Ferromagnetism of the Hubbard Model at Strong Coupling in the Hartree-Fock Approximation

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Abstract
As a contribution to the study of Hartree-Fock theory we prove rigorously that the Hartree-Fock approximation to the ground state of the $d$-dimensional Hubbard model leads to saturated ferromagnetism when the particle density (more precisely, the chemical potential $\mu$) is small and the coupling constant $U$ is large, but finite. This ferromagnetism contradicts the known fact that there is no magnetization at low density, for any $U$, and thus shows that HF theory is wrong in this case. As in the usual Hartree-Fock theory we restrict attention to Slater determinants that are eigenvectors of the $z$-component of the total spin, $S_z = \sum_x n_{x,\uparrow} - n_{x,\downarrow}$, and we find that the choice $2S_z = N = $ particle number gives the lowest energy at fixed $0 < \mu < 4d$.

Keywords: Hubbard model, Ferromagnetism, Hartree-Fock Theory

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1 Introduction

The (one-band) Hubbard model has become a standard model for correlated electrons in condensed matter physics since it is, perhaps, the simplest possible model of itinerant interacting electrons. In spite of its simplicity, its zero temperature phase diagram is rich with different magnetic phases such as paramagnetic, ferromagnetic, and antiferromagnetic phases, depending on the details of the hopping amplitudes, the (relative) coupling constant $U/t$ and the filling parameter $\nu = N/(2|\Lambda|)$.

As the Hubbard model is a many-body fermion model, the computation of its ground state for large lattices is a difficult, if not impossible, task, except in one-dimension \cite{1,2}. Thus various schemes have been developed during the past decades to derive an approximate ground state and then to study its magnetic phase diagram.

In the present paper, we consider the Hartree-Fock approximation of the (repulsive, one-band, nearest-neighbor-hopping) Hubbard model with the intention of studying the validity of the Hartree-Fock approximation. We require the Slater determinants entering the Hartree-Fock energy functional to be eigenfunctions of the operator $S_z := \sum_{x \in \Lambda} \{n_{x,\uparrow} - n_{x,\downarrow}\}$ of total spin in the $z$-direction, and for this reason we refer to the model as the HF$_z$ approximation. Our requirement means that each orbital has the form $\varphi(x) \otimes |\uparrow\rangle$ or $\varphi(x) \otimes |\downarrow\rangle$. This is a restriction in the sense that general orbitals are of the form $\varphi(x,\sigma)$, in which the spin direction depends on position. No other restriction is imposed on the variational states; in particular, no assumption about translation invariance is made a priori. For the HF$_z$ model, at small chemical potential and for sufficiently strong repulsion, we give a mathematical proof of saturated ferromagnetism in the Hartree-Fock ground state. That is, the HF ground state has maximal total spin and maximal ferromagnetic long-range spatial order. The smallness of the chemical potential and the large strength of the repulsion also insure that the HF ground state density is strictly below half-filling.

Before we come to a detailed description of our result and its proof, we discuss it in comparison to other works.

The appearance of ferromagnetic behaviour has been anticipated in many studies of the Hubbard model and approximations thereof. Among these are (restricted) Hartree-Fock approximations \cite{3}, DMFT models in the limit of infinite spatial dimension \cite{4,5,6,7}, exact diagonalizations on small lattices \cite{8}, variational calculations \cite{9} and studies at low filling \cite{10}. These studies support the conjecture that, for large coupling $U/t \gg 1$ and away from half-filling, $\nu \neq 1/2$, \ldots
the ground state of the Hubbard model is ferromagnetic. Ferromagnetism has been established for the (full) Hubbard model in case the dispersion relation leads to a very high density of states around the Fermi energy \[11, 12, 13\] and in case of next-nearest-neigbor hopping \[14, 15\].

As said before, the main purpose of the present paper is to prove ferromagnetic behaviour with mathematical rigor. None of the papers \[4, 5, 6, 7, 8\] cited above match the standards of a mathematical proof: The orbitals in the Hartree-Fock approximation are a priori assumed to be composed of only few Fourier modes; the error terms when taking the limit of infinite spatial dimension in DMFT are not under control; exact diagonalizations are restricted to very small lattices and the implication of these to the thermodynamic limit remains unclear. The work by Mielke and Tasaki \[11, 12, 13\] is mathematically rigorous, but the assumptions made therein about the lattice structure are rather special. On the other hand, by adding next-nearest-neigbor hopping (two-band Hubbard model), Tasaki \[14, 15\] has found a Hubbard model that displays ferromagnetism in all dimensions. Tasaki also reviews rigorous results on ferromagnetism in the Hubbard model in \[16\].

While the prediction of ferromagnetism in the Hubbard model and approximations thereof is supported by the above studies, we also know that HF theory predicts anti-ferromagnetism (in the sense that the total spin is zero) at higher densities, notably at half-filling \[17\]. Furthermore, our proof shows saturated ferromagnetism at low density and sufficiently large coupling in HF theory, even in one-dimension, but the actual ground state always has spin zero in one-dimension as long as there is only nearest-neighbor hopping (see \[13\]).

Even more seriously, our conclusion is opposite to what actually occurs in the Hubbard model. Namely, at very low density (and independent of the value of \( U > 0 \)), there is no magnetization in the ground state of this model. In the ground state \( S_z \) is close to zero and converges to zero, as the particle density tends to zero. This has been pointed out in \[19, 16\], based on arguments similar to the following transcription to lattice systems of the recent work \[20\].

In this paper \[20\] it was shown that fermions in the 3-dimensional continuum \( \mathbb{R}^3 \) (instead of the lattice \( \mathbb{Z}^3 \)), and with a repulsive two-body potential, have a ground state energy density, \( e \), given by

\[
e(\rho_\uparrow, \rho_\downarrow) = \frac{\hbar^2}{2m} \frac{3}{5} (6\pi^2)^{2/3} \left( \rho_\uparrow^{5/3} + \rho_\downarrow^{5/3} \right) + \frac{\hbar^2}{2m} 8\pi a \rho_\uparrow \rho_\downarrow + \text{higher order in } (\rho_\uparrow, \rho_\downarrow),
\]

where \( \rho_\uparrow, \rho_\downarrow \) are the densities of the ‘spin-up’ and the ‘spin-down’ fermions and \( a \)
is the scattering length of the two-body potential. Because $\rho^{5/3}$ dominates $\rho^2$ for small $\rho$, it is clear from [11] that the minimum energy occurs approximately, if not exactly, when $\rho_\uparrow = \rho_\downarrow = \rho/2$. This answers the questions in [21, problem 3].

To show that there is vanishing net magnetization as $\rho \to 0$ one only needs an upper bound for $e$ of the form (1.1). For the Hubbard model (where the two-body potential is a positive delta-function, or even a hard core) this can conveniently be done by a variational wave-function of the form $\Psi = F\Psi_0$, where $\Psi_0$ is a Slater determinant, and $F$ is the projection onto the states with no double occupancy – in imitation of [19, 16, 20]. We omit the details, but we draw attention to the fact that $F\Psi_0$ is not a Slater determinant, reflecting the more complex structure of correlations in the actual ground state of the Hubbard model. The proof of an analog of (1.1) with precise constants is a more complicated matter which is now under investigation, but it is not needed for the present discussion.

Our setting is the usual (repulsive) Hubbard model with nearest-neighbor hopping on a $d$-dimensional cubic lattice $\Lambda$, with periodic boundary conditions and linear size $L$, which we assume to be an even integer. It is defined by the second quantized Hamiltonian

$$H_{\mu,U} = \sum_{x,y \in \Lambda, \sigma = \uparrow, \downarrow} (-\Delta_{x,y} - \mu \delta_{x,y}) c_{x,\sigma}^* c_{y,\sigma} + U \sum_{x \in \Lambda} n_{x,\uparrow} n_{x,\downarrow}. \tag{1.2}$$

We work at fixed chemical potential $\mu$ instead of fixed particle number. The only slightly unusual notation is $\Delta_{x,y} = T_{x,y} - 2d \delta_{x,y}$ for the matrix elements of the discrete Laplacian $\Delta$ on $\Lambda$, with $T_{x,y} := \mathbb{I}[|x-y|_1 = 1]$ being the nearest-neighbor hopping matrix and $\delta_{x,y} = \mathbb{I}[x = y]$ the Kronecker-Delta.

The operators $c_{x,\sigma}^*$, $c_{x,\sigma}$, and $n_{x,\sigma} := c_{x,\sigma}^* c_{x,\sigma}$ are the usual fermion creation, annihilation, and number operators, respectively, at site $x \in \Lambda$ and of spin $\sigma \in \{\uparrow, \downarrow\}$, obeying the canonical anticommutation relations $\{ c_{x,\sigma}^*, c_{y,\tau} \} = \{ c_{x,\sigma}, c_{y,\tau}^* \} = 0$, $\{ c_{x,\sigma}, c_{y,\tau}^* \} = \delta_{x,y} \delta_{\sigma,\tau}$, and $c_{x,\sigma}|0\rangle = 0$, for all $x, y, \sigma, \tau$. Here $|0\rangle$ is the vacuum vector in the usual Fock space $\mathcal{F}_\Lambda := \mathcal{F}_f(\mathbb{C}^\Lambda \otimes \mathbb{C}^2)$ of spin-$\frac{1}{2}$ fermions. The Hamiltonian $H_{\mu,U}$ depends parametrically on the chemical potential $\mu > 0$ and the coupling constant $U > 0$.

Note that the usual hopping parameter $t$ equals 1 here and that the discrete Laplacian $\Delta$ differs from the usual hopping matrix by the inclusion of the diagonal term, i.e., $2d$ times the identity matrix. This difference amounts to a convenient redefinition of the chemical potential $\mu$, so that $\mu = 0$ corresponds precisely to zero filling since the hopping matrix $-\Delta \geq 0$ is a positive semi-definite matrix. Moreover, the boundedness $0 < \mu < 4d$ of $\mu$ together with the assumption that
$U \gg 4d$ insures that the corresponding electron density in the HF ground state is always at low filling, i.e., strictly below half-filling, $0 \leq \rho < 1$.

Our definition of $\mu$ is convenient because in this paper, we are concerned with the Hubbard model at low filling, and our assumption of a bounded chemical potential $0 \leq \mu \leq 2d$.

Apart from this, everything is standard.

The Hamiltonian $H_{\mu,U}$ is a linear operator on the Fock space and the ground state energy $E_{\mu,U}^{(gs)}$ is its smallest eigenvalue,

$$E_{\mu,U}^{(gs)} := \min \left\{ \langle \Psi | H \Psi \rangle \mid \Psi \in \mathcal{F}_\Lambda, \| \Psi \| = 1 \right\} . \tag{1.3}$$

As the dimension $\dim(\mathcal{F}_\Lambda) = 2^{\dim(C^\Lambda \otimes C^2)} = 4^{(L^d)} < \infty$ is finite, the determination of $E_{\mu,U}^{(gs)}$ amounts to diagonalizing the finite-dimensional, selfadjoint matrix $H_{\mu,U}$. The fast growth of this dimension with the number $L^d$ of points in the lattice $\Lambda$, however, allows for an explicit diagonalization of $H_{\mu,U}$ by a modern computer only up to $L = 4$, in three spatial dimensions, $d = 3$.

The Hartree-Fock (HF) approximation is an important method to reduce the high-dimensional many-particle problem given by the diagonalization of $H_{\mu,U}$ to a low-dimensional, but nonlinear variational problem. It is defined by restricting the minimization in (1.3) to Slater determinants $\varphi_1 \wedge \cdots \wedge \varphi_N$, where $\{ \varphi_i \}_{i=1}^N \subseteq C^\Lambda \otimes C^2$ is an orthonormal family of $N$ one-electron wave functions. The HF approximation to the Hubbard model was analyzed in [17] in the special situation when the number of electrons equals the number of lattice sites, $N = |\Lambda|$, which is usually referred to as half-filling.

Note that a priori no other condition but orthonormality is imposed on the orbitals $\{ \varphi_i \}_{i=1}^N$ in the Slater determinants varied over in Hartree-Fock theory. This is sometimes stressed by calling it the unrestricted Hartree-Fock theory. Let us temporarily consider a general many-body Hamiltonian $H$ which commutes with a certain symmetry operator $S$, i.e., $[H, S] = 0$. It is important to note that in this case, the HF ground state $\Phi_{hf}$, i.e., the Slater determinant which minimizes the energy $\langle \Phi_{hf} | H | \Phi_{hf} \rangle$, is not necessarily an eigenstate of $S$. Phrased differently, unrestricted Hartree-Fock theory may (depending on the model) break the symmetry $S$. The following are examples that occur in physically relevant situations: unrestricted HF ground states of atoms are, in general, not eigenfunctions of the angular momentum operator (because in unrestricted HF theory, all shells are filled [22]) - even though the atomic Hamiltonian is rotationally invariant; the ground state in the BCS theory of superconductors (which is a variant of HF theory) is not an eigenfunction of the number operator - even though the BCS Hamil-
tonian preserves the particle number; a HF ground state for the Hubbard model with non-zero spin breaks the invariance of the Hubbard Hamiltonian under global spin rotations; charge density waves (CDW) and spin density waves (SDW) of the Hubbard model are translation invariant only by translation of an even number of lattice sites, breaking the (full) translation symmetry the Hubbard Hamiltonian $H_{\mu,v}$ possesses. As it is impossible to predict a priori whether a symmetry of the Hamiltonian is preserved or not, we call all variations of $\langle \Phi | H | \Phi \rangle$ over Slater determinants $\Phi$ which fulfill an additional constraint restricted Hartree-Fock theory.

In this paper, we consider a restricted Hartree-Fock theory, which we term the HFz approximation. The further restriction imposed is that we minimize in (1.3) only over Slater determinants $\Phi$ that are eigenfunctions of the operator $S_z := \sum_{x \in \Lambda} \{ n_{x,\uparrow} - n_{x,\downarrow} \}$ of total spin in the $z$-direction. One could rephrase our condition by saying that we do not allow for spiral spin density waves (SSDW; see, e.g., [3]) in (1.3). Once again, it is customary to employ this restriction in HF calculations without explicitly drawing attention to the fact that this is a restriction. (In [17] mentioned above, however, we dealt with truly unrestricted HF theory.)

More concretely, our HF wave functions have the form

\[ \Phi = \prod_{i=1}^{N_{\uparrow}} c_{i\uparrow}^* (f_i) \prod_{j=1}^{N_{\downarrow}} c_{j\downarrow}^* (g_i) |0\rangle, \]  

where $c_{i\uparrow}^* (f) = \sum_{x \in \Lambda} f(x) c_{x,\uparrow}^*$, the integers $N_{\uparrow,\downarrow}$ are the particle numbers, and where the $f_i$ and $g_i$ are two families of orthonormal wave functions on the lattice $\Lambda$, i.e., $\langle f_i | f_j \rangle = \langle g_i | g_j \rangle = \delta_{i,j}$, with $\langle f | g \rangle := \sum_{x \in \Lambda} \bar{f}(x) g(x)$ denoting the usual hermitian scalar product for such functions.

It is convenient to rephrase the HFz approximation in terms of one-particle density matrices, i.e., complex, self-adjoint $\Lambda \times \Lambda$ matrices whose eigenvalues lie between 0 and 1. To this end, we denote

\[ K_\mu := -\Delta - \mu \]  

and observe that

\[ \langle \Phi | H | \Phi \rangle = \sum_{i=1}^{N_{\uparrow}} \langle f_i | K_\mu f_i \rangle + \sum_{j=1}^{N_{\downarrow}} \langle g_j | K_\mu g_j \rangle + U \sum_{x \in \Lambda} \left( \sum_{i=1}^{N_{\uparrow}} |f_i(x)|^2 \right) \left( \sum_{j=1}^{N_{\downarrow}} |g_j(x)|^2 \right). \]  

(1.6)
Introducing the one-particle density matrices $\gamma_{\uparrow, \downarrow}$ corresponding to $\Phi$ by

$$\gamma_{\uparrow} := \sum_{i=1}^{N_\uparrow} |f_i\rangle\langle f_i| \quad \text{and} \quad \gamma_{\downarrow} := \sum_{i=1}^{N_\downarrow} |g_i\rangle\langle g_i|,$$

we observe that $\gamma_{\uparrow, \downarrow} = \gamma_{\uparrow, \downarrow}^* = \gamma_{\uparrow, \downarrow}^2$ are orthogonal projections of dimension $N_{\uparrow, \downarrow}$ and that the energy expectation value of the Slater determinant $\Phi$ is given by $\langle \Phi | H \Phi \rangle = E^{(h\!f\!z)}_{\mu, U}(\gamma_{\uparrow}, \gamma_{\downarrow})$, where

$$E^{(h\!f\!z)}_{\mu, U}(\gamma_{\uparrow}, \gamma_{\downarrow}) := \text{Tr}\left\{ K_\mu (\gamma_{\uparrow} + \gamma_{\downarrow}) \right\} + U \sum_{x \in \Lambda} \rho_{\uparrow}(x) \rho_{\downarrow}(x),$$

and the diagonal matrix elements $\rho_{\uparrow, \downarrow}(x) := \gamma_{\uparrow, \downarrow}^{x,x}$ of $\gamma_{\uparrow, \downarrow}$ are the one-particle densities of the electron with spin up ("$\uparrow$") and spin down ("$\downarrow$"), respectively.

The symbol "Tr" denotes the usual trace $\text{Tr}\{A\} = \sum_{x,y \in \Lambda} A_{x,y}$ of a complex $\Lambda \times \Lambda$ matrix $A = (A_{x,y})_{x,y \in \Lambda}$ with $A_{x,y} \in \mathbb{C}$. That is, "Tr" is the trace over the states in $\mathbb{C}^\Lambda$ of a single spinless particle on the lattice $\Lambda$. It does not include spin states, and it is not the trace over states in Fock space.

Let us note that the particle numbers $N_{\uparrow, \downarrow}$ are not determined $ab\ initio$. We are in the grand canonical ensemble, so they are determined by the condition that the total energy (1.8) is minimized.

These observations motivate us to define the $HFz$ energy by the following variational principle over projections:

$$E^{(h\!f\!z)}_{\mu, U} := \min \left\{ E^{(h\!f\!z)}_{\mu, U}(\gamma_{\uparrow}, \gamma_{\downarrow}) \mid \gamma_{\uparrow, \downarrow} = \gamma_{\uparrow, \downarrow}^* = \gamma_{\uparrow, \downarrow}^2 \right\}. \quad (1.9)$$

The two sets of orthogonal projections on $\mathbb{C}^\Lambda$ over which we minimize in (1.9) is not really well-suited for a variational analysis. In particular, they are not convex. An observation in [23], however, states that, because $U \geq 0$, we will obtain the same value for the minimum if we vary over the larger set of all one-particle density matrices, $0 \leq \gamma_{\uparrow, \downarrow} \leq 1$, not only over projections. (Recall that a density matrix is a hermitean $\Lambda \times \Lambda$ matrix $\gamma$ whose eigenvalues lie between 0 and 1, i.e., $0 \leq \gamma \leq 1$, as a matrix inequality.) Our extended $E^{(h\!f\!z)}_{\mu, U}$ is then

$$E^{(h\!f\!z)}_{\mu, U} = \min \left\{ E^{(h\!f\!z)}_{\mu, U}(\gamma_{\uparrow}, \gamma_{\downarrow}) \mid 0 \leq \gamma_{\uparrow, \downarrow} \leq 1 \right\}. \quad (1.10)$$

The evaluation of $E^{(h\!f\!z)}_{\mu, U}$ and the determination of those pairs $(\gamma_{\uparrow}, \gamma_{\downarrow})$ of one-particle density matrices that minimize $E^{(h\!f\!z)}_{\mu, U}$ is the objective of this paper. Our main result is that, for any $0 < \mu < 4d$, the minimal value of $E^{(h\!f\!z)}_{\mu, U}$ is attained for the saturated ferromagnet, provided $U < \infty$ is sufficiently large.
Theorem 1.1 (Ferromagnetism). For any $0 < \mu < 4d$, there is a finite length $L_\#(\mu)$ and a finite coupling constant $U_\#(\mu) \geq 0$, such that, for all even $L \geq L_\#(\mu)$ and all $U \geq U_\#(\mu)$, the minimal HFz energy is given by the sum of the negative eigenvalues of $-\Delta - \mu$,

$$E_{\mu,U}^{(\text{hfz})} = \text{Tr}\{[-\Delta - \mu]_-\}.$$  \hspace{1cm} (1.11)

If $\mu$ is not an eigenvalue of $-\Delta$ and if $(\gamma_\uparrow, \gamma_\downarrow)$ is a minimizer of the HFz functional, i.e., $0 \leq \gamma_\uparrow, \gamma_\downarrow \leq 1$, and $E_{\mu,U}^{(\text{hfz})}(\gamma_\uparrow, \gamma_\downarrow) = E_{\mu,U}^{(\text{hfz})}$, then

- either $\gamma_\uparrow = \mathbb{1}[-\Delta < \mu]$; $\gamma_\downarrow = 0$ (1.12)
- or $\gamma_\uparrow = 0$, $\gamma_\downarrow = \mathbb{1}[-\Delta < \mu]$ (1.13)

where $\mathbb{1}[-\Delta < \mu]$ is the spectral projection of $-\Delta$ onto $(-\infty, \mu)$.

With reference to Eq. (1.11) and elsewhere, note that in our notation, $[X]_- = \min\{X, 0\}$ is negative, whereas elsewhere one often defines $[X]_-$ to be positive, i.e., $[X]_- := \max\{-X, 0\}$. If $X$ is a self adjoint operator then $[X]_-$ denotes the negative part of $X$ and $\text{Tr}[X]_-$ is the sum of the negative eigenvalues of $X$.

Theorem 1.1 is not really as complicated as it looks. It is stated in terms of a length $L_\#$ and coupling constant $U_\#$ in order to make it clear that the state of saturated ferromagnetism is obtained not only asymptotically in the thermodynamic limit and asymptotically as $U \to \infty$, but it holds for all systems with large, finite interaction and sufficiently large size.

Theorem 1.1 states that, for any value of the chemical potential $\mu \in (0, 4d)$, the HFz variational principle yields a ferromagnetic minimizer, provided $U$ and $L$ are chosen sufficiently large (but still finite). A similar statement was proved in [17, Theorem 4.7] for $U = \infty$ (which amounts to requiring $\langle \Phi | n_x,\uparrow n_x,\downarrow \Phi \rangle = 0$, on every lattice site $x \in \Lambda$).

At first sight, Theorem 1.1 seems to contradict another fact proved in [17] that the HF minimizer is antiferromagnetic at half-filling. But as the definition of the chemical potential $\mu$ in present paper differs from its definition in [17] by $2d + U$, the parameter range of the present paper and of [17] never overlap and, hence, there is no contradiction.

As just mentioned, the minimal HF energy and the minimal HFz energy agree in the half-filling case, as shown in [17]. We conjecture that this is also the case for the range of the chemical potential $\mu \in (0, 4d)$ and sufficiently large $U$, but we do not know how to prove this conjecture. This is a topic for future research.
From Theorem 1.1 we conclude that at small filling there is a phase transition (within the context of HFz theory) from paramagnetism for small \( U \) to saturated ferromagnetism for large \( U \). This follows from continuity and the fact that when \( U = 0 \) we can find the ground state explicitly and, as is well known, it has \( S = 0 \) and is obtained from filling up the Fermi sea for both \( \uparrow \) and \( \downarrow \) states.

If \( 0 < \mu \leq \frac{1}{2} \) then we can estimate \( L_{\#}(\mu) \) and \( U_{\#}(\mu) \) in Theorem 1.1 more explicitly. For the precise formulation of these estimates, we introduce the following constants,

\[
L_*(\mu) := 2 \, M_*(\mu) := 24 \left( 4d \right)^2 \mu^{-2}, \tag{1.14}
\]
\[
\kappa(\mu) := \frac{\mu^d}{4^{2d+1} \, e^d \, d^d} \left[ 1 + 2 \ln(2) \left( d^{-1} + 1 \right) + \ln \left( 4d \mu^{-1} \right) \right]^{-2d}, \tag{1.15}
\]
\[
\alpha_*(\mu) := \frac{|S^{d-1}| \, \mu^{(2+d)/2}}{2^{1+d/2} \, (2\pi)^d \, (4d)^d}, \tag{1.16}
\]
\[
\delta_*(\mu, \alpha) := \min \left\{ \frac{\alpha^2}{(12d)^2}, \frac{\alpha}{3\mu \left[ 4M_*(\mu) + 1 \right] d}, \frac{\kappa(\mu)}{2} \right\}, \tag{1.17}
\]
\[
U_*(\mu, \alpha) := \max \left\{ \frac{2\mu}{\delta_*(\mu, \alpha)}, \frac{24d^2}{\alpha \, \delta_*(\mu, \alpha)} \right\}, \tag{1.18}
\]

where \( |S^{d-1}| = 2\pi^{d/2} / \Gamma(d/2) \) is the measure of the unit sphere in \( \mathbb{R}^d \).

**Theorem 1.2.** For any \( 0 < \mu \leq \frac{1}{2} \), Theorem 1.1 holds true with \( L_{\#}(\mu) := L_*(\mu) \) and \( U_{\#}(\mu) := U_*(\mu, \alpha_*(\mu)) \), as defined in (1.14), (1.16), and (1.18).

The explicit form of \( L_*(\mu), \alpha_*(\mu), \) and \( U_*(\mu, \alpha_*(\mu)) \), for a given \( 0 < \mu \leq \frac{1}{2} \), in Theorem 1.2 allows us to estimate the actual minimal size of \( L \) and \( U \) that guarantees saturated ferromagnetism. The distinction between \( \mu \leq 1/2 \) and \( \mu > 1/2 \) is not a fundamental one. It is an artifact of the use in Lemma 3.6 of refs. [24] and [25], whose methods favored this technical distinction.

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2 Proofs of Theorems 1.1 and 1.2

This section contains the proofs of our main results, Theorems 1.1 and 1.2, with the aid of several lemmas which will be proved later in Section 3. Here is a brief outline of the strategy of the proof.

- We first reduce the minimization of $\mathcal{E}_{\mu,U}^{(\text{hfz})}(\gamma_1, \gamma_4)$ in (1.10) over two one-particle density matrices $\gamma_1$ and $\gamma_4$ to the minimization of an effective energy functional $\tilde{\mathcal{E}}_{\mu,U}^{(\text{hfz})}(\gamma)$ which depends only one one-particle density matrix $\gamma$. It is given as a sum of two terms, $\tilde{\mathcal{E}}_{\mu,U}^{(\text{hfz})}(\gamma) = \text{Tr}\{K_\mu\gamma\} + \text{Tr}\{[K_\mu + U\rho]_-\}$, where we recall that $K_\mu = -\Delta - \mu$.

- Given a trial one-particle density matrix $\gamma$ and a small number $\delta > 2\mu U^{-1}$, we introduce the corresponding particle density $\rho(x) := \gamma_{x,x}$ and define the regions $\Omega := \{x | \rho(x) < \delta\}$ and $\Omega^c := \{x | \rho(x) \geq \delta\}$ of low and high density onto which we project by $P_\Omega = \sum_{x \in \Omega} |x\rangle\langle x|$ and $P^c_\Omega = 1 - P_\Omega$, respectively.

- We then use the fact that $\gamma$ is mostly localized in the high density region $\Omega^c$. This leads us to estimate the kinetic energy $\text{Tr}\{-\Delta P_\Omega \gamma P_\Omega\}$ in $\Omega$ by zero and $\text{Tr}\{-\Delta P^c_\Omega \gamma P^c_\Omega\}$ in $\Omega^c$ by the kinetic energy of the free Fermi gas in $\Omega^c$. The localization error is of order of a small constant times the volume $|\partial\Omega|$ of the boundary of $\Omega$. In Lemma 3.1 we give the exact formulation of the bound which we use to estimate the term $\text{Tr}\{K_\mu\gamma\}$ in $\tilde{\mathcal{E}}_{\mu,U}^{(\text{hfz})}(\gamma)$.

- For the analysis of the term $\text{Tr}\{[K_\mu + U\rho]_-\}$ in $\tilde{\mathcal{E}}_{\mu,U}^{(\text{hfz})}(\gamma)$, we use the fact that $\Omega^c$ is a classically forbidden region, because $-\mu + U\rho \geq -\mu + U\delta \geq \mu$ in $\Omega^c$. So, as shown in Lemma 3.2 we can replace $\text{Tr}\{[K_\mu + U\rho]_-\}$ by $\text{Tr}\{P_\Omega(K_\mu + U\rho)P_\Omega_-\}$, up to localization errors of order of a small constant times $|\partial\Omega|$.

- We then pick a (large, but fixed) number $M > 1$ and further split up the low density region $\Omega$ into the subset $\Omega_1$ of those points in $\Omega$ that are at most at distance $2M$ away from the boundary $\partial\Omega$ and the bulk $\Omega_2 \subset \Omega$ of points of distance $2M$ or more to $\partial\Omega$. The contribution of $\Omega_1$ turns out to be negligible because $\Omega_1$ contains at most $(4M + 1)^d|\partial\Omega|$ points, and the density is low in $\Omega_1 \subseteq \Omega$.

- The estimate of the region $\Omega_2 \ni x$ then uses the lower bound on the spatial density $1[K_\mu + U\rho < 0](x,x)$ of the projection onto the negative eigenvalues of $K_\mu + U\rho$ (actually, $\tilde{\rho}$ instead of $\rho$), which we derive in Lemma 3.3.

- Adding up the estimates derived so far, we finally observe that $\tilde{\mathcal{E}}_{\mu,U}^{(\text{hfz})}(\gamma)$ is bounded below by $\text{Tr}\{P_\Omega K_\mu P_\Omega_-\} + \text{Tr}\{P^c_\Omega K_\mu P^c_\Omega_-\} - \eta|\partial\Omega| =: Y - \eta|\partial\Omega|$. 


where \( \eta > 0 \) becomes small when \( U \gg 1 \) and \( \delta > 0 \) is properly chosen. In Lemma 3.6 we reproduce the result from [24, 25] that \( Y \) can be estimated from below by \( \text{Tr} \{ [K_\mu]_- \} + \alpha |\partial \Omega| \), where \( \alpha > 0 \) depends only on \( \mu \). In other words, the introduction of a domain wall at \( \partial \Omega \) drives up the energy by \( \alpha |\partial \Omega| \), which dominates \( \eta |\partial \Omega| \), provided \( \eta \) is small. This establishes that \( \tilde{E}^{(\text{hff})}(\gamma) \geq \text{Tr} \{ [K_\mu]_- \} + (\alpha - \eta)|\partial \Omega| \), which implies the claim.

To carry out the proof in detail, we start with the observation that the minimization over two one-particle density matrices in (1.10) can actually be reduced to the minimization over only one one-particle density matrix. To see this, we observe that

\[
\sum_{x \in \Lambda} \rho_\uparrow(x) \rho_\downarrow(x) = \text{Tr} \{ \rho_\uparrow \gamma_\downarrow \},
\]

(2.1)

where \( \rho_\uparrow \) acts as a multiplication operator, \( (\rho_\uparrow f)(x) := \rho_\uparrow(x) f(x) \). Thus we have

\[
E^{(\text{hff})}_{\mu, U} = \min_{0 \leq \gamma_\uparrow \leq 1} \left[ \text{Tr} \{ K_\mu \gamma_\uparrow \} + \min_{0 \leq \gamma_\downarrow \leq 1} \left( \text{Tr} \{ (K_\mu + U \rho_\uparrow) \gamma_\downarrow \} \right) \right]
\]

(2.2)

\[
= \min_{0 \leq \gamma_\uparrow \leq 1} \left( \text{Tr} \{ K_\mu \gamma_\uparrow \} + \text{Tr} \{ [K_\mu + U \rho_\uparrow]_- \} \right).
\]

(2.3)

(Recall that \( K_\mu = -\Delta - \mu \).) In other words, we have done the minimization over \( \gamma_\downarrow \) in (2.2) by taking \( \gamma_\downarrow \) to be the projection onto the negative eigenspaces of \( K_\mu + U \rho_\uparrow \). Thus, as our minimization principle over only one \( \gamma_\uparrow \), we obtain the following.

\[
E^{(\text{hff})}_{\mu, U} = \min \{ \tilde{E}^{(\text{hff})}_{\mu, U}(\gamma) \mid 0 \leq \gamma \leq 1 \},
\]

(2.4)

\[
\tilde{E}^{(\text{hff})}_{\mu, U}(\gamma) := \text{Tr} \{ K_\mu \gamma \} + \text{Tr} \{ [K_\mu + U \rho]_- \},
\]

(2.5)

where \( \rho(x) := \gamma_{x,x} \). From now on \( \gamma \), with \( 0 \leq \gamma \leq 1 \), is an arbitrary, but fixed one-particle density matrix, for which we bound \( \tilde{E}^{(\text{hff})}_{\mu, U}(\gamma) \) from below. (An upper bound that agrees with Theorem 1.1 is readily obtained simply by choosing the variational function consisting of the unperturbed Fermi sea with all particles spin-up or all spin-down.)

For the next step of the proof we introduce a small number \( \delta > 2\mu U^{-1} \), whose precise value will be chosen in the final step of the proof. Given a one-particle density matrix \( 0 \leq \gamma \leq 1 \) with corresponding density \( \rho(x) := \gamma_{x,x} \), we write the lattice \( \Lambda = \Omega \cup \Omega^c \) as a union of two disjoing subsets of \( \Lambda \) in the following way.

\[
\Omega := \{ x \in \Lambda \mid \rho(x) < \delta \},
\]

(2.6)

\[
\Omega^c := \{ x \in \Lambda \mid \rho(x) \geq \delta \}.
\]

(2.7)
These are the regions of low and high density, respectively. We define the boundary $\partial \Omega$ of $\Omega$ by

$$ \partial \Omega := \{ x \in \Omega \mid \text{dist}_1(x, \Omega^c) = 1 \}, \quad (2.8) $$

where $\text{dist}_1(x, A)$ is the length of (number of bonds in) a shortest path joining $x$ and some point in $y \in A$. Another useful notion of distance which we shall use is $\text{dist}_\infty(x, A)$, which is defined by the condition that $2 \text{dist}_\infty(x, A) + 1$ is the sidelength of the smallest cube centered at $x$ that intersects $A$. When $A$ is a single point $y$ these distances are denoted by $|x - y|_1$ and $|x - y|_\infty$.

We define $P_\Omega$, $P_{\Omega^c} = P_\Omega^\perp$, and $P_{\partial \Omega}$ to be the orthogonal projections onto $\Omega$, $\Omega^c$, and $\partial \Omega$, respectively, where the projection onto an arbitrary set $A \subseteq \Lambda$ is given by

$$ (P_A f)(x) = \begin{cases} f(x) & \text{for } x \in A, \\ 0 & \text{for } x \notin A. \end{cases} \quad (2.9) $$

We further set

$$ \tilde{\rho}(x) := \begin{cases} \rho(x) & \text{for } x \in \Omega^c, \\ \min \left\{ \frac{\mu}{2L}, \rho(x) \right\} & \text{for } x \in \Omega, \end{cases} \quad (2.10) $$

and observe that $\tilde{\rho}(x) \leq \rho(x)$, for all $x \in \Lambda$, which implies that

$$ \tilde{\mathcal{E}}_{\mu, U}^{(h, \mu)}(\gamma) \geq \text{Tr}\{ K_\mu \gamma \} + \text{Tr}\{ [K_\mu + U \tilde{\rho} ]_- \}. \quad (2.11) $$

For brevity, we define $M := M_*(\mu) := 12 \left( \frac{d \mu}{\mu} \right)^2$ and note that, by assumption, $L$ obeys $L \geq 2M$. We further decompose $\Omega$ into two disjoint subsets $\Omega_1$ and $\Omega_2$ defined by

$$ \Omega_1 := \{ x \in \Omega \mid \text{dist}_\infty(x, \Omega^c) \leq 2M \}, \quad (2.12) $$

$$ \Omega_2 := \{ x \in \Omega \mid \text{dist}_\infty(x, \Omega^c) > 2M \}. \quad (2.13) $$

We observe that the $\ell^\infty$-distance of the points in $\Omega_1$ to the boundary $\partial \Omega$ of $\Omega$ is less or equal to $2M$, so $\Omega_1 \subseteq \partial \Omega + Q(2M)$, where $Q(\ell) = \{ -\ell, \ldots, \ell \}^d + LZ^d$. Hence

$$ |\Omega_1| \leq |\partial \Omega| \cdot |Q(2M)| = (4M + 1)^d \cdot |\partial \Omega|, \quad (2.14) $$

and therefore

$$ \sum_{x \in \Omega} \rho(x) = \sum_{x \in \Omega_1} \rho(x) + \sum_{x \in \Omega_2} \rho(x) \leq (4M + 1)^d \delta |\partial \Omega| + \sum_{x \in \Omega_2} \rho(x), \quad (2.15) $$
since $\rho \leq \delta$ on $\Omega$. Eq. (2.15) and Lemma 3.1 yield
\[
\text{Tr}\{K \mu \gamma\} \geq \text{Tr}\{[P^+_{\Omega} K \mu P^+_{\Omega}]_-\} - \left(4d \delta^{1/2} + \mu (4M + 1)d \delta\right) |\partial \Omega| - \mu \sum_{x \in \Omega_2} \rho(x).
\]  

Next, we apply Lemma 3.2 which asserts
\[
\text{Tr}\{[K \mu + U \tilde{\rho}]_-\} \geq \text{Tr}\{[P_{\Omega}(K \mu + U \tilde{\rho})P_{\Omega}]_-\} - \frac{8d^2}{U \delta} |\partial \Omega|.
\]  

Denoting by $\chi := 1_{\{P_{\Omega}(K \mu + U \tilde{\rho})P_{\Omega} < 0\}}$ the orthogonal projection onto the subspace of negative eigenvalues of $P_{\Omega}(K \mu + U \tilde{\rho})P_{\Omega}$ and $\rho_\chi(x) := \chi_{x,x}$ its diagonal matrix element, we observe that
\[
\text{Tr}\{[P_{\Omega}(K \mu + U \tilde{\rho})P_{\Omega}]_-\} = \text{Tr}\{P_{\Omega}(K \mu + U \tilde{\rho}) \chi\} = \text{Tr}\{P_{\Omega} K \mu \chi\} + U \sum_{x \in \Omega} \rho_\chi(x) \tilde{\rho}(x).
\]  

By Lemma 3.3, the density $\rho_\chi$ is bounded below on $\Omega_2$ by the universal constant $\kappa(\mu) > 0$ defined in (3.19). Therefore
\[
\text{Tr}\{[K \mu + U \tilde{\rho}]_-\} \geq \text{Tr}\{[P_{\Omega} K \mu P_{\Omega}]_-\} - \frac{8d^2}{U \delta} |\partial \Omega| + \kappa(\mu) \sum_{x \in \Omega_2} U \tilde{\rho}(x).
\]  

Adding up (2.16) and (2.19), we obtain
\[
\bar{E}^{(hfz)}_{\mu,U}(\gamma) \geq \text{Tr}\{[P_{\Omega} K \mu P_{\Omega}]_-\} + \text{Tr}\{[P^+_{\Omega} K \mu P^+_{\Omega}]_-\} - \left\{4d \delta^{1/2} + \mu (4M + 1)d \delta + \frac{8d^2}{U \delta}\right\} |\partial \Omega| + \sum_{x \in \Omega_2} \left\{\kappa(\mu) U \tilde{\rho}(x) - \mu \rho(x)\right\},
\]  

and Lemma 3.6 further yields
\[
\bar{E}^{(hfz)}_{\mu,U}(\gamma) - \text{Tr}\{[K \mu]_-\} \geq \left\{\alpha(\mu) - 4d \delta^{1/2} - \mu (4M + 1)d \delta - \frac{8d^2}{U \delta}\right\} |\partial \Omega| + \sum_{x \in \Omega_2} \left\{\kappa(\mu) U \tilde{\rho}(x) - \mu \rho(x)\right\}.
\]
We choose
\[ \delta := \delta_*(\mu) = \min \left\{ \frac{\alpha(\mu)^2}{(12d)^2}, \frac{\alpha(\mu)}{3(4M + 1)^2}, \frac{\kappa(\mu)}{2} \right\}, \tag{2.22} \]
and we observe that if
\[ U \geq U_*(\mu, \alpha(\mu)) = \max \left\{ \frac{2\mu}{\delta_*(\mu, \alpha(\mu))}, \frac{24d^2}{\alpha(\mu) \delta_*(\mu, \alpha(\mu))} \right\} \tag{2.23} \]
then our choice for \( \delta \) fulfills the requirement \( \delta > 2\mu U^{-1} \). Moreover, Eqs. (2.22) and (2.23) imply that
\[ 4d^{1/2} + \mu(4M + 1)^d \delta + \frac{8d^2}{U \delta} \leq \frac{\alpha(\mu)}{3} + \frac{\alpha(\mu)}{3} + \frac{\alpha(\mu)}{3} \leq \alpha(\mu). \tag{2.24} \]

We further set \( \Omega'_2 := \{ x \in \Omega_2 | \rho(x) \leq \frac{\mu}{2\delta} \} \) and \( \Omega''_2 := \{ x \in \Omega_2 | \frac{\mu}{2\delta} < \rho(x) \leq \delta \} \), so \( \Omega_2 \) is the disjoint union of \( \Omega'_2 \) and \( \Omega''_2 \), and by the definition (2.10) of \( \bar{\rho} \), we have that
\[ \sum_{x \in \Omega_2} \left\{ \kappa(\mu) U \bar{\rho}(x) - \mu \rho(x) \right\} \tag{2.25} \]
\[ \geq \sum_{x \in \Omega'_2} \left\{ \kappa(\mu) U - \mu \right\} \rho(x) + \sum_{x \in \Omega''_2} \frac{\mu}{2} \left\{ \kappa(\mu) - 2\delta \right\} \geq 0, \]
since \( \delta \leq \frac{1}{2}\kappa(\mu) \) and \( U \geq 2\mu/\delta_*(\mu, \alpha(\mu)) \geq \mu/\kappa(\mu) \). Eqs. (2.24) and (2.25) ensure that the right side of (2.21) is nonnegative, which immediately implies Theorem 1.1.

Theorem 1.2 is obtained by substituting the explicit value of \( \alpha(\mu) \) from (3.60) into (2.23) and using \( L_*(\mu) \) from (3.60). \( \square \)

### 3 Auxiliary Lemmas

In this section we state and prove the lemmas used in the proof of Theorems 1.1 and 1.2 in Section 2.

#### 3.1 The Region \( \Omega^c \) of High Density

In this subsection, we estimate \( \text{Tr} \{ K_{\mu} \gamma \} \) from below. We are guided by the intuition that \( \gamma \) is essentially localized on \( \Omega^c \).
Lemma 3.1.
\[
\text{Tr}\{K_\mu \gamma\} \geq \text{Tr}\{[P^\perp_\Omega K_\mu P^\perp_\Omega]_-\} - 4d \delta^{1/2} |\partial \Omega| - \mu \sum_{x \in \Omega} \rho(x). \tag{3.1}
\]

Proof. Inserting \(\mathbb{I} = P_\Omega + P^\perp_\Omega\) into \(\text{Tr}\{K_\mu \gamma\}\), we obtain
\[
\text{Tr}\{K_\mu \gamma\} = \text{Tr}\{K_\mu P^\perp_\Omega \gamma P^\perp_\Omega\} - 2\text{Re} \text{Tr}\{P^\perp_\Omega \Delta P_\Omega \gamma\} + \text{Tr}\{K_\mu P_\Omega \gamma P_\Omega\} \\
\geq \text{Tr}\{[P^\perp_\Omega K_\mu P^\perp_\Omega]_-\} - 2 \sum_{x \in \Omega, y \in \Omega^c} \Delta_{x,y} |\gamma_{y,x}| - \mu \text{Tr}\{P_\Omega \gamma P_\Omega\} \\
= \text{Tr}\{[P^\perp_\Omega K_\mu P^\perp_\Omega]_-\} - 2 \sum_{x \in \partial \Omega, y \in \Omega^c} \Delta_{x,y} |\gamma_{y,x}| - \mu \sum_{x \in \Omega} \rho(x), \tag{3.2}
\]
where we use that \(-\Delta \geq 0\), that \(P^\perp_\Omega \Delta P_\Omega = P^\perp_\Omega \Delta P^\perp_\Omega\), and that \(0 \leq \gamma \leq 1\). The latter also implies that \(\rho(y) = \gamma_{y,y} \leq 1\), for all \(y \in \Lambda\). Thus, if \(x \in \partial \Omega\) and \(y \in \Omega^c\), the Cauchy-Schwarz inequality yields \(|\gamma_{y,x}| \leq \sqrt{\gamma_{y,y} \gamma_{x,x}} \leq \delta^{1/2}\). Moreover, if \(x \in \partial \Omega\), \(y \in \Omega^c\), and \(\Delta_{x,y} \neq 0\), then \(y\) is a neighbor of \(x\), and we obtain
\[
\sum_{x \in \partial \Omega, y \in \Omega^c} \Delta_{x,y} |\gamma_{y,x}| \leq \delta^{1/2} \sum_{x \in \partial \Omega} \sum_{y \in \Lambda: |x-y|=1} = 2d \delta^{1/2} |\partial \Omega|, \tag{3.3}
\]
which completes the proof of (3.1).

3.2 Decoupling the High and Low Density Regions

This subsection is devoted to showing that \(\text{Tr}\{[K_\mu + U \tilde{\rho}]_-\}\) essentially agrees with the corresponding eigenvalue sum \(\text{Tr}\{[P_\Omega(K_\mu + U \tilde{\rho})P_\Omega]_-\}\) for the operator localized on \(\Omega\), the reason being that \(\Omega^c\) is a classically forbidden region since \(-\mu + U \tilde{\rho} \geq \frac{1}{2} U \delta > 0\) on \(\Omega^c\).

Lemma 3.2.
\[
\text{Tr}\{[K_\mu + U \tilde{\rho}]_-\} \geq \text{Tr}\{[P_\Omega(K_\mu + U \tilde{\rho})P_\Omega]_-\} - \frac{8d^2}{U \delta} |\partial \Omega|. \tag{3.4}
\]

Proof. We wish to apply of the Feshbach projection method. To this end, we first observe the following quadratic form bound,
\[
P^\perp_\Omega (K_\mu + U \tilde{\rho}) P^\perp_\Omega \geq P^\perp_\Omega (U \tilde{\rho} - \bar{\mu}) P^\perp_\Omega \geq \frac{1}{2} U \delta P^\perp_\Omega, \tag{3.5}
\]
for any $\bar{\mu} \in [0, \mu]$, since $\bar{\rho} \geq \delta$ on $\Omega^c$ and $\delta \geq 2\mu U^{-1}$. Thus, $P_\Omega^\perp(K_{\bar{\mu}} + U\bar{\rho})P_\Omega^\perp$ is positive and invertible on $\text{Ran} \ P_\Omega^\perp$, and moreover, we have that

$$ P_\Omega \Delta P_\Omega^\perp [P_\Omega^\perp(K_{\bar{\mu}} + U\bar{\rho})P_\Omega^\perp]^{-1} P_\Omega^\perp \Delta P_\Omega \leq \frac{2}{U \delta} P_{\partial \Omega} \Delta P_\Omega^\perp \Delta P_{\partial \Omega}. \quad (3.6) $$

For $y \in \Omega^c$ and $f \in \mathbb{C}^\Lambda$, the Cauchy-Schwarz inequality implies that

$$ \langle f | P_{\partial \Omega} \Delta \mathbb{I}_y \Delta P_{\partial \Omega} f \rangle = |(\Delta P_{\partial \Omega} f)[y]|^2 = \left| \sum_{x \in \partial \Omega, |x-y|=1} f(x) \right|^2 \quad (3.7) $$

$$ \leq \left( \sum_{x \in \partial \Omega, |x-y|=1} |f(x)|^2 \right) \left( \sum_{x \in \Lambda, |x-y|=1} 1 \right) = 2d \sum_{x \in \partial \Omega, |x-y|=1} |f(x)|^2, $$

which, by summing over all $y \in \Omega^c$, yields

$$ \langle f | P_{\partial \Omega} \Delta P_\Omega^\perp \Delta P_{\partial \Omega} f \rangle = \sum_{y \in \Omega^c} \langle f | P_{\partial \Omega} \Delta \mathbb{I}_y \Delta P_{\partial \Omega} f \rangle \quad (3.8) $$

$$ \leq 2d \sum_{x \in \partial \Omega} \left\{ |f(x)|^2 \cdot \left( \sum_{y \in \Lambda, |x-y|=1} 1 \right) \right\} \leq 4d^2 \sum_{x \in \partial \Omega} |f(x)|^2 = 4d^2 \langle f | P_{\partial \Omega} f \rangle. $$

(We thank D. Ueltschi for pointing out (3.7)-(3.8) to us.) We conclude that

$$ P_\Omega \Delta P_\Omega^\perp [P_\Omega^\perp(K_{\bar{\mu}} + U\bar{\rho})P_\Omega^\perp]^{-1} P_\Omega^\perp \Delta P_\Omega \leq \frac{8d^2}{U \delta} P_{\partial \Omega}. \quad (3.9) $$

The invertibility of $P_\Omega^\perp(K_{\bar{\mu}} + U\bar{\rho} + e)P_\Omega^\perp$ on $\text{Ran} \ P_\Omega^\perp$ implies the applicability of the Feshbach map, for any $e \in [0, \mu]$. I.e., for any $e \in [0, \mu]$,

$$ F(e) := F_{\Omega}(K_{\bar{\mu}} + e + U\bar{\rho}) - e P_\Omega \quad (3.10) $$

$$ = P_\Omega(K_{\bar{\mu}} + U\bar{\rho})P_\Omega - P_\Omega \Delta P_\Omega^\perp [P_\Omega^\perp(K_{\bar{\mu}} + e + U\bar{\rho})P_\Omega^\perp]^{-1} P_\Omega^\perp \Delta P_\Omega $$

is a well-defined matrix on $\text{Ran} \ P_\Omega$, and the isospectrality of the Feshbach map guarantees that $-e \in [-\mu, 0)$ is a negative eigenvalue of $K_{\bar{\mu}} + U\bar{\rho}$ of multiplicity $m(e)$ if and only if $-e$ is an (nonlinear) eigenvalue of $F(e)$, i.e., if the kernel of $F(e) + e$, as a subspace of $\text{Ran} \ P_\Omega$, has dimension $m(e)$. Note that $F$ is monotonically increasing, as a quadratic form, in $e > 0$. In particular,

$$ F(e) \geq F(0) \geq P_\Omega(K_{\bar{\mu}} + U\bar{\rho})P_\Omega - \frac{8d^2}{U \delta} P_{\partial \Omega}, \quad (3.11) $$
additionally taking (3.9) into account.

We claim that, for all \( \lambda \in (0, \infty) \), the number of eigenvalues of \( K_\mu + U\tilde{\rho} \) below \(-\lambda\) is smaller than the number of negative eigenvalues of \( F(\lambda) + \lambda \),

\[
\text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda] \} \leq \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda) + \lambda < 0] \},
\]

where \( \text{Tr}_{\Omega} \) denotes the trace on \( \text{Ran} \, P_\Omega \). Both sides of Eq. (3.12) are zero and thus fulfill the claimed inequality, for \( \lambda \geq \mu \). Assume that (3.12) is violated, for some \( \lambda \in (0, \infty) \), i.e., that \( \lambda_* := \inf\{ \lambda \in (0, \infty) | \text{Eq. (3.12) holds true} \} > 0 \). We show that this assumption leads to a contradiction. Obviously, \(-\lambda_*\) must be an eigenvalue of \( K_\mu + U\tilde{\rho} \), and hence also of \( F(\lambda_*) \), of multiplicity \( m(\lambda_*) \geq 1 \), because only then the left or the right side of (3.12) changes (increases, in fact). Moreover, Eq. (3.12) holds true for \( \lambda = \lambda_* \), itself, i.e., the infimum in the definition of \( \lambda_* \) is a minimum. Hence, for all sufficiently small \( \varepsilon > 0 \), the definition of \( \lambda_* \) and the monotony of \( F(\varepsilon) \) in \( \varepsilon \) yield

\[
\begin{align*}
\text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda_*] \} & \leq \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda_*) + \lambda_* < 0] \} \\
\text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda_* + \varepsilon] \} & > \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda_*) - \varepsilon + \lambda_* - \varepsilon < 0] \} \\
& \geq \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda_*) + \lambda_* - \varepsilon < 0] \}.
\end{align*}
\]

Choosing \( \varepsilon > 0 \) so small that \(-\lambda_*\) is the only eigenvalue of \( K_\mu + U\tilde{\rho} \) in the interval \([-\lambda_*, -\lambda_* + \varepsilon] \), we hence obtain

\[
m(\lambda_*) = \text{Tr}\{ \mathbbm{1}[0 \leq K_\mu + U\tilde{\rho} + \lambda_* < \varepsilon] \} \\
= \text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda_* + \varepsilon] \} - \text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda_*] \} \\
> \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda_*) + \lambda_* < \varepsilon] \} - \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda_*) + \lambda_* < 0] \} \\
= \text{Tr}_{\Omega}\{ \mathbbm{1}[0 \leq F(\lambda_*) + \lambda_* < \varepsilon] \} = m(\lambda_*),
\]

arriving at a contradiction, which proves (3.12), for all \( \lambda \in (0, \infty) \). From (3.12) and (3.11), we finally conclude

\[
\begin{align*}
\text{Tr}\{[K_\mu + U\tilde{\rho}]_-\} & = -\int_0^\infty \text{Tr}\{ \mathbbm{1}[K_\mu + U\tilde{\rho} < -\lambda] \} \, d\lambda \\
& \geq -\int_0^\infty \text{Tr}_{\Omega}\{ \mathbbm{1}[F(\lambda) + \lambda < 0] \} \, d\lambda \\
& \geq -\int_0^\infty \text{Tr}_{\Omega}\{ \mathbbm{1}[F(0) + \lambda < 0] \} \\
& = \text{Tr}\{[F(0)]_-\} = \text{Tr}_{\Omega}\{[F(0)]_-\} \\
& \geq \text{Tr}\{[P_{\Omega}(K_\mu + U\tilde{\rho})P_{\Omega}]_-\} - \frac{8d^2}{U\delta} \text{Tr}\{P_{\Omega}\}.
\end{align*}
\]
which is the assertion of Lemma 3.2.

QED

3.3 The Electron Density in the Bulk

In this subsection we consider the spectral projection

\[ \chi := \mathbb{1} \left[ P_\Omega (K_\mu + U\tilde{\rho}) P_\Omega < 0 \right] = \mathbb{1} \left[ P_\Omega (-\Delta - \mu + U\tilde{\rho}) P_\Omega < 0 \right] \quad (3.17) \]

of \( P_\Omega (-\Delta - \mu + U\tilde{\rho}) P_\Omega \) onto its negative eigenvalues. Writing \( \Delta_\Omega := P_\Omega \Delta P_\Omega \), i.e., \( (\Delta_\Omega)_{x,y} = \Delta_{x,y} \) for \( x, y \in \Omega \), and = 0, otherwise, and \( V \equiv \sum_{x \in \Omega} V(x) \cdot \mathbb{1}_x \),

\[ \chi = \mathbb{1} \left[ -\Delta_\Omega - V < 0 \right] \quad \text{and} \quad \forall x \in \Omega : \frac{1}{2 \mu} \leq V(x) \leq \mu \]  

(3.18)
due to the definition (2.9) of \( \tilde{\rho} \). Naive semiclassical intuition tells us that, for \( x \in \Omega \), the particle density \( \rho_{\chi}(x) := \chi_{x,x} \) corresponding to the one-particle density matrix \( \chi \) should be bounded below by the particle density of the Fermi gas given by the one-particle density matrix \( \mathbb{1} \left[ -\Delta < \mu/2 \right] \). The purpose of this subsection is to prove such a bound (up to a constant factor) where it can be expected to hold, namely, for those points \( x \) that are sufficiently far away from the boundary of \( \Omega \).

Lemma 3.3. Let \( 0 < \mu \leq 4d \), define \( M := M_* := 12 \left( \frac{4d}{\mu} \right)^2 \). Suppose that \( L \) obeys \( L \geq 2M \) and that \( x \in \Omega \), with \( \text{dist}_\infty (x, \partial \Omega) > 2M \). Then

\[ \rho_{\chi}(x) \geq \kappa(\mu) := \frac{\mu^d}{4^{2d+1} d! e^d} \left[ 1 + 2 \ln(2) \left( d^{-1} + 1 \right) + \ln \left( 4d \mu^{-1} \right) \right]^{-2d}. \quad (3.19) \]

Proof. For any \( \beta > 0 \), we note that the map \( \mathbb{R}^\Omega \to \mathbb{R}, W \mapsto (e^{-\beta(-\Delta_\Omega - W)})_{x,x} \) is monotonically increasing in \( W \). Namely, as \( T_{\Omega} = P_\Omega TP_\Omega \) has nonnegative matrix elements, so does \( e^{\beta \Delta_\Omega} \),

\[ (e^{\beta \Delta_\Omega})_{w,z} = e^{-2de} (e^{\beta T_{\Omega}})_{w,z} = e^{-2de} \sum_{k=0}^{\infty} \frac{e^k}{k!} (T_{\Omega}^k)_{w,z} \geq 0, \quad (3.20) \]

for all \( w, z \in \Omega \). So, if \( n \) is an integer and \( W, \tilde{W} \in \mathbb{R}^\Omega \) with \( W(z) \leq \tilde{W}(z) \), for
all \( z \in \Omega \), then we have that

\[
\left( \left[ e^{\beta \Delta_\Omega/n} e^{\beta W/n} \right]^n \right)_{z_0, z_n} = \sum_{z_1, \ldots, z_{n-1} \in \Omega} \left\{ \prod_{j=1}^n \left( e^{\beta \Delta_\Omega/z_j} e^{\beta W(z_j)/n} \right) \right\}
\]

\[
\leq \sum_{z_1, \ldots, z_{n-1} \in \Omega} \left\{ \prod_{j=1}^n \left( e^{\beta \Delta_\Omega/z_j} e^{\beta \tilde{W}(z_j)/n} \right) \right\}
\]

\[
= \left( \left[ e^{\beta \Delta_\Omega/n} e^{\beta \tilde{W}/n} \right]^n \right)_{z_0, z_n},
\]

(3.21)

for all \( z_0, z_n \in \Omega \). Setting \( z_0 := z_n := x \in \Omega \) and taking the limit \( n \to \infty \), the Lie-Trotter product formula and Eq. (3.21) imply that

\[
\left( e^{-\beta (\Delta_\Omega + W)} \right)_{x,x} \leq \left( e^{-\beta (\tilde{\Delta}_\Omega + \tilde{W})} \right)_{x,x},
\]

(3.22)

indeed. In particular,

\[
e^{\beta \mu} \left( e^{\beta \Delta_\Omega} \right)_{x,x} \leq \left( e^{-\beta (\Delta_\Omega + V)} \right)_{x,x},
\]

(3.23)

since \( V \geq \frac{1}{2} \mu \) on \( \Omega \). On the other hand, \( -\Delta_\Omega - V \geq -\mu \) and \( \chi^\perp (-\Delta_\Omega - V) \chi^\perp \geq 0 \), as quadratic forms. The spectral theorem thus implies that

\[
\chi e^{-\beta (\Delta_\Omega + V)} \chi \leq \chi e^{\beta \mu} \chi = e^{\beta \mu} \chi,
\]

(3.24)

\[
\chi^\perp e^{-\beta (\Delta_\Omega + V)} \chi^\perp \leq \chi^\perp \leq P_\Omega.
\]

(3.25)

Putting together (3.23), (3.24), and (3.25), using that \( \chi \) and \( -\Delta_\Omega - V \) commute, we arrive at

\[
e^{\beta \mu} \left( e^{\beta \Delta_\Omega} \right)_{x,x} \leq \left( e^{-\beta (\Delta_\Omega + V)} \right)_{x,x}
\]

\[
= \left( \chi e^{-\beta (\Delta_\Omega + V)} \chi \right)_{x,x} + \left( \chi^\perp e^{-\beta (\Delta_\Omega + V)} \chi^\perp \right)_{x,x}
\]

\[
\leq e^{\beta \mu} \chi_{x,x} + 1.
\]

(3.26)

Solving for \( \rho^\chi(x) = \chi_{x,x} \), we therefore have

\[
\rho^\chi(x) \geq e^{-\beta \mu/2} \left[ (e^{\beta \Delta_\Omega})_{x,x} - e^{-\beta \mu/2} \right],
\]

(3.27)

for any \( x \in \Omega \) and any \( \beta > 0 \).

Next, recall that \( Q(M) = \{-M, \ldots, M\}^d + L \mathbb{Z}^d = \{ y \in \Lambda : |y|_\infty \leq M \} \) is the box of sidelength \( 2M + 1 \) centered at \( 0 \in \Lambda \). Since \( \text{dist}_\infty (x, \partial \Omega) > 2M \), by assumption, we have that

\[
Q(M) - z + x \subseteq \Omega,
\]

(3.28)
for all \( z \in Q(M) \). By Lemma 3.4, this inclusion implies that
\[
(\exp[\beta \Delta \Omega])_{x,x} \geq (\exp[\beta \Delta Q(M)_{-z+x}])_{x,x} = (\exp[\beta \Delta Q(M)])_{z,z},
\]
and by averaging this inequality over \( z \in Q(M) \), we obtain
\[
(\exp[\beta \Delta \Omega])_{x,x} \geq \frac{1}{|Q(M)|} \sum_{z \in Q(M)} (\exp[\beta \Delta Q(M)])_{z,z}.
\]
Now, we apply Lemma 3.5 and arrive at
\[
\frac{1}{|Q(M)|} \sum_{z \in Q(M)} (\exp[\beta \Delta Q(M)])_{z,z} \geq \frac{e^{-d\beta/M}}{(2\pi)^d} \int_{[-\pi,\pi]^d} \exp[-\beta \omega(k)] d^d k
\]
\[
= \left( \frac{2 e^{-\beta/M}}{\pi} \int_0^{\pi/2} \exp[-4 \beta \sin^2(t)] dt \right)^d,
\]
where \( \omega(k) = \omega(-k) = \sum_{\nu=1}^d \{1 - \cos(k_\nu)\} = \sum_{\nu=1}^d 4 \sin^2(k_\nu/2) \). Choosing \( \beta \geq 1 \), we observe that
\[
\frac{1}{\pi} \int_0^{\pi/2} e^{-t^2} dt \geq \frac{1}{\pi} \int_0^{\pi} e^{-t^2} dt = \frac{1}{2\sqrt{\pi}} \text{erf}[\pi] \geq \frac{1}{4}.
\]
Using this and \( \sin^2(t) \leq t^2 \), we have the following estimate,
\[
\frac{2 e^{-\beta/M}}{\pi} \int_0^{\pi/2} \exp[-4 \beta \sin^2(t)] dt \geq \frac{e^{-\beta/M}}{\beta^{1/2}} \cdot \frac{1}{\pi} \int_0^{\pi} e^{-t^2} dt \geq \frac{e^{-\beta/M}}{4 \beta^{1/2}}.
\]
Inserting this estimate into (3.31) and then the result in (3.30) and (3.27), we obtain, for any \( \beta \geq 1 \), that
\[
\rho_\chi(x) \geq e^{-\beta \mu/2} \left[ \frac{e^{-d\beta/M}}{4d \beta^{1/2}} - e^{-\beta \mu/2} \right] = e^{-\tau d} \left[ \left( e^{1-2d \tau/(M \mu)} \right)^{d/2} \left( \frac{\mu}{16\pi d} \frac{e^{\tau}}{\tau} \right)^{d/2} - 1 \right],
\]
where \( \tau := \beta \mu/d \). Note that if we require \( \tau \geq 4 \) then \( \beta = \tau d/\mu \geq 1 \), since \( \mu \leq 4d \). We may thus replace \( \beta \in [1, \infty) \) by \( \tau \in [4, \infty) \). Our goal is to choose \( \tau \) such that
\[
\left( \frac{\mu}{16\pi d} \frac{e^{\tau}}{\tau} \right)^{d/2} \geq 2 \iff \tau - \ln(\tau) \geq Y := 1 + 2 \ln(2) \left( \frac{1}{d} + 1 \right) + \ln \left( \frac{4d}{\mu} \right).
\]
Note that, due to \( \mu \leq 4d \),
\[
2.38 \leq 1 + 2 \ln(2) \leq Y \leq 3 \ln \left( 16 d \mu^{-1} \right).
\]
We choose \( \tau := Y + 2 \ln(Y) \) and observe that \( Y \geq 2.38 \) insures \( \tau \geq 4.11 \geq 4 \), as required. Moreover, with this choice, we have

\[
\tau - \ln(\tau) - Y = 2 \ln(Y) - \ln \left[ Y + 2 \ln(Y) \right] \\
\geq \ln(Y) - \ln \left[ 1 + 2 \ln(Y) Y^{-1} \right] \\
\geq \ln(Y) - 2 \ln(Y) Y^{-1} = 2 \ln(Y) \left( \frac{1}{2} - \frac{1}{Y} \right) > 0 ,
\]

using that \( \ln(1 + \varepsilon) \leq \varepsilon, \) for \( \varepsilon \geq 0 \), and \( Y \geq 2.38 > 2 \). Thus, (3.35) and (3.34) hold true. Additionally, we observe that \( Y \leq 3 \ln \left( \frac{16}{d} \mu \right) \) and

\[
\tau \leq Y \cdot \max_{r > 0} \left\{ 1 + 2 \left( \frac{\ln r}{r} \right) \right\} = (1 + 2/e)Y \leq 2Y
\]

insures that \( \frac{2d\tau}{\mu} \leq \frac{12d}{\mu} \ln \left( \frac{16}{d} \mu \right) \leq 12 \left( \frac{4d}{\mu} \right)^{2} \leq M_{s} \leq M \). This, in turn, yields

\[
\exp \left[ 1 - \frac{2d\tau}{M \mu} \right] \geq 1 ,
\]

and by inserting (3.39) and (3.34) into (3.33), we arrive at

\[
\rho(x) \geq e^{-\tau d} = \frac{\mu d}{4^{2d+1}e^{d}d^{d}} \left[ 1 + 2 \ln(2) \left( d^{-1} + 1 \right) + \ln \left( 4d\mu^{-1} \right) \right]^{-2d} .
\]

QED

**Lemma 3.4.** Let \( A, B \subseteq \Lambda \), with \( A \subseteq B \), and denote \( \Delta_{A} := P_{A} \Delta P_{A} \) and \( \Delta_{B} := P_{B} \Delta P_{B} \). For all \( x \in A \) and all \( \beta > 0 \),

\[
\left( \exp[\beta \Delta_{A}] \right)_{x,x} \leq \left( \exp[\beta \Delta_{B}] \right)_{x,x} .
\]

**Proof.** We first define the nearest-neighbor hopping matrix \( T \) on \( \Lambda \) by \( T_{w,z} := 1 \) if \( |w - z|=1 \) and \( T_{w,z} := 0 \), otherwise. For a given subset \( C \subseteq \Lambda \), the matrix \( T_{C} := P_{C} T P_{C} \) denotes the hopping matrix restricted to \( C \). Note that \( \Delta_{C} = T_{C} - 2dP_{C} \) is the difference of the two commuting matrices \( T_{C} \) and \( 2dP_{C} \). Hence, for \( x \in C \),

\[
\left( \exp[\beta \Delta_{C}] \right)_{x,x} = \left( \exp[\beta T_{C}] \exp[-2d\beta P_{C}] \right)_{x,x} = e^{-2d\beta} \left( \exp[\beta T_{C}] \right)_{x,x} .
\]

Due to this identity and the fact that \( x \in A \subseteq B \), Eq. (3.41) is equivalent to

\[
\left( \exp[\beta T_{A}] \right)_{x,x} \leq \left( \exp[\beta T_{B}] \right)_{x,x} .
\]
Now, \( 0 \leq (T_A)_{w,z} \leq (T_B)_{w,z} \), and hence \((T^*_n)_{x,x} \leq (T^*_n)_{x,x} \), for all integers \( n \). Thus, (3.43) follows from an expansion of the exponentials in Taylor series,

\[
\left( \exp[\beta T_A] \right)_{x,x} = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (T^n_A)_{x,x} \leq \sum_{n=0}^{\infty} \frac{\beta^n}{n!} (T^n_B)_{x,x} = \left( \exp[\beta T_B] \right)_{x,x}.
\]

(3.44)

\[\text{QED}\]

**Lemma 3.5.** Let \( Q = \{-m, \ldots, m\}^d \subset \mathbb{Z}^d \) be a cube. Denote by \( \Delta_Q \) the nearest-neighbor Laplacian on \( Q \), i.e., \( \Delta_Q = P_Q \Delta P_Q = -2dP_Q + T_Q, T_Q := P_Q T P_Q \), and \( T_{x,y} = \mathbb{1}(|x - y|_1 = 1) \). Then, for all \( \beta > 0 \),

\[
\frac{1}{|Q|} \sum_{z \in Q} \left( \exp[\beta \Delta_Q] \right)_{z,z} \geq e^{-d\beta/m} \int_{[-\pi,\pi]^d} \exp[-\beta \omega(k)] d^d k,
\]

(3.45)

where \( \omega(k) := \sum_{\nu=1}^{d} 2\{1 - \cos(k_\nu)\} \).

**Proof.** We may pick an even integer \( r \), choose \( L := r \cdot (2m + 1) \), and identify \( Q + L \mathbb{Z}^d \subset \Lambda \). (Note that the statement of the lemma makes no reference to the Hubbard model analyzed before, and for the purpose of the proof, \( L \) can be taken an arbitrarily large integer multiple of \( 2m + 1 \).) Given \( s \in \mathbb{Z}^d_r \), we define \( Q(s) := Q + (2m+1) s \) and observe that the family \( \{Q(s)\}_{s \in \mathbb{Z}^d_r} \) of cubes define a disjoint partition of \( \Lambda \), i.e.,

\[
\Lambda = \bigcup_{s \in \mathbb{Z}^d_r} Q(s) \quad \text{and} \quad \forall s \neq s' : Q(s) \cap Q(s') = \emptyset.
\]

(3.46)

Hence

\[
\hat{\Delta} := \sum_{s \in \mathbb{Z}^d_r} \Delta_Q(s)
\]

(3.47)

is the sum of translated, but mutually disconnected copies of \( \Delta_Q \). We observe that

\[
\text{Tr}\{ \exp[\beta \hat{\Delta}] \} = \sum_{x \in \Lambda} \left( \exp[\beta \hat{\Delta}] \right)_{x,x} = \sum_{s \in \mathbb{Z}^d_r} \sum_{z \in Q} \left( \exp[\beta \hat{\Delta}] \right)_{z+(2m+1)s,z+(2m+1)s} = r^d \sum_{z \in Q} \left( \exp[\beta \Delta_Q] \right)_{z,z}.
\]

(3.48)
As an intermediate result, we thus have
\[
\frac{1}{|Q|} \sum_{z \in Q} \left( \exp[\beta \Delta_Q] \right)_{z,z} = \frac{1}{|\Lambda|} \Tr \left\{ \exp[\beta \hat{\Delta}] \right\},
\]
(3.49)
since $|\Lambda| = L^d = r^d |Q|$.

Next, we translate $\hat{\Delta}$ by the elements of $Q$, i.e., for $\eta \in Q$, we introduce $\hat{\Delta}^{(\eta)}$ on $\mathbb{C}^{\Lambda}$ by
\[
\hat{\Delta}^{(\eta)} := \sum_{q \in \mathbb{Z}^d} \Delta_{Q(q)+\eta} = \sum_{q \in \mathbb{Z}^d} \Delta_{Q+\eta+(2m+1)q}.
\]
(3.50)
Of course, $\hat{\Delta}^{(\eta)}$ is unitarily equivalent to $\hat{\Delta}$. We observe that
\[
\frac{1}{|Q|} \sum_{\eta \in Q} \hat{\Delta}^{(\eta)} = \frac{1}{|Q|} \sum_{y \in \Lambda} \Delta_{Q+y} = -2d \cdot \mathbb{1}_{\mathbb{C}^{\Lambda}} + \frac{1}{|Q|} \sum_{y \in \Lambda} T_{Q+y},
\]
(3.51)
where, for $w, z \in \Lambda$,
\[
\left( \sum_{y \in \Lambda} T_{Q+y} \right)_{w,z} = \sum_{y \in \Lambda} \mathbb{1}_{Q}(w-y) \mathbb{1}_{Q}(z-y) T_{w,z}
\]
\[
= \left( (Q+w) \cap (Q+z) \right) \cdot T_{w,z} = 2m(2m+1)^{d-1} T_{w,z},
\]
(3.52)
since $T_{w,z} \neq 0$ only if $w - z$ are neighboring lattice sites. Hence,
\[
\frac{1}{|Q|} \sum_{\eta \in Q} \hat{\Delta}^{(\eta)} = -2d \cdot \mathbb{1}_{\mathbb{C}^{\Lambda}} + \frac{2m}{2m+1} T = -\frac{2d}{2m+1} \cdot \mathbb{1}_{\mathbb{C}^{\Lambda}} + \frac{2m}{2m+1} \Delta
\]
\[
\geq -\frac{d}{m} \cdot \mathbb{1}_{\mathbb{C}^{\Lambda}} + \Delta
\]
(3.53)
where $\Delta \leq 0$ is the nearest-neighbor Laplacian on $\Lambda$ (with periodic b.c.). This and the convexity of $A \mapsto \Tr \{ \exp[A] \}$ therefore imply that
\[
\Tr \{ \exp[\beta \hat{\Delta}] \} = \frac{1}{|Q|} \sum_{\eta \in Q} \Tr \{ \exp[\beta \hat{\Delta}^{(\eta)}] \} \geq \Tr \left\{ \exp \left[ \frac{\beta}{|Q|} \sum_{\eta \in Q} \hat{\Delta}^{(\eta)} \right] \right\}
\]
\[
\geq e^{-\beta d/m} \Tr \{ \exp[\beta \Delta] \}.
\]
(3.54)
We diagonalize $\Delta$ by discrete Fourier transformation on $\mathbb{C}^{\Lambda}$. The eigenvalues of $-\Delta$ are given by $\omega(k)$, where $k \in \Lambda^* = \frac{2\pi}{L} \mathbb{Z}^d_L$ is the variable dual to $x \in \Lambda$. Since $|\Lambda^*| = L^d = |Q| r^d$, we therefore have
\[
\frac{1}{|Q|} \sum_{z \in Q} \exp[\beta \Delta_Q]_{z,z} = \frac{1}{|\Lambda|} \Tr \{ \exp[\beta \hat{\Delta}] \} \geq \frac{e^{-\beta d/m}}{|\Lambda^*|} \sum_{k \in \Lambda^*} e^{-\beta \omega(k)}.
\]
(3.55)
Inequality (3.55) holds for every \( L = r(2m + 1) \), and hence also in the limit \( L \to \infty \). Since the right side of (3.50) is a Riemann sum approximation to the integral in (3.45), this limit yields the asserted estimate (3.45). QED

3.4 The Discrete Laplacians on \( \Omega \), \( \Omega^c \), and their Eigenvalue Sums

In this final subsection, we compare the sum of the eigenvalues of

\[
-\tilde{\Delta} := P_\Omega (-\Delta) P_\Omega + P_{\Omega^c}^\perp (-\Delta) P_{\Omega^c}^\perp
\]

(3.56)

below \( \mu \) to the sum of the eigenvalues of

\[-\Delta \]

below \( \mu \), where \( \Omega \subseteq \Lambda \) is an arbitrary, but henceforth fixed, subset of \( \Lambda \), and \( \Omega^c := \Lambda \setminus \Omega \) is its complement. To this end, we introduce the difference of these eigenvalue sums,

\[
\delta E(\mu, \Omega) := \text{Tr}\{[-\tilde{\Delta} - \mu]_-\} - \text{Tr}\{[\Delta - \mu]_-\}
\]

(3.57)

where \( \tilde{P}_- := \mathbb{1}[-\tilde{\Delta} \leq \mu] \) and \( P_- := \mathbb{1}[-\Delta \leq \mu] \). We further set \( \tilde{P}_+ := \tilde{P}_\perp \) and \( P_+ := P_\perp \). Since \( \tilde{P}_- \) commutes with \( P_\Omega \), we have that

\[
\text{Tr}\{(-\tilde{\Delta} - \mu) \tilde{P}_-\} = \text{Tr}\{(-\Delta - \mu) P_-\},
\]

and thus

\[
\delta E(\mu, \Omega) = \text{Tr}\{(-\Delta - \mu) (\tilde{P}_- - P_-)\}
\]

(3.58)

is manifestly nonnegative. The derivation of a nontrivial lower bound on \( \delta E(\mu, \Omega) \) of the form \( \delta E(\mu, \Omega) \geq \alpha(\mu) |\partial \Omega| \), where \( \alpha(\mu) > 0 \) is a positive constant which depends only on \( \mu \) and the spatial dimension \( d \geq 1 \) (but not on \( \Omega \)), is a task that was first addressed by Freericks, Lieb, and Ueltschi in [24]. Shortly thereafter, Goldbaum [25] improved the numerical value for \( \alpha(\mu) > 0 \), especially if \( \mu \) is close to \( 2d \). As a consequence of the estimates in [24, 25], we have the following lemma.

Lemma 3.6 (Freericks, Lieb, and Ueltschi (2002), Goldbaum (2003)).

(i) Let \( \frac{1}{2} < \mu < 4d \). There is \( L_*(\mu) < \infty \) and \( \alpha(\mu) > 0 \) such that, for all \( L \geq L_*(\mu) \) and all subsets \( \Omega \subseteq \Lambda \),

\[
\delta E(\mu, \Omega) \geq \alpha(\mu) |\partial \Omega|.
\]

(3.59)
(ii) Let $0 < \mu \leq \frac{1}{2}$, and define

$$\alpha(\mu) := \frac{|S^{d-1}| \mu^{(2+d)/2}}{2^{1+d/2} (2\pi)^d (4d)^5} \quad \text{and} \quad L_*(\mu) := \frac{4\pi d}{\mu}. \quad (3.60)$$

where $|S^{d-1}|$ is the surface volume of the $d$-dimensional sphere. Then, for all $L \geq L_*(\mu)$ and all subsets $\Omega \subseteq \Lambda = \mathbb{Z}_L^d$, we have

$$\delta E(\mu, \Omega) \geq \alpha(\mu) |\partial \Omega|. \quad (3.61)$$

Proof. We only give the proof of (ii), which amounts to reproducing the proof of Lemma 3.1 in [23]. By $\{\psi_k\}_{k \in \Lambda^*} \subseteq \mathcal{C}^{\Lambda}$ we denote the orthonormal basis (ONB) of eigenvectors of $\Delta$, i.e.,

$$\psi_k(x) := |\Lambda|^{-1/2} e^{-i k \cdot x}, \quad k \in \Lambda^* = \frac{2\pi}{L} \mathbb{Z}_L^d, \quad (3.62)$$

and we have that $-\Delta \psi_k = \omega(k) \psi_k$, with $\omega(k) = \sum_{\nu=1}^{d} 2 \{1 - \cos(k_{\nu})\}$. Evaluating the traces in Eq. (3.58) by means of this ONB, we obtain

$$\delta E(\mu, \Omega) = \sum_{k \in \Lambda^*} \left\{ \left[ \mu - \omega(k) \right]_+ \langle \psi_k | \tilde{P}_+ \psi_k \rangle + \left[ \omega(k) - \mu \right]_+ \langle \psi_k | \tilde{P}_- \psi_k \rangle \right\}. \quad (3.63)$$

Let $\{\varphi_j\}_{j=1}^{|\Lambda|} \subseteq \mathcal{C}^{\Lambda}$ be an ONB of eigenvectors of $\tilde{\Delta}$, i.e., $-\tilde{\Delta} \varphi_j = e_j \varphi_j$. For any $k \in \Lambda^*$ and $1 \leq j \leq |\Lambda|$, we observe that

$$\left( e_j - \omega(k) \right)^2 |\langle \psi_k | \varphi_j \rangle|^2 = |\langle \psi_k | (\Delta - \tilde{\Delta}) \varphi_j \rangle|^2$$

$$= |\langle \psi_k | (P_{\Omega} \Delta P_{\Omega}^+ + P_{\Omega}^+ \Delta P_{\Omega}) \varphi_j \rangle|^2$$

$$= |\langle P_{\Omega} \Delta P_{\Omega}^+ \psi_k | \varphi_j \rangle|^2 + |\langle P_{\Omega}^+ \Delta P_{\Omega} \psi_k | \varphi_j \rangle|^2$$

$$\geq |\langle P_{\partial \Omega} \Delta P_{\Omega}^+ \psi_k | \varphi_j \rangle|^2, \quad (3.64)$$

using that either $P_{\Omega} \varphi_j = 0$ or $P_{\Omega}^+ \varphi_j = 0$ and that $P_{\Omega} \Delta P_{\Omega}^+ = P_{\partial \Omega} \Delta P_{\Omega}^+$. Since $|e_j - \omega(k)| \leq 4d$, Eq. (3.64) implies that

$$(4d)^2 |\langle \psi_k | \varphi_j \rangle|^2 \geq |\langle b_k | \varphi_j \rangle|^2, \quad (3.65)$$
where \( b_k := P_{\partial\Omega} \Delta P_{\Omega} \psi_k \) is the boundary vector that plays a crucial role in [24]. By summation over all \( j \) corresponding to eigenvalues \( e_j > \mu \), we obtain

\[
\langle \psi_k | \tilde{P}_+ \psi_k \rangle \geq (4d)^{-2} \langle b_k | \tilde{P}_+ b_k \rangle ,
\]

for all \( k \in \Lambda^* \). Next, the convexity of \( \lambda \mapsto [\lambda]_+ \) and the fact that \( \tilde{P}_+ = \mathbb{1}[-\Delta > \mu] \geq (4d)^{-1}[-\Delta - \mu]_+ \) yield

\[
\langle b_k | \tilde{P}_+ b_k \rangle \geq \frac{1}{4d} \langle b_k | [-\Delta - \mu]_+ b_k \rangle \geq \frac{1}{4d} \left[ \langle b_k | (-\Delta - \mu) b_k \rangle \right]_+ = \frac{1}{4d} \left[ \langle b_k | (-\Delta - \mu) b_k \rangle \right]_+ .
\]

(3.67)

Now, for any \( x \in \partial\Omega \) there is, by definition, at least one point \( x + e \in \Omega \), with \( |e|_1 = 1 \). Since \( b_k \) is supported in \( \partial\Omega \), we have \( b_k(x + e) = 0 \), and thus

\[
\langle b_k | (-\Delta - \mu) b_k \rangle = \sum_{x \in \partial\Omega} \left\{ \sum_{|e|_1 = 1} |b_k(x) - b_k(x + e)|^2 - \mu|b_k(x)|^2 \right\}
\geq (1 - \mu) \sum_{x \in \partial\Omega} |b_k(x)|^2 = (1 - \mu) \|b_k\|^2 .
\]

(3.68)

Inserting (3.66)–(3.68) into (3.63), we arrive at

\[
\delta E(\mu, \Omega) \geq \frac{(1 - \mu)}{(4d)^3} \sum_{k \in \Lambda^*} [\mu - \omega(k)]_+ \|b_k\|^2 .
\]

(3.69)

Next, we use that in the sum in (3.69) only those \( k \in \Lambda^* \) contribute, for which \( \omega(k) = \sum_{\nu=1}^d 2\{1 - \cos(k\nu)\} \leq \frac{1}{2}, \) as \( 0 < \mu \leq 1 \). This implies that \( \cos(k\nu) \geq \frac{1}{2}, \) for all \( \nu \in \{1, 2, \ldots, d\} \). Hence, for these \( k \), we have that

\[
\|b_k\|^2 = \frac{1}{|\Lambda|} \sum_{x \in \partial\Omega} \left| \sum_{\sigma = \pm} \sum_{\nu=1}^d e^{i\sigma k\nu} \mathbb{1}[x + \sigma e_{\nu} \in \Omega^e] \right|^2
\geq \frac{1}{|\Lambda|} \sum_{x \in \partial\Omega} \left( \sum_{\sigma = \pm} \sum_{\nu=1}^d \cos(k\nu) \mathbb{1}[x + \sigma e_{\nu} \in \Omega^e] \right)^2
\geq \frac{1}{4|\Lambda|} \sum_{x \in \partial\Omega} 1 = \frac{|\partial\Omega|}{4|\Lambda|} ,
\]

(3.70)
since there is at least one choice for \((\sigma, \nu)\) such that \(x + \sigma e_\nu \in \Omega^c\). Inserting this estimate into (3.69), we obtain

\[
\delta E(\mu, \Omega) \geq \frac{|\partial \Omega|}{8 (4d)^3} \left( \frac{1}{|\Lambda^*|} \sum_{k \in \Lambda^*} [\mu - \omega(k)]_+ \right). \tag{3.71}
\]

Now define \(q : \mathbb{T}^d \to \Lambda^*\) by the preimages

\[
q^{-1}(k) := k + \left[ -\frac{\pi}{L}, \frac{\pi}{L} \right]^d,
\tag{3.72}
\]

for \(k \in \Lambda^*\). In other words, given \(\xi \in \mathbb{T}^d\), the point \(q(\xi) \in \Lambda^*\) is the closest point to \(\xi\). In particular, \(|\xi - q(\xi)|_\infty \leq \frac{\pi}{L}\), which implies that \(|\omega(q(\xi)) - \omega(\xi)| \leq \frac{2\pi d}{L}\), by Taylor’s theorem. Hence,

\[
\frac{1}{|\Lambda^*|} \sum_{k \in \Lambda^*} [\mu - \omega(k)]_+ = \int_{\mathbb{T}^d} [\mu - \omega(q(\xi))]_+ \frac{d^d \xi}{(2\pi)^d} \geq \int_{\mathbb{T}^d} [\mu - 2\pi dL^{-1} - \omega(\xi)]_+ \frac{d^d \xi}{(2\pi)^d} \geq \int_{\mathbb{T}^d} [\mu - 2\pi dL^{-1} - \omega(\xi)]_+ \frac{d^d \xi}{(2\pi)^d}. \tag{3.73}
\]

Since, by assumption, \(\frac{2\pi d}{L} \leq \frac{2\pi d}{L^*} = \frac{\mu}{2}\) and \(\omega(\xi) \leq \xi^2\), we have

\[
\int_{\mathbb{T}^d} [\mu - 2\pi dL^{-1} - \omega(\xi)]_+ d^d \xi \geq \int_{\mathbb{T}^d} \left[ \frac{\mu}{2} - \xi^2 \right]_+ d^d \xi = \frac{|S^{d-1}|}{2^{d/2} d(d + 2)} \mu^{1+(d/2)}. \tag{3.74}
\]

Inserting (3.73)–(3.74) into (3.71), we arrive at the asserted estimate. \(\text{QED}\)

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