat{\gamma}_0 \hat{X} \hat{\gamma}_0] \geq -\text{const.} \text{Tr}_1[\hat{X} \hat{\gamma}_gs] \cdot \text{min} \left( 1, \sqrt{\text{Tr}_1[\hat{X} (\hat{1}_1 - \hat{\gamma}_0) \hat{\gamma}_gs (\hat{1}_1 - \hat{\gamma}_0)]} \right).
\]

Lemma 3.

\[
\frac{\Delta E(n)}{|\Lambda|} \geq -\text{const.} U \sqrt{n} \sqrt{\text{Tr}_1[(\hat{1}_1 - \hat{\gamma}_{gs}) \hat{\gamma}_0]} \equiv -\text{const.} U \sqrt{n} A.
\]

The final element of the proof is to find an estimate of the constant \( A \). It can be expressed in terms of the spectrum of the noninteracting \( (U = 0) \) system, i.e. on the eigenvalues of the hopping matrix \( \{x_{k,y}\} \) and the corresponding density of states (DOS). Since the hopping matrix has been assumed to be translationally invariant, it can be diagonalized with the help of the (discrete) Fourier transform. This brings the \( \hat{T} \) operator (and, hence, the free Hamiltonian) into the diagonal form:

\[
\hat{T} = \sum_{k \in BZ} \sum_{\sigma} \epsilon(k) c_{k,\sigma}^\dagger c_{k,\sigma},
\]

where \( BZ = [-\pi, \pi)^d \cap (\pi/L)\mathbb{Z}^d \) is the first Brillouin zone, the function \( \epsilon(k) \) (the ‘free-particle spectrum’, or the ‘dispersion relation’) is the discrete Fourier transform of the hopping matrix:

\[
\epsilon(k) = \hat{t}(k) = \sum_{x \in \Lambda} t(x) e^{ik \cdot x},
\]

and the operators \( c_{k,\sigma}^\dagger \) and \( c_{k,\sigma} \) are given by

\[
c_{k,\sigma}^\dagger = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} e^{ik \cdot x} c_{x,\sigma}, \quad c_{k,\sigma} = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} e^{-ik \cdot x} c_{x,\sigma}.
\]

Of course, the vectors \( |k, \sigma\rangle = c_{k,\sigma}^\dagger |0\rangle \) form an orthonormal basis of \( \mathcal{H} \) and the ground state \( |\Psi_0\rangle \) (belonging to the \( F_{N+, N-} \) subspace) of the \( U = 0 \) Hubbard model can be, assuming that \( \epsilon(k_j) \leq \epsilon(k_i) \) for \( j < i \), written as \( (N_+ + N_- = N) \)

\[
|\Psi_0\rangle = \left( \prod_{j_1=1}^{N_+} c_{k_{j_1},+}^\dagger \right) \left( \prod_{j_2=1}^{N_-} c_{k_{j_2},-}^\dagger \right) |0\rangle.
\]

This allows to introduce the Fermi energy \( \epsilon_F \) as the highest energy of the occupied one-particle states, that is \( \epsilon_F = \epsilon(k_{j_{\text{max}}}) \), where \( j_{\text{max}} = \text{max}(N_+, N_-) \).

The density of states (of the non-interacting system, \( U = 0 \)), is defined by the formula

\[
\rho_d(E) = \int_{[-\pi, \pi]^d} d^d k \delta(\epsilon(k) - E) \equiv \frac{dN_d(E)}{dE},
\]

\[7\]
where
\[ N_d(E) = \int_{[-\pi,\pi]^d} d^d k \chi(\epsilon(k) \leq E). \] (30)

The necessary estimate of the constant \( A \) appearing in the inequality (24) is now provided by Lemma 4. (the ‘bootstrap’ estimate).

There exist constants \( c_1, c_2, c_3 \) such that for every \( \epsilon > 0 \) the constant \( A \) satisfies the bound \( (2L = |\Lambda|^{1/d} \) is the width of the lattice):

\[ A^2 \leq \frac{c_1}{\epsilon} U A \sqrt{n} + c_2 \int_{-\epsilon-c_3/L}^{c_3/L} d\lambda \rho_d(\epsilon_F + \lambda) \equiv \frac{c_1}{\epsilon} U A \sqrt{n} + c_2 I(\epsilon, L; n). \] (31)

Solving the inequality (31) one obtains the upper bound on \( A \)
\[ A \leq \frac{c_1}{2\epsilon} U \sqrt{n} + \sqrt{\left( \frac{c_1}{2\epsilon} U \right)^2 n + c_2 I(\epsilon, L; n)}. \] (32)

Combined with the inequality (24), this bound provides the general form (obtained in [1]) of the the lower bound on the difference (10) of the true ground state energy and the H-F approximation to it. The precise form of this bound, i.e. its final dependence on \( n \) and \( U \) (and on the lattice dimension \( d \)), depends on the estimate of the integral \( I(\epsilon, L; n) \). The latter depends on the general form of density of states \( \rho_d(E) \) (which is a property of the type of the lattice and the number of dimensions \( d \)) and also on the filling of the lattice. Estimating \( I(\epsilon, L; n) \) is straightforward in those cases in which \( \rho_d(E) \) is a bounded function; in some cases it has, however, (integrable) singularities which introduce some complications in estimating \( I(\epsilon, L; n) \). These will be discussed in the next Section.

### 4 Examples of estimates

In this Section we show how the machinery developed in [1] and presented above works in practice. In Sections 4.1 and 4.2 we repeat (for the illustration) the derivation of the estimates obtained in [1], and in the subsequent two sections we present our extension of this approach to the versions of the Hubbard models not considered in [1]: to the single band model on the body centered cubic (bcc) lattice and to the flat band systems.

#### 4.1 A prototype calculation: the (hyper)cubic lattice in \( d \geq 3 \)

Let the elements of the hopping matrix be non-zero and equal \( t \) only for the nearest neighbour sites of the \( d \)-dimensional simple (hyper)cubic lattice (sc). The dispersion function has then the form

\[ \epsilon_{sc}(k) = -2t (\cos k_1 + \ldots + \cos k_d). \] (33)
It is therefore a Morse function (i.e., it has only non-degenerate critical points). For \( d \geq 3 \) the corresponding DOS function, which is given by a non-elementary integral [10], is bounded and the integral \( I(\varepsilon, L; n) \) defined by (31) can be easily estimated (\( c_4 = \max\{4c_3, 1\} \)):

\[
I(\varepsilon, L; n) \leq \left( \frac{2c_3}{L} + \varepsilon \right) \sup(\rho_d) \equiv c_4 \left( |\Lambda|^{1/d} + \varepsilon \right) \sup(\rho_d).
\]

The resulting bound [22]

\[
A \leq \frac{c_1}{2\varepsilon} U \sqrt{n} + \sqrt{\frac{c_1^2 U^2 n}{4\varepsilon^2} + c_4 \varepsilon + c_4 |\Lambda|^{1/d}}
\]

is valid for any \( \varepsilon > 0 \) and can be, therefore, brought into a reasonably optimal form (using the inequality \( \sqrt{a + b} < \sqrt{a} + \sqrt{b} \)) by simply setting \( \varepsilon = \text{const.} n^{1/3} U^{2/3} \):

\[
A \leq \text{const.} \left( n^{1/6} U^{1/3} + \text{const.'} |\Lambda|^{1/d} \right).
\]

Combining this with the relation [24] we obtain the lower bound

\[
\frac{\Delta E(n)}{|\Lambda|} \geq -\text{const.} \left( n^{2/3} U^{4/3} + \text{const.'} n^{1/2} U |\Lambda|^{1/d} \right).
\]

### 4.2 The square lattice in \( d = 2 \)

In the case of the two-dimensional square lattice with a nonzero hopping amplitude for nearest neighbor sites only the density of states is given by a complete elliptic integral of the first kind [10] :

\[
\rho(\varepsilon) = \frac{1}{2|t|\pi^2} K(1 - (\varepsilon/4t)^2),
\]

(the plot is given in Figure 1a of this reference). From the well-known properties of the elliptic integral \( K(k) \) which logarithmically diverges at \( k = 1 \) it follows that \( \rho(\varepsilon) \) has such a singularity at \( \varepsilon = 0 \). Depending on the value of the Fermi energy \( \varepsilon_F \), which is determined by the filling, the integration domain in \( I(\varepsilon, L; n) \) may or may not contain this singularity. In the latter case, the density of states is (within the integration domain) bounded and essentially the same estimate of \( I(\varepsilon, L; n) \) as in the case of the hypercubic lattice in \( d \geq 3 \). The condition on density \( n \) which distinguishes this case from the other one is rather involved. We therefore do not show details of this analysis and concentrate on the opposite case of sufficiently high filling in which the presence of the singularity affects the estimate of \( I(\varepsilon, L; n) \).

It this case, using the asymptotic form of the elliptic relevant integral, one can write

\[
I(\varepsilon, L; n) \leq C \left( \frac{c}{L} + \varepsilon \right) \ln \left( \frac{c}{L} + \varepsilon \right) + \varepsilon + \frac{c}{L} \ln \frac{c}{L} + 2\frac{c}{L}.
\]

Setting here \( \varepsilon = \text{const.} n^{1/3} U^{2/3} \) (which again is a simple but reasonable choice) we obtain as the upper bound

\[
A \leq C' \left( n^{1/6} U^{1/3}
\right.

\[
+ \sqrt{n^{1/3} U^{2/3} + \left( \frac{1}{L} + n^{1/3} U^{2/3} \right) \ln \left( \frac{1}{L} + n^{1/3} U^{2/3} \right) + \frac{1}{L} \ln \frac{1}{L} + \frac{2}{L} \right).
\]

(36)
In conjunction with the inequality (24) this suffices to conclude that for small $U$ and large $|\Lambda|$ the H-F approximation becomes exact. We note also that the bound on $A$ given in [1] for this particular case, although more transparent, is slightly less stringent than the one given above. Nevertheless, it too leads to the same overall conclusion. This bound follows from the one given above if one takes into account that the constraint $0 \leq n \leq 2$ implies boundedness of $n \ln n$; using the inequality $\sqrt{a+b} \leq \sqrt{a} + \sqrt{b}$ after a bit lengthy but elementary algebra one arrives at

$$A \leq C \left\{ n^{1/6} U^{1/3} (\ln |U| + 1) + |\Lambda|^{-1/4} \ln (|\Lambda|^{-1/2} + 1) \right\}, \quad (37)$$

which leads to

$$\frac{\Delta E(n)}{|\Lambda|} \geq -C \left[ n^{2/3} U^{4/3} (\ln |U| + 1) + n^{1/2} U |\Lambda|^{-1/4} \ln (|\Lambda|^{-1/2} + 1) \right]. \quad (38)$$

We remark that the above estimate is universally applicable at all densities (fillings) in view of the fact that it is weaker than the one obtained for high densities.

### 4.3 Body-centered cubic lattice in $d = 3$

The body-centered cubic lattice (bcc) is an example of a lattice on which the period of the hopping matrix $t_{x,y}$ is greater than 1. Application to this case of the machinery developed in [1] requires again its slight generalization. Here we consider only the simplest case that is, we assume that the hopping constants (nonzero entries of the matrix $t_{x,y}$) are all equal $t$. The dispersion relation which originates from the periodic structure of such a bcc lattice is [10]

$$\epsilon_{\text{bcc}}(k) = -8t \cos k_1 \cos k_2 \cos k_3. \quad (39)$$

The corresponding DOS function $\rho_{\text{bcc}}(\epsilon)$ cannot be expressed in terms of elementary functions. It is nevertheless possible to extract those its properties which are important for estimating the integral $I(\epsilon, L; n)$. It turns out that the DOS function in question does have a singularity near the zero energy $\rho_{\text{bcc}}(\epsilon) \sim (4\pi)^{-3} \ln^2 \epsilon [10]$. The singularity originates from the neighbourhood of the point $(\pi/2, \pi/2, \pi/2)$ at which all the cosine functions in (39) simultaneously vanish. In estimating the integral $I(\epsilon, L; n)$, assuming that the singularity of the DOS function lies within the integration domain, we follow, therefore, the steps taken in [1] in deriving the estimate for the $d = 2$ square lattice (in which case the DOS function has also a logarithmic singularity, $\sim \ln \epsilon$). The estimate of the integral $I(\epsilon, L; n)$ obtained using the asymptotic form of $\rho_{\text{bcc}}$ reads ($c$ is some constant):

$$I(\epsilon, L; n) \leq C \left\{ 4 + \ln^2 \frac{c}{L} + 2 \left| \ln \frac{c}{L} \right| \right\} + 2 \epsilon$$

$$\quad + \left( \frac{c}{L} + \epsilon \right) \left\{ \ln^2 \left( \epsilon + \frac{c}{L} \right) + 2 \left| \ln \left( \epsilon + \frac{c}{L} \right) \right| \right\}. \quad (40)$$

Setting again $\epsilon = \text{Const.} n^{1/3} U^{2/3}$ we get a reasonably stringent, but unfortunately having a rather complicated form, bound on $A$ as a function of $L$, $n$ and $U$ (it is somewhat analogous to (36)). Instead of reproducing it here we will content ourselves
with a less stringent but more transparent bound which, combined with the inequality (24), leads to the lower bound
\[
\frac{\Delta E(n)}{|\Lambda|} \geq -C \left[ n^{2/3} U^{1/3} \left( 1 + \ln^2 |U| + \ln |U| \right) + n^{1/2} U \times \mathcal{O}(|\Lambda|^{-1/6}) \right].
\] (41)

### 4.4 Flat-band systems

We now turn to systems the dispersion functions \( \epsilon(k) \) of which are completely flat, i.e. independent of \( k \). (In general, the dispersion relations of such systems consist of several subbands; some of them may be non-constant, but at least one is). Such lattices play a crucial role in the emergence of the flat-band ferromagnetism [11]. Perhaps, the most famous one is the Kagomé lattice. Another one is the simple one-dimensional lattice, called the sawtooth chain. A completely flat subband with a macroscopic degeneracy of the ground state (the number of states having the lowest possible value of energy is proportional to \( |\Lambda| \)) implies that the corresponding DOS function has the delta function form with a spectral weight \( w \) (\( w = 1/3 \) for the Kagomé lattice, \( w = 1/2 \) for the sawtooth one).

The fundamental inequality (31) takes in this case the form
\[
A^2 \leq c_1 U \sqrt{n} A + w |\Lambda|,
\]
and implies the upper bound
\[
A \leq \frac{c_1 U \sqrt{n}}{2 \varepsilon} + \frac{c_1 U \sqrt{n}}{2 \varepsilon} + 4w |\Lambda|.
\]

Optimizing again with respect to \( \varepsilon \) by setting \( \varepsilon = \infty \) we get
\[
A \leq 2 \sqrt{w |\Lambda|},
\]
which, in conjunction with (24), leads to the estimate
\[
\frac{\Delta E(n)}{|\Lambda|} \geq -\text{Const.} U \sqrt{n |\Lambda|}.
\] (42)

Although correct, this result is clearly useless. The lesson that, nevertheless, can be drawn from this example is: the more singular is the DOS function, the worse is the estimate of \( \Delta E \).

### 5 Multiband models

In the common opinion the single-band version of the Hubbard model considered in the preceding sections is too simple to be capable of capturing all relevant features of realistic systems exhibiting ferromagnetism. One is therefore naturally led to consider various extensions of the original Hubbard model which allow to introduce a variety of interaction terms in order to model both charge and magnetic - e.g. the Hund
one - interactions \cite{12,13}. In this Section we point out that the technique of Bach and Poelchau \cite{1} can be immediately extended to give estimates of the ground state energies of at least two simplest such extensions: the $M$-band model with the coulombic interactions only and the $SU(M)$ symmetric extension of the single-band model which correspond to spin $M$ fermions the interactions of which are spin independent ($SU(M)$ is then an “accidental” extension of the usual $SU(2)$ symmetry associated with the usual rotational invariance). Up to now we were not able to apply the same approach to models with the Hund-type interactions.

5.1 The $M$-band Hubbard Model

Allowing for $M$-bands enlarges the dimension of the single particle Hilbert space $\mathcal{H}$ to $2M|\Lambda|$ so that now the dimension of the Fock space $\mathcal{F}(\mathcal{H})$ constructed in the same way as in Section 2 is $2^{2M}|\Lambda|$. The natural basis of $\mathcal{H}$ is in this case formed by the state-vectors $|x,a,\sigma\rangle$ where $a = 1, \ldots, M$ is the band label, and $\sigma = \pm$ (as previously we consider spin 1/2 fermions) is the spin label. In terms of the creation and annihilation operators associated with this basis of $\mathcal{H}$ the Hamiltonian of the considered $M$-band version of the Hubbard model reads

$$H = - \sum_{(x,x)} \sum_{a=1}^{M} t_{x,x} c_{x,a,\sigma}^\dagger c_{y,a,\sigma} + U \sum_{x} \sum_{a=1}^{M} n_{x,a,+} n_{x,a,-} + U' \sum_{x} \sum_{a\neq a'=1}^{M} \sum_{\sigma,\sigma' = \pm} n_{x,a,\sigma} n_{x,a',\sigma'}.$$  \hspace{1cm} (43)

$U$ and $U'$ (both positive) represent here the Coulomb repulsion of fermions in the same and in different bands, respectively.

Below we consider only a particular version of (44) with $U = U'$. In this case the notation can be made more concise by introducing the multi-index $A \equiv (a, \sigma)$:

$$H = - \sum_{x,y} \sum_{A} t_{x,y} c_{x,A}^\dagger c_{y,A} + U \sum_{x} \sum_{A \neq A'} n_{x,A} n_{x,A'}.$$  \hspace{1cm} (44)

To estimate the ground state energy of this model one can introduce the 1- and 2-particle density operators in full analogy with the definitions (17) and (18), respectively. The only difference is the replacement of the spin index $\sigma$ with the multi-index $A$ introduced above. With the help of the density operators the quantity of interest, the difference $\Delta E_1(n)$ defined as in (10), can be estimated by essentially repeating the steps taken in the preceding sections. To this end one introduces the projection Hermitian operators

$$\hat{X}_x = \sum_{A} |x, A\rangle \langle x, A|,$$

which allow to write the interaction term in (44) in the form

$$\hat{V}_2 = U \sum_{x} \hat{X}_x \otimes \hat{X}_x,$$  \hspace{1cm} (46)

analogous to (15). All considerations used for the single-band Hubbard Model can now be repeated without any modifications leading to bounds on $\Delta E$ analogous to (34).
5.2 \textit{SU}(M) symmetric Hubbard Model

Another version of the Hubbard model to which the method of \cite{1} of bounding the difference $\Delta E$ of the ground state energies can be immediately applied is one in which there are $M$ kinds (‘flavours’) of fermions. Its Hamiltonian has the form

\[
H = -\sum_{x,y} \sum_{m} t_{x,y} c_{x,m}^{\dagger} c_{y,m} + U \sum_{x} \sum_{m \neq m'} n_{x,m} n_{x,m'}
\]

\[
= -\sum_{x,y} \sum_{m} t_{x,y} c_{x,m}^{\dagger} c_{y,m} + \frac{U}{2} \sum_{x} (n_{x}^{2} - n_{x}), \tag{47}
\]

where $n_{x}$ is the total number density of particles on the site $x$; it can be written in terms of the fermionic creation and annihilation operators: $n_{x} = \sum_{m=1}^{M} c_{x,m}^{\dagger} c_{x,m}$. The operator $n_{x}$ is invariant under local $U(M)$ rotations which mix flavours labeled by different values of $m$. The hopping term, which involves operators at different sites, reduces this invariance to the global $U(M)$ symmetry only. The $SU(M)$-symmetric Hubbard model is obtained by stripping off the global $U(1)$ phase factor. (A certain variant of such a $SU(M)$ Hubbard model, with $M$ having the interpretation of the number of hyperfine states, has been used in \cite{14} to model cold fermionic gases). Also in this case, the introduction of the Hermitian projectors

\[
\hat{X}_{x} = \sum_{m} |x,m\rangle\langle x,m|, \tag{48}
\]

having all the necessary properties of the projectors \cite{13} and \cite{45} allows to rewrite the interaction term of (47) in the form analogous to (15) and (46) and, therefore, the bound on $\Delta E$ established above holds.

6 Summary

In this paper we have shown that the method of Bach and Poelchau \cite{1} of estimating the difference of the true and the approximate, obtained using the Hartree-Fock approach, ground state energies of the simplest versions of the Hubbard models can be extended to more complicated cases of the Hubbard models with period of the lattice greater than the unit one and to certain versions of the multi-band Hubbard models.

One possible route to prove the existence of the itinerant ferromagnetism is to consider the multiband Hubbard model with the Hund interaction, and obtain a sufficiently tight estimate of $\Delta E$ in this case. The original motivation for our investigation was the hope that the machinery developed in \cite{1} can be extended to obtain the bounds explicitly depending on the polarization for such a realistic version of the Hubbard model of spin 1/2 fermions on lattices allowing thereby for rigorous statements about the existence of ordered phase (at zero temperature) of such systems. This ambitious goal still remains a challenge - we don’t see how the Hund interactions could be written in the form similar to \cite{15}, \cite{46}, which is needed for applying to it the technique of \cite{1}. While we still believe that a lower bound $\Delta E$ can be derived in this case as well, we at present we have no idea how to obtain it. Nevertheless the method allowed to obtain valuable lower bounds on the difference of the true ground state energy and the
Hartree Fock approximation to it in some cases which are currently of prime interest but were not considered in the original work [1].

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