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Hund's Rule and Metallic Ferromagnetism

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We study tight-binding models of itinerant electrons in two different bands, with effective on-site interactions expressing Coulomb repulsion and Hund's rule. We prove that, for sufficiently large on-site exchange anisotropy, all ground states show metallic ferromagnetism: They exhibit a macroscopic magnetization, a macroscopic fraction of the electrons is spatially delocalized, and there is no energy gap for kinetic excitations.

KEY WORDS: Metallic ferromagnetism; Hund's rule; two-band tight-binding models.

1. INTRODUCTION

Ferromagnetism is known to originate from strongly correlated states of quantum mechanical electrons with a very large total spin but small total energy. Microscopic mechanisms giving rise to a coexistence of metallic behavior with ferromagnetic ordering at sufficiently low temperatures have been proposed, but are not well understood, mathematically, yet. Ferromagnetism in conjunction with a positive electric conductivity (metallic behavior) is a collective phenomenon arising from a competition of *spatial motion* (hopping) of quantum mechanical charged particles with half-integer spin obeying *Pauli's exclusion principle*, i.e., of electrons, in a periodic background with *Coulomb repulsion* between pairs of such particles. A mathematically precise description of this phenomenon is difficult because there are two kinds of *gapless* excitations: electron–hole pairs very close to

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the Fermi surface, and spin waves in ferromagnetically ordered spin configurations. In a perturbative analysis of states of very low total energy, there are therefore two sources of infrared divergences, or of "small energy denominators", namely electron–hole excitations with an energy arbitrarily close to the groundstate energy, and spin waves, or magnons, of very long wave length.

In this paper, we study some tight-binding models of metallic compounds with two bands partly filled with electrons. In a ground state, the low-lying band is at most half-filled, due to strong on-site Coulomb repulsion between pairs of electrons in a spin-singlet state, while the higher-lying band is assumed to be weakly filled, so that a Fermi surface is expected. It is assumed that an electron from the low-lying band and an electron from the higher-lying band occupying the *same* site of the underlying lattice obey *Hund's rule*, i.e., their interaction energy is minimized if they form a *spin-triplet state*. A two-electron spin-triplet state is symmetric under exchange of the two spins. The Pauli principle then requires the *microscopic* orbital wave function of the two electrons to be antisymmetric under exchange of their positions, which makes the Coulomb repulsion between the two electrons *small*. (Concretely, an antisymmetric microscopic wave function for two electrons moving in the field of an ion may be constructed as a Slater determinant of, e.g., two different d-shell orbitals.) It may be of interest to remark that a mathematically rigorous derivation of Hund's rule in atomic physics from first principles has not been found, yet. That it is assumed to hold in our models must therefore be considered to be a reasonable, but heuristic ansatz. In order to eliminate small energy denominators due to spin waves of very long wavelength, we choose the couplings between the spins of an electron from the lower band and of an electron from the higher band occupying the *same* site to be *anisotropic*. Hund's rule cannot be invoked to justify this feature. Our results can be expected to hold for isotropic spin–spin couplings, in accordance with Hund's rule, too; but we have not been able to rigorously prove this.

The models studied in this paper are arguably the simplest physically relevant models in which metallic ferromagnetism can be exhibited.

The feature that magnetic ordering emerges from a cooperation between electron hopping and local, on-site electron–electron interactions appears to be inherent in several tight-binding models and has been studied intensely. *Antiferromagnetic* ordering, for example, can be seen to emerge in the half-filled (single-band) Hubbard model in second-order perturbation theory in t/U, where t measures the strength of hopping and U the strength of on-site Coulomb repulsion. This was discovered by Anderson;[1] (for a more precise analysis, see also ref. 6). A model

simpler than the Hubbard model is the Falicov–Kimball model. There are many rigorous results about the Falicov–Kimball model starting with refs. 4 and 11. A fairly systematic perturbative analysis can be found in ref. 5, and references given there. These and many further results show how long-range correlations in ground states or low-temperature equilibrium states can arise from a cooperation between electron hopping and on-site interactions. Unfortunately, the perturbative methods in refs. 4, 5 and 11 can only be applied to the analysis of insulators, i.e., of states where electrons are essentially localized, because, in such situations, there are no small energy denominators or infrared divergences. The analysis of long-range correlations in *metals* calls for different, non-perturbative methods.

One approach towards understanding simple examples of itinerant ferromagnetism is based on studying the Hubbard model on very special lattices that give rise to a macroscopic degeneracy of the ground state energy of the Hubbard Hamiltonian (i.e., to a "flat band", or to a nearly flat band; see refs. 12 and 13. A Hartree–Fock study of the Hubbard model also provides useful insights.[2,3] More recently, there has been some interest in studying manganites described by models with several bands. Numerical studies indicate that there is ferromagnetic ordering at sufficiently low temperatures (see, e.g., refs. 9, 10 and 14), and references given there. The models studied in this paper are similar to models used to describe manganites. They have ground states involving macroscopically large domains of essentially free electrons but with aligned spins. Electrons are discouraged to leave such a domain, because, in neighboring domains, the direction of their spin violates Hund's rule, and this would result in a state of comparatively large energy. At the technical level, our analysis is very much based on ref. 7 (see also refs. 8 and 15). The methods developed in these references enable us to prove lower bounds on the ground state energy which, when combined with rather simple variational upper bounds, lead to the conclusion that the boundaries between domains of electrons of opposite spin have a total length growing much less rapidly than the total number of sites in the system, and this enables us to exhibit ferromagnetic ordering in the ground states. The fact that there are only two preferred spin orientations, $\uparrow$ and $\downarrow$, is, of course, due to the anisotropy in the on-site spin–spin coupling for two electrons in different bands occupying the same site. (The analysis of isotropic models would be considerably more difficult.) Within large domains of a fixed preferred spin orientation, electrons are completely delocalized, so that the ground state energy is *not* separated from the energies of excited states by a uniformly positive energy gap.

2. SETTING, MODELS, AND SUMMARY OF MAIN RESULTS

We consider a lattice model with electrons in two different bands, indexed by $a=1,2$. We let $c^\dagger_{a\sigma}(x)$ and $c_{a\sigma}(x)$ denote the creation and annihilation operators for an electron of band a and spin $\sigma=\uparrow,\downarrow$, at site $x\in\mathbb{Z}^d$. The state space of the system in a finite domain $\Lambda\subset\mathbb{Z}^d$ is the Hilbert space

$$\mathcal{H}_\Lambda=\mathcal{F}_\Lambda\otimes\mathcal{F}_\Lambda, \tag{2.1}$$

where $\mathcal{F}_\Lambda$ is the usual Fock space for electrons,

$$\mathcal{F}_\Lambda=\bigoplus_{N\geqslant 0} P_-\Big[\ell^2(\Lambda)\otimes\mathbb{C}^2\Big]^{\otimes N}. \tag{2.2}$$

Here P_- is the projector onto antisymmetric functions. The energy of electrons is partly kinetic and partly due to interactions among themselves. The kinetic energy is represented by standard hopping terms. Interactions are of two different kinds. First, Coulomb interactions are approximated by on-site operators of the Hubbard type. Second, a pair interaction involving the spins of electrons of different bands reminds of the Hund rule for the filling of atomic eigenstates. Precisely, we define the "2-band Hund–Hubbard Hamiltonian" as

$$\begin{aligned} H_\Lambda^{\mathrm{HH}} = &-\sum_{a=1,2} t_a \sum_{\sigma=\uparrow,\downarrow} \sum_{\substack{x,y\in\Lambda\\ |x-y|=1}} c^\dagger_{a\sigma}(x)c_{a\sigma}(y) + \sum_{a=1,2} U_a \sum_{x\in\Lambda} n_{a\uparrow}(x)n_{a\downarrow}(x) \\ &+U_{12}\sum_{x\in\Lambda} n_1(x)\,n_2(x) - J\sum_{x\in\Lambda} \boldsymbol{S}_1(x)\cdot\boldsymbol{S}_2(x). \end{aligned} \tag{2.3}$$

The parameters t_a control the kinetic energy of electrons of each band and they are related to the effective mass of electrons. We suppose that $t_1>t_2$ and refer to electrons of band 1 as "light" (they move fast) and electrons of band 2 as "heavy" (they move slowly). The parameters U_1, U_2, U_{12} are positive and represent the Coulomb interaction energy between two particles of band 1, two particles of band 2, and one particle of each band, respectively. The number operators are defined by $n_{a\sigma}(x)=c^\dagger_{a\sigma}(x)c_{a\sigma}(x)$ and $n_a(x)=n_{a\uparrow}(x)+n_{a\downarrow}(x)$. Finally, $J>0$ measures the strength of the coupling between the spins; spin operators are given by

$$S^{(j)}_a(x)=\sum_{\sigma,\sigma'}\tau^{(j)}_{\sigma\sigma'}c^\dagger_{a\sigma}(x)c_{a\sigma'}(x), \tag{2.4}$$

where $\tau^{(j)}$, $j=1,2,3$, are the Pauli matrices $\frac{1}{2}\left(\begin{smallmatrix}0&1\\1&0\end{smallmatrix}\right)$, $\frac{1}{2}\left(\begin{smallmatrix}0&-\mathrm{i}\\\mathrm{i}&0\end{smallmatrix}\right)$, $\frac{1}{2}\left(\begin{smallmatrix}1&0\\0&-1\end{smallmatrix}\right)$. We will consider a simpler model with anisotropic spin interactions (the third components of the spins interact more strongly) and with the property that one of the two bands is nearly flat. The Hamiltonian of this model is introduced in Eq. (2.9), below. The following discussion applies to general Hund–Hubbard models, isotropic and anisotropic ones.

We note that neither the hopping terms alone nor the Hund couplings alone give rise to global magnetization. Without on-site interactions the ground state favored by the hopping terms is not magnetic; the kinetic energy is minimized by a state where half the electrons have spin $\uparrow$, and half the electrons have spin $\downarrow$. As for the Hund couplings, they are local (on-site) and do not yield the long-range correlations that are present in a ferromagnetic state. Ferromagnetism in this model results from a cooperation of the two terms.

This model was numerically studied in ref. 9 for $t_1 = t_2$. Ferromagnetic phases were identified at low temperatures and for some intervals of electronic densities. The present model with $t_1 < t_2$ actually behaves more like the two-band Hubbard model with Kondo spins of ref. 10; heavy electrons here play a rôle similar to that of Kondo spins. Ferromagnetic phases were also numerically observed for this model.

In this paper, we study a phase with spontaneous magnetization. The total spin operator in a domain $\Lambda \subset \mathbb{Z}^d$ is denoted $\boldsymbol{M}_\Lambda$ and is given by

$$\boldsymbol{M}_\Lambda = \sum_{x\in\Lambda} \big[\boldsymbol{S}_1(x) + \boldsymbol{S}_2(x)\big]. \tag{2.5}$$

The norm of $\boldsymbol{M}_\Lambda$ is

$$\|\boldsymbol{M}_\Lambda\| = \Big(\sum_{i=1}^{3} (M_\Lambda^{(i)})^2\Big)^{1/2}, \tag{2.6}$$

with $M_\Lambda^{(i)}$ the ith component of $\boldsymbol{M}_\Lambda$. We expect that the system displays extensive magnetization. That is, in a domain Λ the expectation of $\|\boldsymbol{M}_\Lambda\|$ in the ground state should be proportional to $|\Lambda|$. We are not able to prove this, but we can prove that the system is magnetized at least on a "mesoscopic" scale. To be precise, we consider the following definition of the magnetization per site: Given a state $\Upsilon \in \mathcal{H}_\Lambda$ and a subdomain $\Lambda' \subset \Lambda$, we define

$$\begin{aligned} m_{\Lambda,\Lambda'} &= \frac{1}{|\Lambda|} \sum_{x:\Lambda'+x\subset\Lambda} \frac{1}{|\Lambda'|} \big(\Upsilon, \|\boldsymbol{M}_{\Lambda'+x}\|\Upsilon\big); \\ m^{(3)}_{\Lambda,\Lambda'} &= \frac{1}{|\Lambda|} \sum_{x:\Lambda'+x\subset\Lambda} \frac{1}{|\Lambda'|} \big|(\Upsilon, M^{(3)}_{\Lambda'+x}\Upsilon)\big|. \end{aligned} \tag{2.7}$$

Note that we consider the expectation value of the norm of $\boldsymbol{M}_{\Lambda'}$ in the state Υ, averaged over all translates of Λ' such that $\Lambda'+x$ remains in Λ. The number of terms in the sum is $|\Lambda|$, up to a negligible boundary correction. We clearly have that $m_{\Lambda,\Lambda'} \geqslant m^{(3)}_{\Lambda,\Lambda'}$. We will prove that, for the anisotropic model introduced in Eq. (2.9), below, the third component of the ground state magnetization per site, $m^{(3)}_{\Lambda,\Lambda'}$, satisfies

$$\lim_{\Lambda' \nearrow \mathbb{Z}^d} \lim_{\Lambda \nearrow \mathbb{Z}^d} m^{(3)}_{\Lambda,\Lambda'} > 0.$$

The limits are over boxes of increasing size, and electron densities are kept constant.

Perturbation methods shed some light onto the structure of the phases of this model. The situation is similar to the one in the Hubbard model at half-filling and with strong on-site repulsion, which behaves like the antiferromagnetic Heisenberg model. Perturbative methods along the lines of refs. 5 and 6 can be used for many rational densities. However, such methods can be applied only when electrons are localized, and this is not the case in a conducting metal. Here we focus our attention on regimes where there does not exist an energy gap separating excitations from the ground state energy, and where some electrons have delocalized wave functions.

The Hamiltonian Eq. (2.3) is symmetric with respect to spin rotations, and this makes the study difficult. We simplify the model by replacing the term $\boldsymbol{S}_1(x) \cdot \boldsymbol{S}_2(x)$ by $S^{(3)}_1(x) \cdot S^{(3)}_2(x)$. Furthermore, we let $t_2 \to 0$. We can fix the energy scale by choosing $t_1 = 1$. We then obtain the following simplified Hamiltonian ("2-band Ising-Hubbard model")

$$\begin{aligned} H^{\mathrm{IH}}_\Lambda = & -\sum_\sigma \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} c^\dagger_{1\sigma}(x) c_{1\sigma}(y) + \sum_{a=1,2} U_a \sum_{x\in\Lambda} n_{a\uparrow}(x) n_{a\downarrow}(x) \\ & + U_{12} \sum_{x\in\Lambda} n_1(x) n_2(x) \\ & - \frac{J}{4} \sum_{x\in\Lambda} [n_{1\uparrow}(x) - n_{1\downarrow}(x)] \cdot [n_{2\uparrow}(x) - n_{2\downarrow}(x)]. \end{aligned} \tag{2.8}$$

Let ρ_1, ρ_2 denote the densities of light and heavy particles, respectively. We prove the following statement in Section 4. Our proof works in dimension larger or equal to 2 (Eq. (3.19) holds for $d \geqslant 2$ only). We do not have results for the one-dimensional models.

Theorem 2.1. Let $d \geqslant 2$. For arbitrary $0 < \rho_1 < \rho_2 \leqslant 1$, there exists $J_0 < \infty$ such that, for $\frac{J}{4} - U_{12} > J_0$, all ground states Υ of H_Λ^{IH} satisfy

$$\lim_{\Lambda' \nearrow \mathbb{Z}^d} \lim_{\Lambda \nearrow \mathbb{Z}^d} m^{(3)}_{\Lambda,\Lambda'} = \frac{\rho_1 + \rho_2}{2}.$$

This theorem suggests that the ground state displays "saturated ferromagnetism", as it has maximum total spin. Notice that for large enough J it holds independently of $U_1, U_2 \geqslant 0$.

The proof of Theorem 2.1 reduces to the study of the ground state energy for fixed configurations of heavy electrons, since the latter do not have kinetic energy. To a configuration of heavy electrons we can assign domains of $\uparrow$ and $\downarrow$ spins. A light electron of spin $\uparrow$, say, is in a state that is essentially localized on the domain where heavy electrons also have spin $\uparrow$. Hund interactions suppress other configurations. In the limit $J \to \infty$, the ground state energy is purely kinetic and it is minimal in a configuration of heavy electrons with large domains of identical spins. This allows us to show that the size of the boundary of these domains is less than $|\Lambda|^{1-\frac{1}{d}}$, meaning that spins are locally aligned. See Section 4 for details.

The constant J_0 in Theorem 2.1 depends on ρ_1, and there are good reasons for it. There is no ferromagnetism for $\rho_1 = 0$ or $\rho_1 = \rho_2 = 1$. The former case results in independent spins at each site. The latter case can be treated with perturbation methods. Non-empty sites are typically occupied by two particles of spin $\uparrow$, or by two particles of spin $\downarrow$. An effective interaction of strength $\frac{2}{U_1 + \frac{J}{2}}$ stabilizes antiferromagnetic chessboard phases in the ground state and at low temperatures. This interaction can be obtained using the method described in ref. 6. The case $\rho_1 = \rho_2 < 1$ is more subtle.

We can improve the result of Theorem 2.1 and consider a model that interpolates between Eqs. (2.3) and (2.8). We refer to the following Hamiltonian as "the asymmetric 2-band Hund–Hubbard model":

$$\begin{aligned} H_\Lambda^{\mathrm{aHH}} = & -\sum_{a=1,2} t_a \sum_{\sigma=\uparrow,\downarrow} \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} c^\dagger_{a\sigma}(x) c_{a\sigma}(y) \\ & + \sum_{a=1,2} U_a \sum_{x\in\Lambda} n_{a\uparrow}(x) n_{a\downarrow}(x) \\ & + U_{12} \sum_{x\in\Lambda} n_1(x)\, n_2(x) - J \sum_{x\in\Lambda} S_1^{(3)}(x) S_2^{(3)}(x) \\ & - J^\perp \sum_{x\in\Lambda} \big(S_1^{(1)}(x) S_2^{(1)}(x) + S_1^{(2)}(x) S_2^{(2)}(x) \big). \end{aligned} \tag{2.9}$$

Let us again fix the energy scale by setting $t_1 = 1$.

Theorem 2.2. Let $d \geqslant 2$. For arbitrary $0 < \rho_1 < \rho_2 \leqslant 1$, there are constants $J_0 < \infty$ and $c > 0$ (both depend on the densities) such that if $\frac{J}{4} - U_{12} > J_0$ and $t_2, J^\perp < c$, all ground states Υ of H_Λ^{aHH} satisfy

$$\lim_{\Lambda' \nearrow \mathbb{Z}^d} \lim_{\Lambda \nearrow \mathbb{Z}^d} m_{\Lambda,\Lambda'} = \frac{\rho_1 + \rho_2}{2}.$$

This theorem again holds uniformly in $U_1, U_2 \geqslant 0$.

Our paper is organized as follows. We discuss the properties of the ground state of a simple model in Section 3. The results for the simple model are then used in Section 4 where Theorem 2.1 is proved. Finally, it is shown in Section 5 that the claims for the Ising–Hubbard Hamiltonian Eq. (2.8) can be extended to certain perturbations, that include the asymmetric Hund–Hubbard model (2.9). This proves Theorem 2.2.

3. INTERACTING ELECTRONS IN A MAGNETIC POTENTIAL

We introduce in this section a Hubbard model of electrons in an external potential that involves the third components of the spins. We do not insist on the physical relevance of this model. The sole motivation for this section stems from applications to Hund–Hubbard systems. We will use Propositions 3.1–3.3 in Sections 4 and 5 in order to prove Theorems 2.1 and 2.2 — these theorems being physically motivated.

The results below extend the bounds for the ground state energy of spinless electrons in binary potentials proposed in ref. 7. We work in the Fock space $\mathcal{F}_\Lambda$ of spin $\frac{1}{2}$ electrons in Λ. Let V be a "magnetic potential", that is, V is a collection of non-negative numbers $V_x^\uparrow, V_x^\downarrow$ indexed by sites $x \in \mathbb{Z}^d$. The Hamiltonian is

$$H_\Lambda(V) = -\sum_{\substack{x,y \in \Lambda \\ |x-y|=1}} \sum_{\sigma=\uparrow,\downarrow} c_\sigma^\dagger(x) c_\sigma(y) + U \sum_{x \in \Lambda} n_\uparrow(x) n_\downarrow(x) + \sum_{x \in \Lambda} \sum_{\sigma=\uparrow,\downarrow} V_x^\sigma \, n_\sigma(x). \tag{3.1}$$

Here, $c_\sigma^\dagger(x)$ and $c_\sigma(x)$ are creation and annihilation operators of fermions of spin σ at x, and $n_\sigma(x) = c_\sigma^\dagger(x) c_\sigma(x)$. We suppose that a gap V_0 separates the minimum value from other values of the potential. Introducing

$$A_\sigma = \{x \in \Lambda : V_x^\sigma = 0\}, \quad A = A_\uparrow \cup A_\downarrow \tag{3.2}$$

(the sites where the potential is zero for some spin), we define

$$V_0 = \min_{\sigma=\uparrow,\downarrow} \inf_{x \notin A_\sigma} V_x^\sigma. \tag{3.3}$$

We assume that V_0 is strictly positive.

In order to understand the bounds on the ground state energy given below, it is useful to consider the situation where $V_0 \to \infty$. Assuming that $A_\uparrow \cap A_\downarrow = \emptyset$, the domain Λ is partitioned into $A_\uparrow$, $A_\downarrow$, and $\Lambda \setminus A$. Electrons of spin σ are described by wave functions with support in A_σ, the energy being infinite otherwise. Electrons do not interact and their ground state energy is purely kinetic. It mainly consists of a bulk term that depends on the electronic density inside A_σ and that is proportional to the volume $|A_\sigma|$. The effect of the boundary of A_σ is to increase the ground state energy by a term proportional to the size of the boundary. The ground state energy of non-interacting spinless electrons in arbitrary finite domains was studied in ref. 7; upper and lower bounds were established that confirm the discussion above. As V_0 decreases from infinity to a finite value, electrons delocalize somewhat, but the situation does not change in any essential way.

Estimates for the ground state energy involve the energy density of free spinless electrons in the limit of infinite volume. As is well-known, the energy per site $e(\rho)$ for a density $0 < \rho < 1$ of electrons is given by

$$e(\rho) = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_F(\rho)} \varepsilon_k \, dk, \quad \varepsilon_k = -2 \sum_{i=1}^{d} \cos k_i, \tag{3.4}$$

where $\varepsilon_F(\rho)$ is the Fermi energy, defined by the equation

$$\rho = \frac{1}{(2\pi)^d} \int_{\varepsilon_k < \varepsilon_F(\rho)} dk. \tag{3.5}$$

Notice that $e(\rho) < 0$ for $0 < \rho < 1$. We need to define the boundary $B(A)$ of a set $A \subset \mathbb{Z}^d$; it is convenient to define it as the number of bonds that connect A with its complement,

$$B(A) = \#\{(x, y) : x \in A, y \notin A, |x - y| = 1\}. \tag{3.6}$$

We first give a bound for fixed densities of electrons of each spin. In the absence of interactions ($U = 0$) the following proposition merely rephrases similar results in ref. 7. We define $E_\Lambda(V; N_\uparrow, N_\downarrow)$ as the ground

state energy of $H_\Lambda(V)$ when the number of spin $\uparrow$ (spin $\downarrow$) electrons is $N_\uparrow$ ($N_\downarrow$, respectively). We introduce a notation for electronic densities inside $A_\uparrow$ and $A_\downarrow$; for $\sigma = \uparrow, \downarrow$, we let $\rho_\sigma = \frac{N_\sigma}{|A_\sigma|}$. We have the following bounds for the ground state energy.

Proposition 3.1. Let V be a magnetic potential and $N_\uparrow$, $N_\downarrow$ be numbers with the properties that:

- $A_\uparrow \cap A_\downarrow = \emptyset$.
- $V_0 > 2d(\sqrt{d}+1)$.
- $N_\uparrow \leqslant |A_\uparrow|$, $N_\downarrow \leqslant |A_\downarrow|$.

Then there exists $\alpha(\rho) > 0$ (independent of V_0), for $0 < \rho < \frac{|A|}{|\Lambda|}$, such that

$$\sum_{\sigma=\uparrow,\downarrow} \Big[e(\rho_\sigma)|A_\sigma| - \tfrac{e(\rho_\sigma)}{2d} B(A_\sigma) \Big] \geqslant E_\Lambda(V; N_\uparrow, N_\downarrow) \geqslant \sum_{\sigma=\uparrow,\downarrow} \Big[e(\rho_\sigma)|A_\sigma| + \big(\alpha(\rho_\sigma) - \gamma(V_0)\big) B(A_\sigma) \Big]$$

with

$$\gamma(V_0) = \tfrac{4d}{V_0 - 2d} + \tfrac{16d^3}{(V_0-2d)^2 - 4d^3}.$$

The inequalities in this proposition hold uniformly in U. The proof of Proposition 3.1 is based on results in ref. 7, where the sum, $S_{\Lambda,N}$, of the N lowest eigenvalues of the discrete Laplacian $t_{xy} = -\delta_{|x-y|,1}$, $x, y \in \Lambda$ is estimated, with Λ a finite set of lattice points of arbitrary shape. Two of the results in ref. 7 are relevant for our analysis:

- We have upper and lower bounds,

$$e(\rho)|\Lambda| - \tfrac{e(\rho)}{2d} B(\Lambda) \geqslant S_{\Lambda,N} \geqslant e(\rho)|\Lambda| + a(\rho) B(\Lambda), \tag{3.7}$$

  where $\rho = \frac{N}{|\Lambda|}$, and $a(\rho)$ is strictly positive for any $0 < \rho < 1$. Recall that $e(\rho)$ is negative, so that all boundary terms in the above equation are positive. (The notation in ref. 7 is slightly different, the Hamiltonian being shifted by $2d$ and the boundary is defined differently.)
- If $S^U_{\Lambda,N}$ denotes the sum of the N lowest eigenvalues of the operator $-\delta_{|x-y|,1} + U\chi_{\Lambda^c}(x)$, where χ_{Λ^c} is the characteristic function of the complement, Λ^c, of the set Λ, and if U is positive, we have

$$S_{\Lambda,N} \geqslant S^U_{\Lambda,N} \geqslant S_{\Lambda,N} - \gamma(U)B(\Lambda), \tag{3.8}$$

for some $\gamma(U) \to 0$ as $U \to \infty$.

The upper bound for $E_\Lambda(V; N_\uparrow, N_\downarrow)$ does not depend on V_0. Increasing the values of the potential actually incresases the energy, so it is enough to prove the statement in the limit $V_0 \to \infty$. Electrons with different spins are independent, and the upper bound follows from the one in Eq. (3.7).

Let us turn to the lower bound. The operator that represents interactions between electrons is positive; we get a lower bound for the ground state energy by taking $U \to 0$. For $V_0 = \infty$ we are in the situation of ref. 7. For finite V_0 we use Eq. (3.8) with minor modifications. Namely, starting with Eqs. (4.3)–(4.5) of ref. 7 but introducing our measure $B(\Lambda)$ of the boundary, the upper bound in Eq. (4.8) can be replaced by $\frac{4d}{V_0 - 2d} B(\Lambda)$. It is useful to modify the bound for the number of sites at distance n from the domain Λ (recall that we are using the ℓ^1 distance here). It is not hard to check that

$$\begin{aligned} &\#\{x : \operatorname{dist}(x, \Lambda) = 1\} \leqslant B(\Lambda); \\ &\#\{x : \operatorname{dist}(x, \Lambda) = n\} \leqslant d \cdot \#\{x : \operatorname{dist}(x, \Lambda) = n - 1\} \quad \text{if } n \geqslant 2. \end{aligned} \tag{3.9}$$

We therefore have that $\#\{x : \operatorname{dist}(x, \Lambda) = n\} \leqslant d^{n-1} B(\Lambda)$. This allows to bound $N - \operatorname{Tr} \tilde{\rho}$ in Eq. (4.11) by $\frac{4d^2}{(V_0 - 2d)^2 - 4d^3} B(\Lambda)$, leading to the present definition of $\gamma(V_0)$. The bound given here is better for large V_0 than the one in ref. 7.

The considerations above show that Proposition 3.1 is a mild extension of ref. 7. The following proposition needs, however, a more detailed proof.

Proposition 3.2. Under the same hypotheses as in Proposition 3.1, we have that, for all normalized ground states Υ of $H_\Lambda(V)$,

$$\sum_{\sigma = \uparrow, \downarrow} \sum_{x \notin A_\sigma} (\Upsilon, n_\sigma(x) \Upsilon) \leqslant \tfrac{3}{V_0 - 4d} [B(A_\uparrow) + B(A_\downarrow)].$$

Proof. Let M_σ be the number of electrons of spin σ that are outside of A_σ, and $P_{M_\uparrow M_\downarrow}$ be the projector onto the subspace spanned by states with exactly M_σ particles outside A_σ, $\sigma = \uparrow, \downarrow$. A state Υ can be decomposed as

$$\Upsilon = \sum_{M_\uparrow = 0}^{N_\uparrow} \sum_{M_\downarrow = 0}^{N_\downarrow} c_{M_\uparrow M_\downarrow} \Upsilon_{M_\uparrow M_\downarrow}, \tag{3.10}$$

with $c_{M_\uparrow M_\downarrow} = \| P_{M_\uparrow M_\downarrow} \Upsilon \| \geqslant 0$, $\sum c^2_{M_\uparrow M_\downarrow} = 1$, and $\Upsilon_{M_\uparrow M_\downarrow} = c^{-1}_{M_\uparrow M_\downarrow} P_{M_\uparrow M_\downarrow} \Upsilon$ is normalized. The goal is to estimate

$$\sum_{\sigma=\uparrow,\downarrow} \sum_{x \notin A_\sigma} (\Upsilon, n_\sigma(x) \Upsilon) = \sum_{M_\uparrow, M_\downarrow} c^2_{M_\uparrow M_\downarrow} (M_\uparrow + M_\downarrow). \tag{3.11}$$

The strategy is to obtain a lower bound for $E_\Lambda(V; N_\uparrow, N_\downarrow)$ that involves the expression above. Comparison with the upper bound of Proposition 3.1 will prove the claim.

The ground state energy is increasing in U so that we can again set $U = 0$ when discussing a lower bound. The Hamiltonian $H_\Lambda(V)$ can be split into

$$\begin{aligned} H_\Lambda(V) = & \sum_{\sigma=\uparrow,\downarrow} \Big(H^\sigma_{A_\sigma}(V) + H^\sigma_{\Lambda \setminus A_\sigma}(V) \Big) \\ & - \sum_{\sigma=\uparrow,\downarrow} \sum_{\substack{x \in A_\sigma, y \notin A_\sigma \\ |x-y|=1}} \big[c^\dagger_\sigma(x) c_\sigma(y) + c^\dagger_\sigma(y) c_\sigma(x) \big]. \end{aligned} \tag{3.12}$$

Hamiltonians $H^\sigma_\cdot(V)$ consist in kinetic terms for particles of spin σ in the corresponding domains, and of the potentials given by V^σ. They leave the subspace with fixed $M_\uparrow$ and $M_\downarrow$ invariant. The norm of the last operator is smaller than $2B(A_\uparrow) + 2B(A_\downarrow)$. Therefore

$$\begin{aligned} (\Upsilon, H_\Lambda(V) \Upsilon) \geqslant & \sum_{M_\uparrow, M_\downarrow} c^2_{M_\uparrow M_\downarrow} \sum_\sigma (\Upsilon_{M_\uparrow M_\downarrow}, [H^\sigma_{A_\sigma}(V) + H^\sigma_{\Lambda \setminus A_\sigma}(V)] \Upsilon_{M_\uparrow M_\downarrow}) \\ & - 2B(A_\uparrow) - 2B(A_\downarrow). \end{aligned} \tag{3.13}$$

Inserting the lower bound for the sum of the lowest eigenvalues of the discrete Laplacian in a finite domain, neglecting the positive boundary correction term, we get the lower bound

$$(\Upsilon_{M_\uparrow M_\downarrow}, H^\sigma_{A_\sigma}(V) \Upsilon_{M_\uparrow M_\downarrow}) \geqslant e\left(\tfrac{N_\sigma - M_\sigma}{|A_\sigma|} \right) |A_\sigma| \geqslant e(\rho_\sigma) |A_\sigma| - \varepsilon_{\mathrm{F}}(\rho_\sigma) M_\sigma . \tag{3.14}$$

The second inequality holds because $e(\rho + \eta) \geqslant e(\rho) + \eta \varepsilon_{\mathrm{F}}(\rho)$ (indeed, $e(\rho)$ is convex and its derivative is $\varepsilon_{\mathrm{F}}(\rho)$).

The Hamiltonian $H^\sigma_{\Lambda \setminus A_\sigma}(V)$ is the second-quantized version of a one-body Hamiltonian, whose eigenvalues are bigger than $V_0 - 2d$. Since $\varepsilon_{\mathrm{F}}(\rho) \leqslant 2d$, we have

$$(\Upsilon, H_\Lambda(V)\Upsilon) \geqslant \sum_{\sigma=\uparrow,\downarrow} e(\rho_\sigma)|A_\sigma| + (V_0 - 4d) \times \sum_{M_\uparrow, M_\downarrow} c^2_{M_\uparrow M_\downarrow}(M_\uparrow + M_\downarrow) - 2B(A_\uparrow) - 2B(A_\downarrow). \tag{3.15}$$

The right side must be less than the upper bound for $E_\Lambda(V; N_\uparrow, N_\downarrow)$ stated in Proposition 3.1. Using $-\frac{e(\rho)}{2d} \leqslant 1$, we get Proposition 3.2. ∎

We turn to the situation where the total number of electrons is specified, but not their spins. Let $E_\Lambda(V; N)$ be the ground state energy of $H_\Lambda(V)$ with N electrons. In the proof of the following proposition we have to assume that the dimension of the system is at least 2.

Proposition 3.3. We suppose $d \geqslant 2$. Let V be a magnetic potential and N be a number, that satisfy

- $A_\uparrow \cap A_\downarrow = \emptyset$.
- $V_0 > 2d(\sqrt{d} + 1)$.
- $N \leqslant |A|$.

Let $\rho = \frac{N}{|A|} < 1$; then there exists $\bar{\alpha}(\rho) > 0$ such that

$$e(\rho)|A| - \tfrac{e(\rho)}{2d}[B(A_\uparrow) + B(A_\downarrow)] \geqslant E_\Lambda(V; N) \geqslant e(\rho)|A| + \big(\bar{\alpha}(\rho) - \gamma(V_0)\big)[B(A_\uparrow) + B(A_\downarrow)].$$

Proof. The upper bound follows from the upper bound of Proposition 3.1 that holds for all U. We can set $U = 0$ for the lower bound. Because electrons of different spins do not interact, the ground state energy is given by a sum of lowest eigenvalues of the corresponding one-body Hamiltonians for particles of given spin. Let $N_\uparrow$ be the number of spin $\uparrow$ electrons in the ground state. Taking into account multiplicities, there are $|A_\uparrow|$ available eigenvalues in $(-2d, 2d)$ for spin $\uparrow$ electrons, and $|A_\downarrow|$ eigenvalues for spin $\downarrow$ electrons. Other eigenvalues are larger than $V_0 - 2d$. Since $N \leqslant |A|$, we must have $0 \leqslant N_\uparrow \leqslant |A_\uparrow|$ and $0 \leqslant N - N_\uparrow \leqslant |A_\downarrow|$.

Let us introduce $\rho = \frac{N}{|A|}$, $\rho' = \frac{N_\uparrow}{|A|}$, and $\eta = \frac{|A_\uparrow|}{|A|}$. We have $\rho_\uparrow = \frac{\rho'}{\eta}$ and $\rho_\downarrow = \frac{\rho - \rho'}{1-\eta}$. Using the lower bound of Proposition 3.1, we obtain

$$E_\Lambda(V; N) \geqslant \big\{\eta e(\tfrac{\rho'}{\eta}) + (1-\eta)e(\tfrac{\rho-\rho'}{1-\eta})\big\}|A| + \big[\alpha(\tfrac{\rho'}{\eta}) - \gamma(V_0)\big]B(A_\uparrow) + \big[\alpha(\tfrac{\rho-\rho'}{1-\eta}) - \gamma(V_0)\big]B(A_\downarrow). \tag{3.16}$$

This bound does not hold for all ρ', but it holds when ρ' corresponds to a ground state. We get a lower bound by minimizing over ρ'. A difficulty arises, namely that the coefficient of $B(A_\uparrow)$ or of $B(A_\downarrow)$ could be negative. The term in braces reaches its minimum for $\frac{\rho'}{\eta} = \frac{\rho-\rho'}{1-\eta} = \rho$. Let ϵ be such that the minimizer for the whole right side be $\frac{\rho'}{\eta} = \rho - \frac{\epsilon}{\eta}$ (and $\frac{\rho-\rho'}{1-\eta} = \rho + \frac{\epsilon}{1-\eta}$). The fractions $\frac{\epsilon}{\eta}$ and $\frac{\epsilon}{1-\eta}$ are small, because α and γ are small. Hence ϵ is small, too. Let $f(\epsilon)$ denote the term in braces,

$$f(\epsilon) = \eta e(\rho - \tfrac{\epsilon}{\eta}) + (1-\eta) e(\rho + \tfrac{\epsilon}{1-\eta}). \tag{3.17}$$

The second derivative is

$$f''(\epsilon) = \tfrac{1}{\eta} \varepsilon_{\mathrm{F}}'(\rho - \tfrac{\epsilon}{\eta}) + \tfrac{1}{1-\eta} \varepsilon_{\mathrm{F}}'(\rho + \tfrac{\epsilon}{1-\eta}). \tag{3.18}$$

One easily verifies that $\varepsilon_{\mathrm{F}}'(\rho) \geqslant c$, with c strictly positive when $d \geqslant 2$. This implies that

$$f(\epsilon) \geqslant e(\rho) + \tfrac{c}{2\eta(1-\eta)} \epsilon^2. \tag{3.19}$$

Then

$$\begin{aligned} E_\Lambda(V; N) \;\geqslant\; & e(\rho)|A| + \tfrac{c\epsilon^2}{\eta(1-\eta)}|A| + \big[\alpha(\rho - \tfrac{\epsilon}{\eta}) - \gamma(V_0)\big] B(A_\uparrow) \\ & + \big[\alpha(\rho + \tfrac{\epsilon}{1-\eta}) - \gamma(V_0)\big] B(A_\downarrow). \end{aligned} \tag{3.20}$$

The right side should be $e(\rho)|A| + \bar{\alpha}[B(A_\uparrow) + B(A_\downarrow)]$. We must show that the brackets are strictly positive, depending on ρ and V_0, but uniformly in η. Four situations need to be carefully investigated: (1) if ρ is small and $\frac{\epsilon}{\eta} > 0$ is of the order of ρ; (2) if ρ is small and $\frac{\epsilon}{1-\eta} < 0$ is of the order of ρ; (3) if ρ is close to 1 and $\frac{\epsilon}{\eta} < 0$ is of the order of $1-\rho$; and (4) if ρ is close to 1 and $\frac{\epsilon}{1-\eta} > 0$ is of the order of ρ. These four cases are similar, so it is enough to consider case (1). The factor in front of $B(A_\downarrow)$ is bounded away from 0 because $\rho + \frac{\epsilon}{1-\eta}$ is bounded away from 0 and 1 (uniformly in η), so that $\alpha(\rho + \frac{\epsilon}{1-\eta}) > 0$ (uniformly in η). We can assume that $\frac{\epsilon}{\eta} > \frac{\rho}{2}$ (the bound is uniform in η otherwise), and we consider the factor in front of $B(A_\uparrow)$. We take advantage of the second term in $|A|$, observing that

$$\tfrac{c\epsilon^2}{\eta(1-\eta)}|A| > \tfrac{c}{1-\eta}(\tfrac{\rho}{2})^2 \eta |A|. \tag{3.21}$$

Now $\eta|A| = |A_\uparrow| \geqslant \frac{1}{2d} B(A_\uparrow)$, and we see that the factor in front of $B(A_\uparrow)$ is uniformly bounded away from zero as $\eta \to 0$. ∎

4. THE ISING APPROXIMATION

In this section we prove Theorem 2.1. Heavy electrons are static and they can be treated classically. Their state is represented by a classical spin configuration $s_\Lambda \in \{0, \uparrow, \downarrow, 2\}^\Lambda$, and the model (2.8) corresponds to a Hamiltonian, $H_\Lambda(s_\Lambda)$, acting on $\mathcal{F}_\Lambda$. The expression for $H_\Lambda(s_\Lambda)$ is given by Eq. (2.8), with the understanding that the operators $c^\dagger_{1\sigma}(x), c_{1\sigma}(x)$ act on $\mathcal{F}_\Lambda$ (instead of $\mathcal{F}_\Lambda \otimes \mathcal{F}_\Lambda$), and the operators $n_{2\sigma}(x)$ are replaced by numbers as follows:

$$n_{2\uparrow}(x) \mapsto \begin{cases} 1 & \text{if } s_x = \uparrow \\ 0 & \text{if } s_x = \downarrow, \end{cases}$$

$$n_{2\downarrow}(x) \mapsto \begin{cases} 0 & \text{if} s_x = \uparrow \\ 1 & \text{if } s_x = \downarrow. \end{cases}$$

Thus $H_\Lambda(s_\Lambda)$ is a Hubbard Hamiltonian with an external potential (or "field") given by s_Λ. It is convenient to add a constant $\frac{J}{4} - U_{12}$ to the energy so that the potential is non-negative. For given s_Λ we define the potential $V^\uparrow$ by

$$V^\uparrow_x = \begin{cases} 0 & \text{if } s_x = \uparrow \\ \frac{J}{2} & \text{if } s_x = \downarrow \\ \frac{J}{4} - U_{12} & \text{if } s_x = 0 \\ \frac{J}{4} + U_{12} & \text{if } s_x = 2. \end{cases} \tag{4.1}$$

Next, we define $V^\downarrow$ in the same way, by flipping the spins. With $N_1 = \rho_1|\Lambda|$, the Hamiltonian for the Ising–Hubbard model can be expressed using the Hamiltonian $H_\Lambda(V)$ defined in Eq. (3.1), namely

$$H_\Lambda(s_\Lambda) + (\tfrac{J}{4} - U_{12})N_1 = H_\Lambda(V) + U_2 \sum_{x\in\Lambda} \delta_{s_x,2}. \tag{4.2}$$

The strategy of our proof of Theorem 2.1 is as follows:

- A state where all electrons have spin $\uparrow$ gives us an upper bound for the ground state energy (Eq. (4.3)).
- We derive a lower bound for the ground state energy that involves "classical excitations" of s_Λ — regions where heavy particles do not have parallel spins. See Proposition 4.1.

• By combining the upper and lower bounds for the ground state energy, we find that any ground state configuration necessarily has only few excitations (see Eq. (4.5)). This suffices to prove Theorem 2.1.

Let $E(s_\Lambda; \rho_1)$ denote the ground state energy of Eq. (4.2), and let N_2 be the number of heavy electrons in s_Λ. A candidate for the ground state is a purely ferromagnetic state, where all particles have spin $\uparrow$. Heavy electrons occupy a domain $A_\uparrow$ with $|A_\uparrow| = N_2$, and they are described by the configuration $s_x = \uparrow$ for all $x \in A_\uparrow$. Light electrons also have spin $\uparrow$; electrons of identical spins do not interact, so that the ground state is given by the $\rho_1|\Lambda|$ lowest eigenstates of the hopping matrix in Λ. By the upper bound in Proposition 3.1, we have that

$$\min_{s_\Lambda} E(s_\Lambda; \rho_1) \leqslant e(\tfrac{\rho_1}{\rho_2}) N_2 + 4d N_2^{1-\frac{1}{d}}. \tag{4.3}$$

The ratio $\frac{\rho_1}{\rho_2} = \frac{N_1}{N_2}$ represents the effective density of light electrons when they all reside in $A_\uparrow$. The second term on the right side is an upper bound for the boundary contribution to the energy of an optimal domain with N_2 sites.

Next, we turn to a lower bound. It is useful to introduce

$$\xi(\rho) = \rho \varepsilon_{\mathrm{F}}(\rho) - e(\rho). \tag{4.4}$$

Notice that $0 \leqslant \xi(\rho) \leqslant 2d$, and $\xi'(\rho) = \rho \varepsilon'_{\mathrm{F}}(\rho) > 0$ so that $\xi(\rho)$ is increasing. Recall the definition (3.2) for sets $A_\uparrow$ and $A_\downarrow$ that are determined by the potential (4.1). Notice that A is the set of sites occupied by exactly one heavy particle, and that $A_\uparrow \cap A_\downarrow = \emptyset$.

Proposition 4.1. For $0 < \rho_1 < \rho_2 \leqslant 1$, there exist $J_0 < \infty$ and $\widetilde{\alpha} > 0$ (both independent of Λ) such that if $\frac{J}{4} - U_{12} > J_0$, we have that

$$E(s_\Lambda; \rho_1) \geqslant e(\tfrac{\rho_1}{\rho_2}) N_2 + \big[\xi(\tfrac{\rho_1}{\rho_2}) + \tfrac{1}{2} U_2\big](N_2 - |A|) + \widetilde{\alpha}\big[B(A_\uparrow) + B(A_\downarrow)\big],$$

for arbitrary s_Λ.

Remark. A similar bound can be proven when $0 < \rho_1 < 2 - \rho_2 \leqslant 1$.

One main consequence of Proposition 4.1 can be obtained by combining it with the upper bound Eq. (4.3). We get

$$\begin{cases} |A| \geqslant N_2(1 - \mathrm{const} \cdot N_2^{-1/d}) \\ B(A_\uparrow) + B(A_\downarrow) \leqslant \mathrm{const} \cdot N_2^{1-\frac{1}{d}} \end{cases} \tag{4.5}$$

for constants that are uniform in the size of the system. These inequalities imply Theorem 2.1, as is shown below.

Proof of Proposition 4.1. We observe that $\sum_x \delta_{s_x,2} = \frac{1}{2}(N_2 - |A|)$ yielding the term involving U_2. To alleviate our notation we suppose now that $U_2 = 0$. Let $\zeta > 0$ be a small number; we first consider configurations such that $\frac{N_1}{|A|} \leqslant 1 - \zeta$. Proposition 3.3 gives

$$E(s_\Lambda; \rho_1) \geqslant e\left(\frac{N_1}{|A|}\right)|A| + \left(\bar{\alpha}\left(\frac{N_1}{|A|}\right) - \gamma\left(\frac{J}{4} - U_{12}\right)\right)[B(A_\uparrow) + B(A_\downarrow)]. \quad (4.6)$$

The function $\nu e(\frac{\rho}{\nu})$ is convex in ν, and its derivative with respect to ν is equal to $-\xi(\frac{\rho}{\nu})$. Therefore

$$e\left(\frac{N_1}{|A|}\right)|A| = e\left(\frac{\rho_1}{\rho_2}\frac{N_2}{|A|}\right)\frac{|A|}{N_2}N_2 \geqslant e\left(\frac{\rho_1}{\rho_2}\right)N_2 + \xi\left(\frac{\rho_1}{\rho_2}\right)(N_2 - |A|). \quad (4.7)$$

Since $\frac{N_1}{|A|} < 1 - \zeta$ the function $\bar{\alpha}\left(\frac{N_1}{|A|}\right)$ is uniformly bounded away from zero, and we obtain a strictly positive $\tilde{\alpha}$, provided $\frac{J}{4} - U_{12}$ is large enough (see Proposition 3.1).

We now consider configurations such that $1 - \zeta < \frac{N_1}{|A|} \leqslant 1$. Equation (4.6) is still valid but $\bar{\alpha}\left(\frac{N_1}{|A|}\right)$ may be very small and we ignore it; it is positive. Convexity of $e(\rho)$ yields

$$e\left(\frac{N_1}{|A|}\right) \geqslant e(1) + \left(\frac{N_1}{|A|} - 1\right)\varepsilon_{\mathrm{F}}(1) \geqslant -2d\zeta. \quad (4.8)$$

We have used that $e(1) = 0$ and $\varepsilon_{\mathrm{F}}(1) = 2d$. Because $B(A_\uparrow) + B(A_\downarrow) \leqslant 2d|A|$, we obtain from Eq. (4.6)

$$E(s_\Lambda; \rho_1) \geqslant -2d\left[\zeta + \gamma\left(\frac{J}{4} - U_{12}\right) + \tilde{\alpha}\right]|A| + \tilde{\alpha}\left[B(A_\uparrow) + B(A_\downarrow)\right]. \quad (4.9)$$

In order to complete the proof of Proposition 4.1, we need to check that

$$-2d\left[\zeta + \gamma\left(\frac{J}{4} - U_{12}\right) + \tilde{\alpha}\right]|A| \geqslant e\left(\frac{\rho_1}{\rho_2}\right)N_2 + \xi\left(\frac{\rho_1}{\rho_2}\right)(N_2 - |A|). \quad (4.10)$$

We have that $N_2 - |A| = N_2[1 - \frac{\rho_1}{\rho_2}\frac{|A|}{N_1}] = N_2[1 - \frac{\rho_1}{\rho_2} + O(\zeta)]$. As $|A| \leqslant N_2$ and because the term in brackets can be arbitrary small (depending on ρ_1, ρ_2), it is enough to check that

$$0 > e\left(\frac{\rho_1}{\rho_2}\right) + \xi\left(\frac{\rho_1}{\rho_2}\right)\left(1 - \frac{\rho_1}{\rho_2}\right). \quad (4.11)$$

Using the definition (4.4) of ξ, the condition can be reduced to $\xi(\rho) - \varepsilon_F(\rho) > 0$ for $0 < \rho < 1$. This is easy to verify, as this function is strictly decreasing and $\xi(1) - \varepsilon_F(1) = 0$.

Finally, the case where $N_1 > |A|$ is easy because we can use Proposition 4.1 for the lowest $|A|$ eigenvalues, and remaining eigenvalues are larger than $\frac{J}{4} - U_{12} - 2d \geqslant 0$. ∎

Proof of Theorem 2.1. We have established inequalities (4.5) that show that ground state configurations of heavy electrons consist of large domains with one particle of spin $\uparrow$ at each site, large domains with one particle of spin $\downarrow$, or domains void of particles. Boundaries of these domains are "sparse". Recall that definition (2.7) of the magnetization $m_{\Lambda,\Lambda'}$ involves an average over translates of Λ'. It is enough to restrict to boxes that are fully in $A_\uparrow$ or in $A_\downarrow$. Indeed, few boxes are intersecting their boundaries, and there are virtually no electrons outside of A.

It is clear that $m^{(3)}_{\Lambda,\Lambda'} \leqslant \frac{\rho_1+\rho_2}{2}$ for all states with densities ρ_1 and ρ_2 of light and heavy electrons, so that it suffices to establish the converse inequality. The definition of $m^{(3)}_{\Lambda,\Lambda'}$ involves a sum over translates of Λ' that are inside Λ. All terms are positive, so we get a lower bound by restricting the sum to translates that are contained in either $A_\uparrow$ or $A_\downarrow$:

$$\sum_{x:\Lambda'+x\subset\Lambda} \left|(\Upsilon, M^{(3)}_{\Lambda'+x}\Upsilon)\right| \geqslant \sum_{x:\Lambda'+x\subset A_\uparrow} (\Upsilon, M^{(3)}_{\Lambda'+x}\Upsilon) - \sum_{x:\Lambda'+x\subset A_\downarrow} (\Upsilon, M^{(3)}_{\Lambda'+x}\Upsilon). \tag{4.12}$$

Let us recall the definition of $M^{(3)}_{\Lambda'}$:

$$M^{(3)}_{\Lambda'} = \sum_{x\in\Lambda'} M^{(3)}(x), \tag{4.13}$$

with

$$M^{(3)}(x) = \tfrac{1}{2} \sum_{a=1,2} \big(n_{a\uparrow}(x) - n_{a\downarrow}(x)\big). \tag{4.14}$$

Since $\|M^{(3)}(x)\| \leqslant 1$, we have from Eq. (4.12)

$$\sum_{x:\Lambda'+x\subset\Lambda} (\Upsilon, |M^{(3)}_{\Lambda'+x}|\Upsilon) \geqslant \sum_{x\in A_\uparrow} (\Upsilon, M^{(3)}(x)\Upsilon) - \sum_{x\in A_\downarrow} (\Upsilon, M^{(3)}(x)\Upsilon) - |\Lambda'|[B(A_\uparrow) + B(A_\downarrow)]. \tag{4.15}$$

Let $N_{1\uparrow} = \sum_{x\in\Lambda}(\Upsilon, n_{1\uparrow}(x)\Upsilon)$; then

$$\sum_{x\in A_\uparrow}(\Upsilon, M^{(3)}(x)\Upsilon) = \tfrac{1}{2}|A_\uparrow| + \tfrac{1}{2}N_{1\uparrow} - \sum_{x\notin A_\uparrow}(\Upsilon, n_{1\uparrow}(x)\Upsilon). \tag{4.16}$$

The latter term is less than $\frac{3}{\frac{J}{4}-U_{12}-4d}B(A_\uparrow)$ by Proposition 3.2. The same argument applies to spin $\downarrow$ electrons. Using inequalities (4.5), we see that $m_{\Lambda,\Lambda'}$ is larger than $\frac{1}{2}\rho_2 + \frac{1}{2}\rho_1$, up to a term of order $|\Lambda|^{-1/d}$ (it depends on Λ'). This term vanishes in the limit $\Lambda \nearrow \mathbb{Z}^d$. ∎

5. THE ASYMMETRIC HUND–HUBBARD MODEL

We now turn to the proof of Theorem 2.2. The asymmetric Hund–Hubbard model (2.9) can be expressed as a perturbation of the Ising–Hubbard model (2.8). Namely, with $t_1 = 1$,

$$\begin{aligned} H_\Lambda^{\mathrm{aHH}} = H_\Lambda^{\mathrm{IH}} &- t_2 \sum_{\sigma=\uparrow,\downarrow} \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} c_{2\sigma}^\dagger(x)c_{2\sigma}(y) \\ &- J^\perp \sum_{x\in\Lambda}\left[S_1^{(1)}(x)S_2^{(1)}(x) + S_1^{(2)}(x)S_2^{(2)}(x)\right]. \end{aligned} \tag{5.1}$$

In the previous section we showed that any ground state configuration of the Ising–Hubbard model satisfies inequalities Eq. (4.5). Heavy electrons are now quantum particles and a classical configuration cannot be an eigenstate. We can extend Eq. (4.5) by expanding the ground state in the basis of configurations of heavy particles, and show that Eq. (4.5) holds in average. Namely, we denote by $\Phi(s_\Lambda) \in \mathcal{F}_\Lambda$ the normalized state of heavy electrons in the configuration s_Λ. Clearly, $(\Phi(s_\Lambda))$ is a basis of $\mathcal{F}_\Lambda$. Any state $\Upsilon \in \mathcal{F}_\Lambda \otimes \mathcal{F}_\Lambda$ has a unique decomposition as

$$\Upsilon = \sum_{s_\Lambda} c(s_\Lambda)\Psi(s_\Lambda)\otimes\Phi(s_\Lambda), \tag{5.2}$$

where $c(s_\Lambda) \geqslant 0$ satisfies $\sum_{s_\Lambda} c^2(s_\Lambda) = 1$, and $\Psi(s_\Lambda)$ is *some* normalized state that represents the light particles. Notice the asymmetry in notation: $\Psi(s_\Lambda)$ is indexed by s_Λ, but the configuration of spins of light particles may be very different from the configuration s_Λ, in general. In particular, $\Psi(s_\Lambda)$ describes a state with N_1 particles, while $\Phi(s_\Lambda)$ has N_2 particles. Let $X(s_\Lambda)$ denote the number of "excitations" of s_Λ; namely,

$$X(s_\Lambda) = (N_2 - |A|) + B(A_\uparrow) + B(A_\downarrow). \tag{5.3}$$

The extension of Eq. (4.5) is as follows.

Proposition 5.1. Let $d \geqslant 2$, and $0 < \rho_1 < \rho_2 \leqslant 1$. There are constants $J_0 < \infty$ and $\gamma > 0$ such that if $\frac{J}{4} - U_{12} > J_0$ and $t_2, J^\perp < \gamma$, and if $c(s_\Lambda)$ are the coefficients defined in Eq. (5.2) for a ground state of H_Λ^{aHH}, we have

$$\sum_{s_\Lambda} c^2(s_\Lambda) X(s_\Lambda) \leqslant \mathrm{const} \cdot N_2^{1-\frac{1}{d}},$$

for a constant that is independent of Λ.

Proof. We again define V by Eq. (4.1) and $H_\Lambda(V)$ by Eq. (4.2). U_2 plays no rôle here, just as in Section 4; so we set it to 0 from now on. By the variational principle we find an upper bound for the ground state energy by considering a state where all electrons have spin $\uparrow$. Heavy electrons are packed together and light ones are in appropriate delocalized wave functions with support on $A_\uparrow$. Neither the t_2 term nor the $J^\perp$ term contributes to the energy of this state, and Eq. (4.3) therefore continues to be an upper bound for the ground state energy.

The goal is now to find a lower bound with the same bulk term as in the equation above, plus a correction that involves the average of $X(s_\Lambda)$. For Υ expanded as in (5.2), we have

$$\begin{aligned}
(\Upsilon, H_\Lambda^{\mathrm{aHH}}\Upsilon) + (\tfrac{J}{4} - U_{12})N_1 = {} & \sum_{s_\Lambda} c^2(s_\Lambda)\Big(\Psi(s_\Lambda), H_\Lambda(V)\Psi(s_\Lambda)\Big) \\
& - t_2 \sum_{s_\Lambda, s'_\Lambda} \sum_{\sigma=\uparrow,\downarrow} \sum_{\substack{x,y\in\Lambda \\ |x-y|=1}} c(s_\Lambda)c(s'_\Lambda)\Big(\Psi(s_\Lambda), \Psi(s'_\Lambda)\Big) \\
& \times \Big(\Phi(s_\Lambda), c_{2\sigma}^\dagger(x)c_{2\sigma}(y)\Phi(s'_\Lambda)\Big) \\
& - J^\perp \sum_{s_\Lambda, s'_\Lambda} \sum_{x\in\Lambda} c(s_\Lambda)c(s'_\Lambda)\Big(\Psi(s_\Lambda)\otimes\Phi(s_\Lambda), \\
& \qquad \big[S_1^{(1)}(x)S_2^{(1)}(x) + S_1^{(2)}(x)S_2^{(2)}(x)\big]\Psi(s'_\Lambda)\otimes\Phi(s'_\Lambda)\Big).
\end{aligned} \tag{5.4}$$

The first term involves the same $H_\Lambda(V)$ that appears in Eq. (4.2); this gives us the right bulk contribution. The other two terms are actually irrelevant and it is enough to find estimates.

We observe that the second term on the right side of Eq. (5.4) is less than

$$t_2 \sum_{s_\Lambda, s'_\Lambda}{}' c(s_\Lambda) c(s'_\Lambda) \leqslant t_2 \Big(\sum_{s_\Lambda, s'_\Lambda}{}' c^2(s_\Lambda) \Big)^{1/2} \Big(\sum_{s_\Lambda, s'_\Lambda}{}' c^2(s'_\Lambda) \Big)^{1/2} = t_2 \sum_{s_\Lambda, s'_\Lambda}{}' c^2(s_\Lambda). \tag{5.5}$$

Primed sums are over configurations that are identical except for a heavy electron moved to a neighboring site. Given s_Λ, there are less than $2d(N_2 - |A|) + B(A_\uparrow) + B(A_\downarrow)$ such configurations s'_Λ (recall that $\frac{1}{2}(N_2 - |A|)$ is the number of sites that are occupied by two heavy electrons). It follows that Eq. (5.5) is smaller than $2dt_2 \sum_{s_\Lambda} c^2(s_\Lambda) X(s_\Lambda)$ (and it is larger than the negative of this expression).

The third term of the right side of Eq. (5.4) can be treated in the same spirit. It is necessary to cast the perpendicular Hund interactions in a form that shows that their contribution is no more than the boundary between domains of identical spins. We therefore introduce standard operators $S_a^{(+)}(x)$, $S_a^{(-)}(x)$, by

$$\begin{aligned} S_a^{(+)}(x) &= S_a^{(1)}(x) + \mathrm{i} S_a^{(2)}(x), \\ S_a^{(-)}(x) &= S_a^{(1)}(x) - \mathrm{i} S_a^{(2)}(x). \end{aligned} \tag{5.6}$$

Perpendicular spin interactions become

$$S_1^{(1)}(x) S_2^{(1)}(x) + S_1^{(2)}(x) S_2^{(2)}(x) = \tfrac{1}{2} \big[S_1^{(+)}(x) S_2^{(-)}(x) + S_1^{(-)}(x) S_2^{(+)}(x) \big]. \tag{5.7}$$

Let $x \in A$, and s_Λ^x be the configuration obtained from s_Λ by flipping the spin at x. The third term of Eq. (5.4) is equal to

$$-\tfrac{1}{2} J^\perp \sum_{s_\Lambda} \sum_{x \in A} c(s_\Lambda) c(s_\Lambda^x) \Big(\Psi(s_\Lambda), S_1^{(\#)}(x) \Psi(s_\Lambda^x) \Big), \tag{5.8}$$

with #="+" if $s_x = \downarrow$, and #="−" if $s_x = \uparrow$. Since $S_1^{(+)}(x) = c_{1\uparrow}^\dagger(x) c_{1\downarrow}(x)$, the Schwarz inequality yields the bound

$$\Big| \Big(\Psi(s_\Lambda), S_1^{(+)}(x) \Psi(s_\Lambda^x) \Big) \Big| \leqslant \Big(\Psi(s_\Lambda), n_{1\uparrow}(x) \Psi(s_\Lambda) \Big)^{1/2} \Big(\Psi(s_\Lambda^x), n_{1\downarrow}(x) \Psi(s_\Lambda^x) \Big)^{1/2}. \tag{5.9}$$

A similar inequality holds when $S_1^{(+)}(x)$ is replaced with $S_1^{(-)}(x)$; one should simply interchange $n_{1\uparrow}(x)$ and $n_{1\downarrow}(x)$ on the right side. Then echoing Eq. (5.5), the absolute value of Eq. (5.8) is found to be smaller than

$$\tfrac{J^\perp}{2}\Big[\sum_{s_\Lambda}\sum_{x\in A} c^2(s_\Lambda)\Big(\Psi(s_\Lambda), n_{1,-s_x}(x)\Psi(s_\Lambda)\Big)\Big]^{1/2} \cdot \Big[\sum_{s_\Lambda}\sum_{x\in A} c^2(s_\Lambda^x)\Big(\Psi(s_\Lambda^x), n_{1,s_x}(x)\Psi(s_\Lambda^x)\Big)\Big]^{1/2} = \tfrac{J^\perp}{2}\sum_{s_\Lambda}\sum_{x\in A} c^2(s_\Lambda)\Big(\Psi(s_\Lambda), n_{1,-s_x}(x)\Psi(s_\Lambda)\Big). \quad (5.10)$$

This expression is reminiscent of the expression in Proposition 3.2. However, $\Psi(s_\Lambda)$ is *not* a ground state for light electrons in the magnetic potential given by s_Λ and therefore the proposition does not directly apply.

We can nevertheless recycle the ideas underlying the proof of Proposition 3.2.

Let $\mathcal{N} = (N_\uparrow, N_\downarrow, M_\uparrow, M_\downarrow)$ be four positive integers such that $N_\uparrow + N_\downarrow = N_1$, and $M_\sigma \leqslant N_\sigma$. N_σ is the number of light electrons of spin σ, and M_σ is the number of light electrons of spin σ that are not localized on the favorable sites A_σ. We can expand $\Psi(s_\Lambda)$ according to $\mathcal{N}$, in a fashion that is reminiscent of Eq. (3.10),

$$c(s_\Lambda)\Psi(s_\Lambda) = \sum_{\mathcal{N}} c_{\mathcal{N}}(s_\Lambda)\Psi_{\mathcal{N}}(s_\Lambda) \quad (5.11)$$

where coefficients are positive and states are normalized. With this notation we observe that Eq. (5.10) is bounded above by the following expression similar to Eq. (3.11)

$$\tfrac{J^\perp}{2}\sum_{s_\Lambda}\sum_{\mathcal{N}} c^2_{\mathcal{N}}(s_\Lambda)(M_\uparrow + M_\downarrow). \quad (5.12)$$

The Hamiltonian $H_\Lambda(V)$ can be split as in Eq. (3.12) and we obtain the lower bound Eq. (3.13) with $c(s_\Lambda)\Psi(s_\Lambda)$ in lieu of Υ, and $c_{\mathcal{N}}(s_\Lambda)\Psi_{\mathcal{N}}(s_\Lambda)$ in lieu of $c_{M_\uparrow M_\downarrow}\Upsilon_{M_\uparrow M_\downarrow}$. We then get Eqs. (3.14) and (3.15). Explicitly, the lower bound for Eq. (5.4) is

$$e(\tfrac{\rho_1}{\rho_2})N_2 + \sum_{s_\Lambda}\sum_{\mathcal{N}} c^2_{\mathcal{N}}(s_\Lambda) \times\Big\{(\tfrac{J}{4} - U_{12} - 4d - \tfrac{J^\perp}{2})(M_\uparrow + M_\downarrow) - 2B(A_\uparrow) - 2B(A_\downarrow) - 2dt_2 X(s_\Lambda)\Big\}.$$

The bulk term $e(\frac{\rho_1}{\rho_2})N_2$ above comes from Eq. (3.15), minimizing over $N_\uparrow$ and $N_\downarrow$. This expression is less than the upper bound Eq. (4.3); this implies that

$$\sum_{s_\Lambda}\sum_{\mathcal{N}} c^2_{\mathcal{N}}(s_\Lambda)(M_\uparrow + M_\downarrow) \leqslant \frac{4d+2+2dt_2}{\frac{J}{4}-U_{12}-4d-\frac{J^\perp}{2}} \sum_{s_\Lambda} c^2(s_\Lambda)X(s_\Lambda). \tag{5.13}$$

(We used that $N_2^{1-\frac{1}{d}} \leqslant X(s_\Lambda)$.) Notice that the factor on the right side is small. This estimate is necessary to bound Eq. (5.12).

Using Proposition 4.1 for the first term in Eq. (5.4), we then conclude that

$$\sum_{s_\Lambda} c^2(s_\Lambda)\Big(\Psi(s_\Lambda), H_\Lambda(V)\Psi(s_\Lambda)\Big) \geqslant e(\tfrac{\rho_1}{\rho_2})N_2 + \widetilde{\alpha}\sum_{s_\Lambda} c^2(s_\Lambda)X(s_\Lambda). \tag{5.14}$$

(We assume here that $\widetilde{\alpha}$ is smaller than $\xi(\frac{\rho_1}{\rho_2}) + \frac{1}{2}U_2$.) Again invoking the upper bound Eq. (4.3), we obtain

$$\begin{aligned} e(\tfrac{\rho_1}{\rho_2})N_2 + 4dN_2^{1-\frac{1}{d}} \;\geqslant\; & e(\tfrac{\rho_1}{\rho_2})N_2 + \Big[\widetilde{\alpha} - 2dt_2 - \frac{J^\perp}{2}\,\frac{4d+2+2dt_2}{\frac{J}{4}-U_{12}-4d-\frac{J^\perp}{2}}\Big] \\ & \times \sum_{s_\Lambda} c^2(s_\Lambda)X(s_\Lambda). \end{aligned} \tag{5.15}$$

The quantity in brackets is strictly positive when $\frac{J}{4} - U_{12}$ is large enough, and this proves Proposition 5.1. ∎

Proof of Theorem 2.2. The proof is similar to that of Theorem 2.1, except that we use Proposition 5.1 instead of the inequalities Eq. (4.5). All equations until Eq. (4.14) hold without change. Eqs. (4.15) and (4.16) need to be modified because the A_σ's are not fixed here. These equations hold when averaged over s_Λ with weights $c^2(s_\Lambda)$. We obtain

$$\begin{aligned} \sum_{x,\Lambda'+x\subset\Lambda} (\Upsilon, |M^{(3)}_{\Lambda'+x}|\Upsilon) &\geqslant \sum_{s_\Lambda}\sum_{\mathcal{N}} c^2_{\mathcal{N}}(s_\Lambda) \sum_\sigma \Big[\tfrac{1}{2}|A_\sigma| + \tfrac{1}{2}N_\sigma - \tfrac{1}{2}M_\sigma - |\Lambda'|B(A_\sigma)\Big] \\ &\geqslant \tfrac{1}{2}(N_1+N_2) - 2|\Lambda'|\sum_{s_\Lambda} c^2(s_\Lambda)X(s_\Lambda). \end{aligned} \tag{5.16}$$

We have used Eq. (5.13) in order to estimate the contribution of $M_\uparrow$ and $M_\downarrow$. After division by $|\Lambda|$, the last term vanishes in the thermodynamic limit by Proposition 5.1. ∎

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REFERENCES

1. P. W. Anderson, New approach to the theory of superexchange interactions, *Phys. Rev.* **115**:2–13 (1959).
2. V. Bach, E. H. Lieb, and J. P. Solovej, Generalized Hartree-Fock theory and the Hubbard model, *J. Stat. Phys.* **76**:3–90 (1994).
3. V. Bach, E. H. Lieb, and M. V. Travaglia, in preparation.
4. U. Brandt and R. Schmidt, Exact results for the distribution of the f-level ground state occupation in the spinless Falicov-Kimball model, *Z. Phys. B* **63**:45–53 (1986).
5. N. Datta, R. Fernández, and J. Fröhlich, Effective Hamiltonians and phase diagrams for tight-binding models, *J. Stat. Phys.* **96**:545–611 (1999).
6. N. Datta, R. Fernández, J. Fröhlich, and L. Rey-Bellet, Low-temperature phase diagrams of quantum lattice systems. II. Convergent perturbation expansion ans stability in systems with infinite degeneracy, *Helv. Phys. Acta* **69**:752–820 (1996).
7. J. K. Freericks, E. H. Lieb, and D. Ueltschi, Segregation in the Falicov-Kimball model, *Commun. Math. Phys.* **227**:243–79 (2002), Phase separation due to quantum mechanical correlations, *Phys. Rev. Lett.* **88**:106401 (2002).
8. P. S. Goldbaum, Lower bound for the segregation energy in the Falicov-Kimball model, *J. Phys. A* **36**:2227–34 (2003).
9. K. Held and D. Vollhardt, Microscopic conditions favoring itinerant ferromagnetism: Hund's rule coupling and orbital degeneracy, *Eur. Phys. J. B* **5**:473 (1998).
10. K. Held and D. Vollhardt, Electronic correlations in manganites, *Phys. Rev. Lett.* **22**:5168–5171 (2000).
11. T. Kennedy and E. H. Lieb, An itinerant electron model with crystalline or magnetic long range order, *Physica A* **138**:320–358 (1986).
12. A. Mielke and H. Tasaki, Ferromagnetism in the Hubbard model, *Commun. Math. Phys.* **158**:341–371 (1993).
13. H. Tasaki, Ferromagnetism in the Hubbard model: A constructive approach, *Commun. Math. Phys.* **242**:445–472 (2003).
14. M.-T. Tran, Charge ordered ferromagnetic phase in manganites, *Phys. Rev. B* **67**:144404 (2003).
15. D. Ueltschi, Segregation in the asymmetric Hubbard model, *J. Stat. Phys.* **116**:681–697 (2004).