The Hubbard Model

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Abstract

The present work contains a summary of a talk given in the seminar on statistical physics in summer term 2018 at Heidelberg University organized by Andreas Mielke. The Hubbard model is discussed as a simple model in solid state physics describing electron movement on lattices including correlations. After explaining origin, basic properties and symmetries of the model a solution of the Hubbard model with vanishing interaction U is presented and in a mean-field approach the occurence of ferromagnetism is shown. Ferromagnetism in the Hubbard model, however, is a delicate matter and only available under very strong assumptions. Two theorems, the Nagaoka theorem and Lieb's theorem, allowing for ferromagnetic or ferrimagnetic ordering in the Hubbard model are finally presented and proven.

Contents

1 Introduction

The Hubbard model is one of the simplest models incorporating electron-electron correlations in solids. Originally, it was proposed by John Hubbard [1] in 1963 in order to describe the behavior of transition metals. While non local band theory captures the behavior of the outermost electrons in simple metals as alkali earths, the partially filled f shells of rare earth elements can be described to good approximation on a local atomic basis. The partially filled d shells of transition metals, however, show properties of both, band theory and local electron-electron correlations, which lead to rich physical behavior. Among them are the high temperature ferromagnetic materials iron, cobalt and nickel. Thus, understanding the peculiar properties of transition metals may open a path to solve the age-old problem of ferromagnetism. But apart from ferromagnetism the Hubbard model exhibits many more interesting phenomena one can observe in solids: Amongst them a metal-insulator transition, (high T_c) superconductivity and Tomonaga-Luttinger liquids in one dimension. Because covering all interesting properties which may arise would need a course on its own, we will focus on ferromagnetism and some rigorous results concerned with its occurence in the Hubbard model.

The Hamiltonian of the Hubbard model is given by:

Definition 1.1.

$$H = H_{\text{kin}} + H_{\text{int}} = \sum_{x,y\in\Lambda} \sum_{\sigma\in\{\uparrow,\downarrow\}} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} + \sum_{x\in\Lambda} U_x c^\dagger_{x\uparrow} c_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} \tag{1}$$

Here, the $c^\dagger_{x\sigma}$/ $c_{x\sigma}$-operators are the creation and annihilation operators of electrons at lattice sites x on the lattice Λ with spin $\sigma \in \{\frac{1}{2}, -\frac{1}{2}\}$. As representing fermions they obey the canonical anticommutation relations:

$$\{c_{x,\sigma}, c^\dagger_{y,\sigma'}\} = \delta_{xy}\delta_{\sigma\sigma'} \ , \quad \{c_{x,\sigma}, c_{y,\sigma'}\} = \{c^\dagger_{x,\sigma}, c^\dagger_{y,\sigma'}\} = 0 \tag{2}$$

where $\{\cdot,\cdot\}$ denotes the anticommutator. The first term connects different lattice sites via a hopping matrix $(t_{xy})_{x,y\in\Lambda}$. Usually, we assume this matrix to be real and symmetric which is consistent with the interpretation of its entries as overlap integrals of localized, real orbitals. The second term of the Hamiltonian allows for an interaction between electrons being on the same lattice site. Since we would like to model short ranged electron correlations due to Coulomb interaction we usually assume $U_x > 0$. Note that every site can either be vacant, singly occupied by one up or down spin, or doubly occupied by one up **and** one down spin due to the Pauli principle ($(c^\dagger_{x\sigma})^2 = 0$). Moreover, we should mention that one can construct states in the Hilbert space by successively applying the creation operators on the vacuum state $|0>$ ($c_{x\sigma}|0>= 0\ \forall x, \sigma$).
The Hubbard model has several properties and symmetries we want to discuss. First of all, the Hamiltonian (1) commutes with both, the number op. of spin up and spin down particles
($N_{\uparrow(\downarrow)} = \sum_x n_{x\uparrow(\downarrow)}$ with $n_{x\sigma} = c^\dagger_{x\sigma} c_{x\sigma}$), as well as with the total number (op.) of electrons $N_e = N_\uparrow + N_\downarrow$ which means that all three are conserved:

$$[H, N_\uparrow] = [H, N_\downarrow] = [H, N_e] = 0 \tag{3}$$

Therefore, N_e is a fixed quantum number of the model with $0 \leq N_e \leq 2|\Lambda|$ and different subspaces with constant $N_\uparrow$/ $N_\downarrow$ can be considered separately.

Let us now define local and global spin operators:

$$S_{i,x} = \frac{1}{2}\sum_{\alpha,\beta} c^\dagger_{x\alpha}(\sigma_i)_{\alpha\beta}c_{x\beta} \quad , \quad \mathbf{S}_x = (S_{x,x}, S_{y,x}, S_{z,x}) \tag{4}$$

$$S_i = \sum_{x\in\Lambda} S_{i,x} \quad , \quad \mathbf{S} = (S_x, S_y, S_z) \tag{5}$$

where in eq. (4) the first index denotes the vector index of the spin and the second on which lattice site it acts. σ_i are the Pauli matrices with $i \in \{x, y, z\}$. The Hamiltonian has a global $SU(2)$ symmetry which means that it commutes with all global spin operators:

$$[H, S_i] = \left[H, \mathbf{S}^2\right] = 0 \quad \forall i \in \{x, y, z\} \tag{6}$$

This property is quite important for many of the results discussed later as well as for such theorems as the Mermin-Wagner-Hohenberg theorem which will be discussed in another talk. Furthermore, one can show that the standard representation theory for spins (known from quantum mechanics) can be applied to this model and due to the fact that H, S_z and $\mathbf{S}^2$ commute with each other, we can simultaneously diagonalize them. $S(S+1)$ is the eigenvalue of $\mathbf{S}^2$ where S is the total spin of the state with $S = 0, 1, 2, ..., S_{max}$ (if N_e is even) or $\frac{1}{2}, \frac{3}{2}, ..., S_{max}$ (if N_e is odd). S_{max} is the maximal spin a state can have in this model where $S_{max} = \frac{N_e}{2}$ for $0 \leq N_e \leq |\Lambda|$ and $S_{max} = |\Lambda| - \frac{N_e}{2}$ for $|\Lambda| \leq N_e \leq 2|\Lambda|$ because of the Pauli principle.

There is another symmetry of the Hubbard model (so-called particle-hole symmetry) on bibartite lattices at half-filling ($N_e = |\Lambda|$). A bipartite lattice is defined as follows:

Definition 1.2. A lattice Λ is said to be bibartite if there are sublattices $A, B \subseteq \Lambda$ such that $t_{xy} = 0$ for $x, y \in A$ or $x, y \in B$.

Note that this kind of lattice is very conducive to antiferromagnetic order and ferrimagnetism for $|A| \neq |B|$ (see chapter 4). The transformation that leaves the Hamiltonian unchanged in such circumstances is a **particle-hole transformation (PHT)** combined with a sign change of the creation and annihilation operators on just one of the two sublattices A, B:

$$c_{x\sigma} \mapsto \epsilon(x)c^\dagger_{x\sigma} \quad , \epsilon(x) = \begin{cases} 1 & \text{if } x \in A \\ -1 & \text{if } x \in B \end{cases} \tag{7}$$

The particle-hole transformation interchanges the role of creation and annihilation operators and therefore, it also interchanges the occupancy of the sites:

$$n_{x\sigma} = c^\dagger_{x\sigma}c_{x\sigma} \overset{PHT}{\mapsto} c_{x\sigma}c^\dagger_{x\sigma} \overset{anticom.}{=} 1 - c^\dagger_{x\sigma}c_{x\sigma} = 1 - n_{x\sigma} \tag{8}$$

With a brief calculation one can show that the Hamiltonian transforms under (7) as follows:

$$H \mapsto H_{kin} + U\sum_x (1 - c^\dagger_{x\uparrow}c_{x\uparrow})(1 - c^\dagger_{x\downarrow}c_{x\downarrow}) = H + U(|\Lambda| - N_e), \tag{9}$$

i.e. for half-filling we get indeed a particle-hole symmetry.
Finally, we have to define **ferromagnetism** since this is the physical property we will focus on in the following: The Hubbard model exhibits ferromagnetism if **every** ground state of H has the total spin $S = S_{max}$ (see [3] for more details).

2 Mean Field Theory

Like for the study of the Ising Model, we use the mean field approximation to get more insight which physical phenomena the Hubbard model exhibits. In order to analyize the **one dimensional** Hubbard model with this approximation, we first consider the non-interacting limit $U = 0$:

$$H = -t \sum_{<x,y>,\sigma} c^\dagger_{x\sigma} c_{y\sigma} \tag{10}$$

Here, we assumed $t_{xy} = -t \; \forall x, y \in \Lambda$ and considered only nearest neighbor (n.n.) hopping. Since this Hamiltonian is a quadratic form in the $c^\dagger/c$-operators, we can in principle diagonalize it. For that, we consider the canonical transformation $c^\dagger_{k\sigma} = N^{-1/2} \sum_x e^{ikx} c^\dagger_{x\sigma}$, where $c^\dagger_{k\sigma}$ are the creation operators in discrete momentum space. By plugging in the inverted expression $c^\dagger_{x\sigma} = N^{-1/2} \sum_k e^{-ikx} c^\dagger_{k\sigma}$ and using the orthogonality relation $N^{-1} \sum_x e^{ix(l-k)} = \delta_{kl}$, we arrive at:

$$H = \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} = \sum_{k,\sigma} \epsilon_k n_{k\sigma} \quad \text{with} \quad \epsilon_k = -t \sum_x e^{ika_x} \tag{11}$$

Here, we used the n.n. distance $a_x = x - y$. Using periodic boundary conditions in one dimension with $a = 1$, one finds the single-electron energy levels to be
$\epsilon_k = -2t \cdot cos(k)$ $(k \in 2\pi/N\{0, \pm 1, ..., \pm N/2\})$, whereas they belong to the eigenstates $N^{-1/2} e^{ikx}$ (plane waves). Now, the Hamiltonian looks like the one that describes the q. m. harmonic oscillator (sum of independent number operators) and we immediately see that the single-electron energies ϵ_k contain the whole information for calculating the energies of many-particle states: The many-particle ground state can be obtained by filling up the lowest single-particle energy levels obeying the Pauli principle (see Fig. 1). Therefore, it is easy to see that this ground state (if there is no bulk degeneracy) is neither ferromagnetic nor does it have long range order (so-called Pauli Paramagnetism, see [2]).

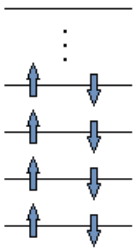

Figure 1: Paramagnetic ground state of the $U = 0$ -limit: Lowest single-particle states are successively filled with electrons, obeying the Pauli principle.

Although the $t = 0$-limit also exhibits paramagnetism ([2]), we will see in the following that the combination of H_{kin} **and** H_{int} is able to produce ferromagnetism. We start with the ansatz $n_{x\uparrow(\downarrow)} = < n_{\uparrow(\downarrow)} > + (n_{x\uparrow(\downarrow)} - < n_{\uparrow(\downarrow)} >)$ and calculate:

$$n_{x\uparrow} n_{x\downarrow} \approx n_{x\uparrow} < n_\downarrow > + n_{x\downarrow} < n_\uparrow > - < n_\uparrow >< n_\downarrow > \tag{12}$$

Here, we neglected the quadratic deviation from the site-independent mean value $< n_{\uparrow(\downarrow)} >$. By plugging in this approximation in H_{int}, we arrive at the following (now quadratic) Hamiltonian:

$$\begin{aligned} H &= -t \sum_{x,\sigma} (c^\dagger_{x\sigma} c_{x+1,\sigma} + c^\dagger_{x+1,\sigma} c_{x\sigma}) \; + \; U \sum_x (n_{x\uparrow} < n_\downarrow > + n_{x\downarrow} < n_\uparrow > - < n_\uparrow >< n_\downarrow >) \\ &= \sum_{k,\sigma} \epsilon_k c^\dagger_{k\sigma} c_{k\sigma} \; + \; U \sum_k (n_{k\uparrow} < n_\downarrow > + n_{k\downarrow} < n_\uparrow >) - U \sum_k < n_\uparrow >< n_\downarrow >, \end{aligned}$$

where in the second step, we diagonalized the H_{kin}- and the H_{int}-term simultaneously in momentum space due to $N_{\uparrow(\downarrow)} = \sum_x n_{x\uparrow(\downarrow)} = \sum_k n_{k\uparrow(\downarrow)}$. Next, we define the magnetization per site m via $< n_{\uparrow(\downarrow)} > = 1/2 \cdot (n_e \pm m)$ in order to calculate the lowest energy E of the Hubbard Model (with given N_e, U and $|\Lambda| >> 1$) as a function of m as follows: First, we read off the single-particle energies from the above Hamiltonian: $\epsilon_{k,\uparrow(\downarrow)} = U/2 \cdot (n_e \mp m) - 2t \cdot cos(k)$ (we neglected the last term of the Hamiltonian, since it is just an offset). Then, we fill up the lowest $N_\uparrow$ single-particle energy levels $\epsilon_{k,\uparrow}$ and the lowest $N_\downarrow$ levels $\epsilon_{k,\downarrow}$, whereas $N_\uparrow$ and $N_\downarrow$ correspond to the magnetization value m. Finally, the **sum** of these single-electron energies has to be corrected by the offset in order to obtain the total energy E for a given m.

The results are plotted in Fig. 2: We observe a first order phase transition at some critical U_c, where the minimum of $E(m)$ hops discontinuously from $m = 0$ to $m = \pm 1$ such that the system becomes ferromagnetic for $U \geq U_c$.

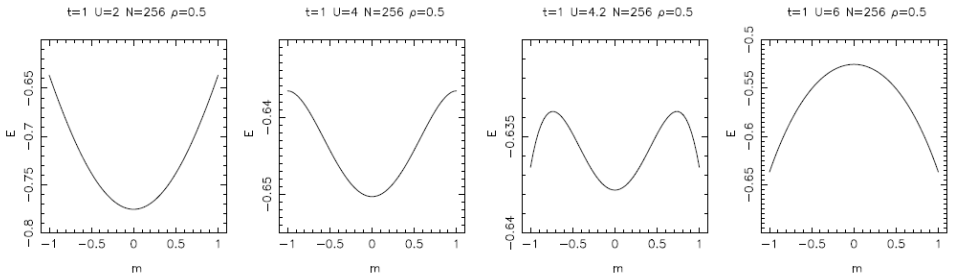

Figure 2: The energy E is plotted against the magnetization m for different U/t at quarter filling $n_e = 1/2$ and lattice size $|\Lambda| = 256$. (Taken from [4])

Interestingly, one can show rigorously (Lieb-Mattis-Theorem, see [2]) that ferromagnetism does not occur in the one dimensional Hubbard model with n.n. hopping and arbitrary U, which is not really surprising since the study of the Ising Model ([5]) also indicates that mean field approximation fails to predict correct results for lower dimensions ($d = 1, 2$), but is increasingly accurate for higher dimensions.

3 Nagaoka's Theorem

In this section we introduce a theorem which states that the Hubbard Model exhibits saturated ferromagnetism in the case of infinite Coulomb repulsion $U \to \infty$ and for one electron less than half filling ($N_e = |\Lambda| - 1$). This result is quite astonishing since we can prove that there is Ferrimagnetism (not saturated ferromagnetism) and preferred antiferromagnetic spin order at half filling for any U on bipartite lattices (Lieb's Theorem). The theorem is stated as follows:

Theorem 3.1. Consider a Hubbard Model with $t_{xy} \geq 0 \; \forall \; x, y \in \Lambda$, $N_e = |\Lambda| - 1$ and $U = \infty$. Moreover, assume that the **Connectivity Condition** holds. Then there exists a non-degenerate ground state (GS) with $S = S_{max} = N_e/2$.

Note that this GS is non-degenerate apart from the trivial $(2S_{max} + 1)$-fold spin degeneracy of $S^{(z)}$. We demonstrate the proof of Tasaki ([3]):

Proof:

We only consider states with finite energies, i.e. states $|\phi >$ which satisfy $H_{int}|\phi >= 0$ (because otherwise $U = \infty$ would lead to states with infinite energies). Thus we only have to consider the finite kinetic part H_{kin} of the Hamiltonian.

In the first part of the proof we are going to construct a ferromagnetic GS and in the second part, we show that this state is indeed unique.

First we construct a Hilbert space basis: Due to $U = \infty$ only one electron is allowed to sit on each single

site in order to avoid infinite energy contributions and $N_e = |\Lambda| - 1$ then implies that there is exactly one site that is not occupied by an electron, called **"hole"** (see Fig. 3).

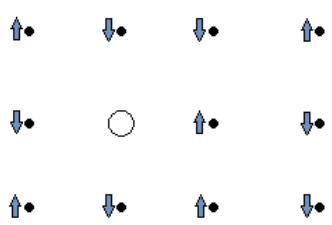

Figure 3: Basis state on a 4×3 square lattice with $S^{(z)} = -1/2$ and exactly one hole.

The basis states can then be written as:

$$|\phi_{x\vec{\sigma}} > = c_{x\uparrow} \left(\prod_{y \in \Lambda} c^{\dagger}_{y\sigma_y^{(1)}} \right) |0> \; = \; c_{x\downarrow} \left(\prod_{y \in \Lambda} c^{\dagger}_{y\sigma_y^{(2)}} \right) |0> \tag{13}$$

where x is the position of the hole, $\vec{\sigma} = (\sigma_y)_{y \in \Lambda \setminus \{x\}} \in S_{\Lambda \setminus \{x\}}$ is the spin configuration of all the occupied sites and it holds: $\sigma_y^{(1)} = \sigma_y^{(2)} = \sigma_y \; \forall \; y \in \Lambda \setminus \{x\}$ with $\sigma_x^{(1)} = \uparrow, \sigma_y^{(2)} = \downarrow$. We note that the equation (13) gives two equivalent definitions of the basis states.
Now, we are able to state the **Connectivity Condition (CC)**:

Definition 3.2. The Hamiltonian H satisfies the CC, if all basis states $|\phi_{x\vec{\sigma}} >$ with the same $S^{(z)} = \sum_{y \in \Lambda \setminus \{x\}} \sigma_y$ are connected via non-vanishing matrix elements of H.

Next, we want to know how the Hamiltonian looks like in this basis. For that we calculate:

$$\begin{aligned} \left(\sum_{\sigma \in \{\uparrow,\downarrow\}} c^{\dagger}_{x\sigma} c_{z\sigma} \right) \phi_{x\vec{\sigma}} &= -c_{z\uparrow} n_{x\uparrow} \left(\prod_{y \in \Lambda} c^{\dagger}_{y\sigma_y^{(1)}} \right) |0> - c_{z\downarrow} n_{x\downarrow} \left(\prod_{y \in \Lambda} c^{\dagger}_{y\sigma_y^{(2)}} \right) |0> \\ &= -\phi_{z,\vec{\sigma}(z \to x)} \quad \text{with} \quad \vec{\sigma}(z \to x) \in S_{\Lambda \setminus \{z\}} \end{aligned} \tag{14}$$

Here we used the two equivalent expressions of the basis states, applied the anticommutation relation and used the fact that in eq. (14) only one term survives depending on the value of σ_z. We observe that the hole hops to the site z and the spin σ_z is now at the site x whereas the spin configuration of all the other sites is unchanged (notation: $\phi_{z,\vec{\sigma}(z \to x)}$). With this result, we are able to derive the matrix elements of the Hamiltonian:

$$< \phi_{y\vec{\tau}} | H | \phi_{x\vec{\sigma}} > \overset{Def.}{=} \sum_{z \in \Lambda} t_{xz} < \phi_{y\vec{\tau}} | \left(\sum_{\sigma \in \{\uparrow,\downarrow\}} c^{\dagger}_{x\sigma} c_{z\sigma} \right) | \phi_{x\vec{\sigma}} > \overset{(14)}{=} -t_{xy} \delta_{\vec{\tau},\vec{\sigma}(y \to x)} \tag{15}$$

We note that in H we did not sum over the site index of the creation operators $c^{\dagger}_{x\sigma}$ since we can only create an electron at the hole in order to avoid infinite energy contributions by doubly occupied sites. Moreover, we observe from eq. (15) that the matrix element vanishes, if the states $|\phi_{y\vec{\tau}} >$ and $|\phi_{x\vec{\sigma}} >$ have **different** $S^{(z)}$**-values**.
By using the expression of an arbitrary ground state in the above basis
($|\psi_{GS} > = \sum_{x,\vec{\sigma}} \alpha_{x\vec{\sigma}} |\phi_{x,\vec{\sigma}} >$ with energy E_{GS}), we can now define a ferromagnetic state $|\psi_F >$:

$$|\psi_F > := \sum_{x \in \Lambda} \beta_x |\phi_{x,(\uparrow)} > \quad \text{with} \quad \beta_x := \left(\sum_{\vec{\sigma} \in S_{\Lambda \setminus \{x\}}} \alpha^2_{x\vec{\sigma}} \right)^{1/2} \tag{16}$$

Note that this state is defined to be ferromagnetic since $|\phi_{x,(\uparrow)}>$ are the basis states with the configuration "all spins up". By using the Cauchy-Schwarz inequality, one can show that the state $|\psi_F>$ is indeed a ground state:

$$\begin{aligned} <\psi_{GS}|H|\psi_{GS}> &\overset{(15)}{=} -\sum_{x,y\in\Lambda} t_{xy} \sum_{\vec{\sigma}\in S_{\Lambda\setminus\{x\}}} \alpha_{y\vec{\sigma}(y\to x)}\alpha_{x\vec{\sigma}} \\ &\overset{t_{xy}\geq 0}{\geq} -\sum_{x,y\in\Lambda} t_{xy} \left(\sum_{\vec{\sigma}\in S_{\Lambda\setminus\{x\}}} \alpha^2_{y\vec{\sigma}(y\to x)}\right)^{1/2} \left(\sum_{\vec{\sigma}\in S_{\Lambda\setminus\{x\}}} \alpha^2_{x\vec{\sigma}}\right)^{1/2} \\ &\overset{Def.}{=} -\sum_{x,y\in\Lambda} t_{xy}\beta_y\beta_x = <\psi_F|H|\psi_F> \end{aligned} \tag{17}$$

In order to show that this ferromagnetic GS is unique, we need the Connectivity Condition to apply the Perron-Frobenius theorem known from linear algebra (a proof is given in [3]):

Lemma 3.3. Let $M = (m_{ij})_{i,j}$ be a real, symmetric matrix with $m_{ij} \leq 0\ \forall i \neq j$ and $\forall i \neq j : \exists(i_1, ..., i_L) : i_1 = i, i_L = j$ with $m_{i_k,i_{k+1}} \neq 0\ \forall k < L$ (M is irreducible). Then it follows:
The lowest eigenvalue of M is non-degenerate.

To apply this Lemma, we identify the matrix M in Lemma 3.3 with the submatrices of the Hamiltonian (15) that connect those basis states with each other, that have the same $S^{(z)}$. Due to $t_{xy} \geq 0$, the first precondition (non-positivity of the matrix) is fulfilled and the second precondition (matrix M has to be irreducible) is obviously equivalent to the Connectivity Condition. Therefore, Lemma 3.3 implies that the ground state in every subspace with constant $S^{(z)}$ is non-degenerate.
At the beginning, we showed that there is a state $|\psi_F>$ with
$H|\psi_F >= E_{GS}|\psi_F >$, $\vec{S}^2|\psi_F >= S_{max}(S_{max}+1)|\psi_F >$ and $S^{(z)}|\psi_F >= S_{max}|\psi_F >$. Due to $[H, \vec{S}^2] = [H, S^{(z)}] = [\vec{S}^2, S^{(z)}] = 0$ there are also states $|\psi_m >$ with $H|\psi_m >= E_{GS}|\psi_m >$ and $\vec{S}^2|\psi_m >= S_{max}(S_{max}+1)|\psi_m >$, but **different**
$S^{(z)}|\psi_m >= m|\psi_m >$ ($m \in \{-S_{max}, -S_{max}+1, ..., S_{max}-1\}$). Therefore, Perron-Frobenius theorem implies that the ferromagnetic GS is unique apart from the trivial $(2S_{max}+1)$-fold spin degeneracy of the $S^{(z)}$-component. ■

We rigorously showed that the combination of quantum mechanical hopping of electrons (H_{kin}) on a lattice with infinitely strong Coulomb repulsion (H_{int}) yields saturated ferromagnetism. The strong Coulomb repulsion is crucial for the appearance of ferromagnetism since one can also prove rigorously that ferromagnetism does not occur for very small U ($0 \leq U < \epsilon_{N_e} - \epsilon_1$ where $\epsilon_i \leq \epsilon_{i+1}$ are the ordered single-electron energies of the $U = 0$- limit) ([3]). Furthermore, the above proof technique does not work for systems with two or more holes (there is indeed no ferromagnetism if $N_e = |\Lambda| - 2$).
At the end of this chapter, we demonstrate a concrete example of the Connectivity Condition:
Consider a square lattice with nearest neighbor (n.n.) hopping ($t_{xy} \neq 0$ for x, y nearest neighbors and $t_{xy} = 0$ else). Then one can create every spin configuration with **constant** $S^{(z)}$ by moving the hole along non-vanishing t_{xy}, whereas this hole hopping is produced by applying the Hamiltonian on $|\phi_{x\vec{\sigma}}>$ (see (14) and (15)).
In Fig. 4 we can see, how one can exchange two spins (belonging to the same loop) by hole movements without changing the spin configuration outside the loop. Therefore, it is possible two get any spin permutation with constant $S^{(z)}$ by iterating this procedure, i.e. the Hubbard Model on a square lattice with n.n. hopping satisfies the Connectivity Condition. This is by the way also true for cubic, triangular, fcc/bcc lattices with n.n. hopping, but not for the one dimensional Hubbard Model with only n.n. hopping since there are no loops in one dimension ([3]).

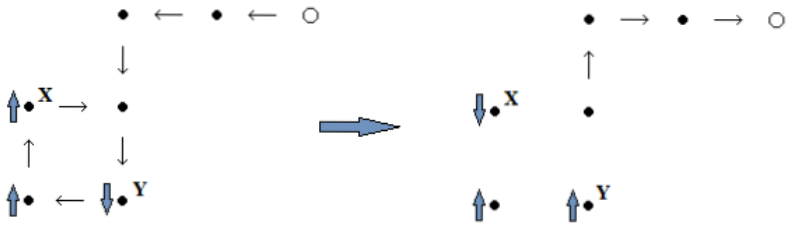

Figure 4: Example of a spin exchange inside a loop of length 4: First, the hole (white dot) is moved to the loop along non-vanishing t_{xy}. Then, the hole hops around the loop once, which leads to the exchange of the spins at x and y. Finally, the hole returns to its former position along the same way as before, such that the spin configuration outside the loop remains unchanged.

4 Lieb's Theorem

In 1989 Elliott Lieb demonstrated that the Hubbard model may display unsaturated ferromagnetism or ferrimagnetism at half-filling. His theorem consists of two parts of which we will only show the second part here. For the complete proof we suggest to read the original paper [6] or its discussion in [7].

Theorem 4.1 (Lieb 1989)**. Lieb I:** Let H be the Hamiltonian given in eq.(1), $U_x \leq 0$ for every $x \in V$ and N_e even. Then, (a) among the ground states of H there is at least one with $S = 0$ and (b) if $U_x < 0$ for every x then the ground state is unique (and hence has S=0).
Lieb II: Let $U_x = U > 0$ be independent of $x \in \Lambda$, $N_e = |\Lambda|$ even (half-filling) and Λ bipartite with $|B| \geq |A|$. Then the ground state of H is unique (apart from the trivial $2S+1$-fold degeneracy) and has total spin $S = \frac{1}{2}(|B| - |A|)$

Remarks : Part II of the theorem allows for an extensive value of the total spin, if $|B| > |A|$. Consider for example the square lattice in Fig. (5) typical of cuprate high-T_c superconductors. Each unit cell contains one atom of type A (blue) and two atoms of type B (green). Thus, according to Lieb's theorem, the total spin per unit cell is given by $S_{uc} = \frac{1}{2}$ and hence the total spin of this lattice is $S_{\text{tot}} = \frac{1}{2}N_{uc}$ where N_{uc} denotes the number of unit cells.
Proof (Lieb II) : Assume $U_x = U > 0$. We apply the particle-hole transformation, defined in eq.(7), only to spin-up operators. The Hamiltonian in eq.(1) then takes the form:

$$H \to \tilde{H} + UN_\downarrow = \sum_{x,y\in\Lambda} \sum_{\sigma\in\{\uparrow,\downarrow\}} t_{xy} c^\dagger_{x\sigma} c_{y\sigma} - U \sum_{x\in\Lambda} c^\dagger_{x\uparrow} c_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} + UN_\downarrow \tag{18}$$

Since the particle-hole transformation is unitary and due to eq.(3) $\tilde{H}$ has the same spectrum as H. However, $\tilde{H}$ is of the same form as the original Hamiltonian but with interaction parameter $\tilde{U} = -U < 0$. Thus, $\tilde{H}$ complies the conditions of the second part of Theorem I and hence the ground state is unique. The ground state is now considered as a function of the parameter U. If the ground state for certain U has total spin $S = \frac{1}{2}(|B| - |A|)$ then it has this spin value for all U since otherwise there would be a degeneracy of the ground state at some U which is impossible because the ground state is unique.
For $\frac{U}{t_{xy}} \gg 1$ we can do the following mapping of the Hubbard Hamiltonian on an effective Hamiltonian which we will recognize as the Hamiltonian of the Heisenberg model.

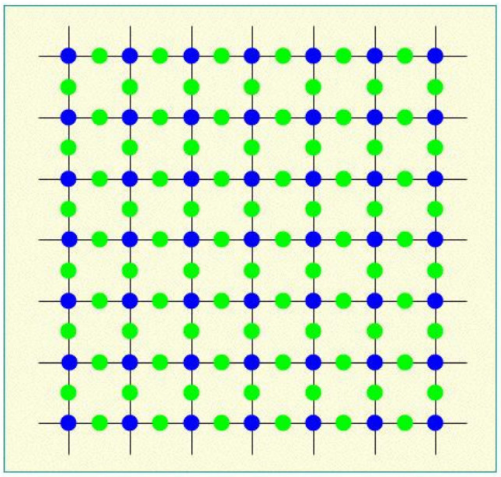

Figure 5: *Two dimensional plane in cuprate high-T_c superconductor: The copper atoms (blue) form an underlying square lattice. In the middle of each bond an oxygen atom (green) is intercalated. In the resulting bipartite lattice the value of the total spin is proportional to the number of unit cells.* (Figure taken from [9])

Consider a unitary transformation given by

$$\exp(R) = \exp\left(\sum_{xy\sigma} r_{x,y,\sigma} c^\dagger_{x\sigma} c_{y\sigma}\right) \tag{19}$$

where we demand R to be antihermitian and real, i.e. $r_{x,y,\sigma} = -r_{y,x,\sigma} \in \mathbb{R}$. According to an important corrollary of the Baker-Campbell-Hausdorff formula we can expand the transformed Hamiltonian in orders of its commutator with R, i.e.

$$H_{\text{eff}} = \exp(R) H \exp(-R) = H + [R,H] + \frac{1}{2}[R,[R,H]] + \sum_{n=3}^{\infty} \frac{[R,H]_n}{n!} \tag{20}$$
$$\text{where } [R,H]_n = \left[R,[R,H]_{n-1}\right] \text{ and } [R,H]_0 = H$$

As we will see later, the terms of order $n \geq 3$ can be neglected for large interaction U. We now split the kinetic part of the Hamiltonian (1) into

$$H_{\text{kin}} = H_{\text{kin},0} + H_{\text{kin},1} \tag{21}$$

where the first part does not change the number of doubly occupied sites and the second one, given by

$$H_{\text{kin},1} = \sum_{x,y,\sigma} t_{xy} \left(n_{x,-\sigma} - n_{y,-\sigma}\right)^2 c^\dagger_{x,\sigma} c_{y,\sigma}, \tag{22}$$

changes it by ± 1. We now choose R such that

$$[R, H_{\text{int}}] + H_{\text{kin},1} = 0 \tag{23}$$

which, by explicit calculation of the first commutator and equating the coefficients of both terms, leads to an explicit expression of $r_{x,y,\sigma}$:

$$[R, H_{\text{int}}] = -U \sum_{xy\sigma} r_{x,y,\sigma}(n_{x,-\sigma} - n_{y,-\sigma}) c^\dagger_{x\sigma} c_{y\sigma} \tag{24}$$
$$\Rightarrow r_{x,y,\sigma} = \frac{t_{xy}}{U}(n_{x,-\sigma} - n_{y,-\sigma})$$

By noticing that $[R, [R, H_{\text{kin}}]] = 0$ we may write the effective Hamiltonian as

$$H_{\text{eff}} = H_{\text{kin},0} + H_{\text{int}} + [R, H_{\text{kin},0}] - \frac{1}{2}[R, [R, H_{\text{int}}]] + \mathcal{O}\left(\left(\frac{t_{xy}}{U}\right)^2\right) \tag{25}$$

where higher order terms can be neglected in first order due to $r_{x,y,\sigma} \sim \frac{t_{xy}}{U}$. Since we are considering a Hubbard model at half-filling ($N_e = |\Lambda|$), the ground state contains exactly one electron per site. We will restrict our Hilbert space to these states using the projection operator P_0. Note, that the following identities hold since in the half-filled state, one electron hopping without changing the number of doubly occupied sites is impossible as well as no interactions between electrons can take place:

$$P_0 H_{\text{kin},0} = P_0 H_{\text{int}} = H_{\text{kin},0} P_0 = H_{\text{int}} P_0 = 0 \tag{26}$$

Thus, we may write the effective Hamiltonian (25) in the half-filled ground state as:

$$H_{\text{H}} = P_0 H_{\text{eff}} P_0 \approx -\frac{1}{2} P_0 [R, [R, H_{\text{int}}]] P_0 = P_0 R [H_{\text{int}}, R] P_0 = U P_0 R^2 P_0 \tag{27}$$

where we used eq.(24) for the half-filled state in the last step.
Inserting the explicit expression for $r_{x,y,\sigma}$ given in eq.(24), we finally obtain

$$H_{\text{H}} = \frac{1}{U} P_0 \sum_{xy\sigma} \sum_{x'y'\sigma'} t_{xy} (n_{x,-\sigma} - n_{y,-\sigma}) c^\dagger_{x\sigma} c_{y\sigma} t_{x'y'} (n_{x',-\sigma'} - n_{y',-\sigma'}) c^\dagger_{x'\sigma'} c_{y'\sigma'} P_0 \tag{28}$$
$$= -\frac{1}{U} P_0 \sum_{xy\sigma\sigma'} t^2_{xy} c^\dagger_{x\sigma} c_{y\sigma} c^\dagger_{y\sigma'} c_{x\sigma'} P_0$$
$$= P_0 \sum_{x,y} \frac{2t^2_{xy}}{U} \left(\mathbf{S}_x \cdot \mathbf{S}_y - \frac{1}{4}\right) P_0 \tag{29}$$

where we dropped a term proportional to the sum over all onsite potentials t^2_{xx} which does not affect the present discussion (we could have done the same for the spin independent term in the last line). We recognize eq.(29) as the Hamiltonian of the Heisenberg model with $J = \frac{2t^2_{xy}}{U} > 0$. This Hamiltonian has a unique ground state with $S = \frac{1}{2}(|B| - |A|)$ which was shown in [8]. Thus, for sufficiently large interactions U we were able to prove the assertion of Theorem II by mapping it to the Heisenberg Hamiltonian which, according to our earlier remarks, proves it for all $U > 0$. ■

5 Summary

We introduced a highly simplified model of electrons in a solid that combines the quantum mechanical hopping H_{kin} of the electrons on a lattice with an on-site (Coulomb-) interaction H_{int}. Although the single Hamiltonians H_{kin} and H_{int} only produce paramagnetism separately, the combination of the two is capable of inducing interesting physical phenomena like ferromagnetism or antiferromagnetic/ ferrimagnetic order. Whereas ferromagnetism is also suggested by mean field theory for sufficiently large repulsion U, we were able to prove rigorously the appearance of ferromagnetism under specific preconditions as infinite repulsion U and that the lattice contains exactly one hole ($N_e = |\Lambda| - 1$). This

result is quite remarkable since one can show that the model does not exhibit ferromagnetism anymore, if there is one additional hole on the lattice and because the Hubbard model prefers antiferromagnetic/ ferrimagnetic order at half-filling ($N_e = |\Lambda|$) on bipartite lattices and arbitrary repulsion U (Lieb's theorem). Finally, we note that further sectors with finite U and away from half-filling can be reached to some extent with aid of the mean field approximation or the renormalization group method.

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