

11 The Hubbard Model and its Properties

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1 Introduction

The Hubbard model, although highly oversimplified, contains the main ingredients to describe interacting quantum mechanical particles, originally fermions, moving in a solid. Its basis is a tight binding description. The Hamiltonian defining the model contains two parts: a single-particle part and a two-particle interaction. The idea is that only one or few energy bands close to the Fermi energy contribute. Therefore, the single-particle part, often called kinetic energy, describes particles hopping on a lattice which may have a single or a few bands. The Coulomb interaction is assumed to be screened. In the Hubbard model, the interaction taken into account is just an on-site interaction, the range of the interaction is thus the shortest possible. With this setup, the Hubbard model is certainly only a caricature of a realistic description of electrons in a solid. Nevertheless, the Hubbard model exhibits almost all interesting phenomena one observes in nature: magnetic ordering of any kind, a metal-insulator transition, superconductivity (it is even used in the context of high temperature superconductivity), a Tomonaga-Luttinger liquid in one space dimension, and even more sophisticated transitions like a Pomeranchuk instability. The Hubbard model can thus be viewed as the simplest possible model of correlated fermions. The Hubbard model contains few independent parameters. If we assume that hopping is only allowed between nearest-neighbor lattice sites, and if we assume translational invariance, the hopping is described by a single parameter. Under the same assumptions, the interaction is described by a single parameter as well. Since the energy scale can be chosen freely, only the ratio between these two parameters is important. The second parameter is the electron density on the lattice. And the third parameter is the lattice itself. In fact, we will see that the lattice is essential for the properties of the model.

Despite its simplicity, only few properties of the Hubbard model have been proven rigorously. Nevertheless, for almost all the different phenomena, rigorous results exist and serve as landmarks for any kind of approximation that is applied to the Hubbard model. Therefore, in this lecture, I concentrate on the rigorous results for the Hubbard model.

2 The Hubbard model

2.1 Definition

The Hamiltonian of the Hubbard model is given by

$$H = H_{\text{kin}} + H_{\text{int}} = \sum_{x,y \in V, \sigma} t_{xy} c_{x,\sigma}^\dagger c_{y,\sigma} + \sum_x U_x c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger c_{x\downarrow} c_{x\uparrow} \quad (1)$$

The model was proposed independently by J. Hubbard [1] for the description of transition metals, by J. Kanamori [2] for the description of itinerant ferromagnetism, and by M.C. Gutzwiller [3] for the description of the metal-insulator transition. In Chemistry, the model is popular as well, and was introduced ten years earlier [4–6]. Under the name Pariser-Parr-Pople model it has been used to describe extended π -electron systems.

Typically, one assumes that the vertex set V forms a translationally invariant lattice and that U_x is independent of x , *i.e.*, $U_x = U$. But more general settings are possible. Especially in the quantum chemical context, V is just a general graph, t_{xy} and U_x depend on the lattice sites.

On a regular lattice, one often assumes nearest-neighbor hopping, *i.e.*, $t_{xy} = t$ for nearest-neighbor sites such that $|x - y| = 1$, and $t_{xy} = 0$ otherwise. Sometimes, a next-nearest-neighbor hopping $t_{xy} = t'$ for $|x - y| = 2$ is introduced. In Sect. 4.5 we will see that such a next nearest-neighbor hopping may change the physical behavior of the system drastically.

For small U and in two or more dimensions, one expects that the Hubbard model describes a Fermi liquid. We will come back to that point later, in Sect. 4, where we sketch how renormalization theory is used to obtain instabilities of the Fermi liquid. Typically, one is interested in the case where the model describes strongly interacting electrons, *i.e.* correlated electrons. In that situations, the interaction U is as large as or larger than typical values of t_{xy} .

For a general overview on the Hubbard model and on correlated fermions in general I refer to the book of Fulde [7]. An overview on rigorous results for the Hubbard model can be found in the article of Lieb [8], an overview on ferromagnetism in the Hubbard model in [9].

2.2 Symmetries of the Hubbard model

The Hubbard model has several symmetries:

Gauge symmetry:

$$c_{x\sigma}^\dagger \rightarrow \exp(i\alpha) c_{x\sigma}^\dagger, \quad c_{x\sigma} \rightarrow \exp(-i\alpha) c_{x\sigma} \quad (2)$$

The Hamiltonian remains invariant if this transformation is applied. As a consequence, the particle number $N_e = \sum_{x\sigma} c_{x\sigma}^\dagger c_{x\sigma}$ is conserved. This is a generic property of almost all models in condensed matter theory that describe fermions.

Spin symmetry: With the help of the Pauli matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (3)$$

we define local

$$S_{\alpha,x} = \frac{1}{2} \sum_{\sigma,\sigma'} c_{x\sigma}^\dagger (\sigma_\alpha)_{\sigma,\sigma'} c_{x\sigma'}, \quad \alpha = x, y, z, \quad \mathbf{S}_x = (S_{x,x}, S_{y,x}, S_{z,x}) \quad (4)$$

and global spin operators.

$$S_\alpha = \sum_x S_{\alpha,x}, \quad \mathbf{S} = (S_x, S_y, S_z) \quad (5)$$

Often one uses

$$S_\pm = S_x \pm iS_y, \quad S_+ = \frac{1}{2} \sum_x c_{x\uparrow}^\dagger c_{x\downarrow}, \quad S_- = S_+^\dagger \quad (6)$$

These operators form an $SU(2)$ algebra. The Hamiltonian commutes with these operators: it has a $SU(2)$ -symmetry. We have

$$[S_x, S_y] = iS_z \quad (7)$$

H , \mathbf{S}^2 and S_z can be diagonalized simultaneously. We denote the eigenvalues of \mathbf{S}^2 as $S(S+1)$, where S is the spin of the eigenstate. $S \propto N_e$, *i.e.*, an extensive value for S , means that the state is ferro- or ferri-magnetic.

Particle-hole transformations: Using the transformation

$$c_{x\sigma}^\dagger \rightarrow c_{x\sigma}, \quad c_{x\sigma} \rightarrow c_{x\sigma}^\dagger \quad (8)$$

the Hamiltonian becomes

$$\begin{aligned} H \rightarrow H' &= \sum_{x,y,\sigma} t_{xy} c_{x\sigma} c_{y\sigma}^\dagger + U \sum_x c_{x\uparrow} c_{x\downarrow} c_{x\downarrow}^\dagger c_{x\uparrow}^\dagger \\ &= - \sum_{x,y,\sigma} t_{xy} c_{y\sigma}^\dagger c_{x\sigma} + U \sum_x (1 - c_{x\uparrow}^\dagger c_{x\uparrow})(1 - c_{x\downarrow}^\dagger c_{x\downarrow}) \\ &= - \sum_{x,y,\sigma} t_{xy} c_{x\sigma}^\dagger c_{y\sigma} + U \sum_x c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger c_{x\downarrow} c_{x\uparrow} + U(|V| - N_e) \end{aligned} \quad (9)$$

$|V|$ is the number of vertices.

Thus, the particle-hole transformation is not a symmetry, but it can be used to obtain eigenstates from other eigenstates.

For a bipartite lattice, *i.e.*, a lattice that splits into two sub-lattices A and B so that $t_{xy} = 0$ if both x and y belong to the same sub-lattice, it is possible to introduce the following transformation:

$$c_{x\sigma}^\dagger \rightarrow c_{x\sigma}^\dagger \text{ if } x \in A, \quad c_{x\sigma}^\dagger \rightarrow -c_{x\sigma}^\dagger \text{ if } x \in B \quad (10)$$

This transformation changes the sign of the kinetic energy. Applying this transformation together with the particle-hole transformation at half filling (*i.e.* $N_e = |V|$) maps the Hamiltonian onto itself. Thus, we have another symmetry for this class of lattices, a particle-hole symmetry. The transformation (10) alone is of some importance since it can be used to change the sign of the hopping matrix elements. Typically, it is assumed that $t_{xy} < 0$ is the natural choice of the sign, at least for nearest neighbors. For bipartite lattices the sign can be changed. In general, the assumption $t_{xy} < 0$, although popular, has no compelling reason [8].

On bipartite lattices at half filling, one can use the particle-hole symmetry to obtain a second $SU(2)$ symmetry. The generators are

$$\hat{S}_z = \frac{1}{2}(N_e - |V|), \quad \hat{S}_+ = \sum_{x \in A} c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger - \sum_{x \in B} c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger, \quad \hat{S}_- = \hat{S}_+^\dagger \quad (11)$$

These generators can be obtained from the original $SU(2)$ generators by performing a particle-hole transformation together with a transformation of type (10) for spin down only. The model

has thus a $SU(2) \times SU(2) = SO(4)$ symmetry at half filling. In discussions concerning high temperature superconductivity, even an approximate $SO(5)$ -symmetry has been proposed. The additional symmetry of the Hubbard model on a bipartite lattice at half filling ($N_e = |V|$) is essential for several of the rigorous results that are valid in this case. The two most important are Lieb's theorem [10], see Sect. 3.1, and the uniform density theorem, Sect. 3.5.

Lattice symmetries: On translationally invariant lattices, the model has the symmetries of the lattice.

The one-dimensional case: The one dimensional Hubbard model has an infinite set of invariants. A special form of the Bethe ansatz yields exact eigenstates of the Hamiltonian. This was first shown by E. Lieb and F. Wu [11]. The ground state is part of these Bethe ansatz eigenstates. Not all the eigenstates of the one-dimensional Hubbard model are Bethe ansatz states. But it was shown by Essler, Korepin, and Schoutens [12], that for even $|V|$, where the lattice is bipartite, all other eigenstates can be obtained by applying the operators \hat{S}_\pm to the Bethe ansatz states.

For an exactly solvable model one should expect an infinite set of invariants. A first attempt to find those is a paper by Heilmann and Lieb [13]. Later Shastry [14] and Grosse [15] presented a large set of such invariants.

The one-dimensional Hubbard model has been investigated by many people, the literature is vast, and a complete overview would be a course in its own. I will not discuss the one-dimensional Hubbard model in this course.

3 Some rigorous results

Most of the rigorous results on the Hubbard model concern the magnetic behavior in the ground state, *i.e.*, at $T = 0$. I discuss the most important rigorous results in the following subsections. For each of the theorems mentioned below I try to explain the main idea of the proof. For the mathematical details I refer to the original papers.

3.1 Lieb's Theorem

In 1989, E. Lieb [10] proved an important theorem and an even more important corollary on the Hubbard model. The theorem is about the attractive Hubbard model. It holds for arbitrary hoppings t_{xy} , with the only assumption that the graph of the hopping matrix is connected. The interaction U_x may depend on x .

Theorem (Lieb 1989) Let H be the Hamiltonian in (1) with real t_{xy} , the graph of $T = (t_{xy})$ should be connected, and negative $U_x < 0$. Let the particle number N_e be even. Then, the ground state is unique and has a total spin $S = 0$.

For the proof, I refer to the original paper by Lieb. He uses a technique called spin reflection positivity. For some details see the remarks below.

On a bipartite lattice, using a particle-hole transformation for spin-down only, together with a transformation (10), the kinetic energy remains the same but the signs of U_x are switched. In that way, one can obtain a result for the attractive Hubbard model. Since S_z transforms with the above transformation to \hat{S}_z , one obtains a result for $\hat{S}_z = 0$, *i.e.*, $N_e = |V|$, *i.e.*, half filling. Therefore, the following corollary holds

Corollary Let H be the Hamiltonian in (1) with real t_{xy} . The graph of t_{xy} should be connected and bipartite, and positive $U_x = U > 0$. Let the particle number $N_e = |V|$. Then, the ground state is unique in the subspace $S_z = 0$. The total spin is $S = \frac{1}{2}||A| - |B||$.

The last statement $S = \frac{1}{2}||A| - |B||$ does not follow directly from the theorem because the theorem makes no statement about \hat{S} . It can be understood in two ways.

The first is to look at weak interactions. For a bipartite lattice, the spectrum of $T = (t_{xy})_{xy \in V}$ is symmetric with respect to 0. For any eigenvalue ε there exists an eigenvalue $-\varepsilon$. Half filling now means that for arbitrary weak interaction all single particle eigenstates with energies $\varepsilon < 0$ are completely filled with two electrons and that the eigenstates with $\varepsilon = 0$ are filled with one electron. For the latter, Hund's rule [16] applies, which means that all electrons have the same spin. The degeneracy of the eigenvalue 0 is $||A| - |B||$, therefore we obtain the a total spin $S = \frac{1}{2}||A| - |B||$.

The second idea is to look at strong interactions and to use a unitary transformation $\exp(R)$ to transform the Hamiltonian to a form where the number of doubly occupied sites is conserved. The ansatz is

$$R = \sum_{x,y,\sigma} r_{x,y,\sigma} c_{x,\sigma}^\dagger c_{y,\sigma} \quad (12)$$

We assume that U is large and expand $\exp(R)H \exp(-R)$ to obtain

$$H \rightarrow H_{\text{int}} + H_{\text{kin}} + [R, H_{\text{int}}] + [R, H_{\text{kin}}] + \frac{1}{2}[R, [R, H_{\text{int}}]] + \dots \quad (13)$$

The kinetic energy H_{kin} can be written as

$$H_{\text{kin}} = H_{\text{kin},0} + H_{\text{kin},1} \quad (14)$$

$H_{\text{kin},0}$ does not change the number of doubly occupied sites, $H_{\text{kin},1}$ changes it by ± 1 . We have

$$H_{\text{kin},1} = \sum_{x,y,\sigma} t_{xy} (n_{x,-\sigma} - n_{y,-\sigma})^2 c_{x,\sigma}^\dagger c_{y,\sigma} \quad (15)$$

We choose R so that

$$H_{\text{kin},1} + [R, H_{\text{int}}] = 0 \quad (16)$$

This yields

$$H \rightarrow H_{\text{eff}} = H_{\text{int}} + H_{\text{kin},0} - \frac{1}{2}[R, [R, H_{\text{int}}]] + \dots \quad (17)$$

We have

$$[R, H_{\text{int}}] = -U \sum_{x,y,\sigma} r_{x,y,\sigma} (n_{x,-\sigma} - n_{y,-\sigma}) c_{x,\sigma}^\dagger c_{y,\sigma} \quad (18)$$

and therefore

$$r_{x,y,\sigma} = \frac{t_{xy}}{U} (n_{x,-\sigma} - n_{y,-\sigma}) \quad (19)$$

Let P_0 be the projector onto states for which each site is occupied by one electron, which is the ground state at half filling and U arbitrarily large. If we restrict the Hilbert space to these states, we get

$$\begin{aligned} H_{\text{eff}} &= P_0 R H R P_0 \\ &= U P_0 R^2 P_0 \\ &= U P_0 \sum_{x,y,\sigma} \frac{t_{xy}}{U} (n_{x,-\sigma} - n_{y,-\sigma}) c_{x,\sigma}^\dagger c_{y,\sigma} \sum_{x',y',\sigma'} \frac{t_{x',y'}}{U} (n_{x',-\sigma'} - n_{y',-\sigma'}) c_{x',\sigma'}^\dagger c_{y',\sigma'} P_0 \\ &= -\frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t_{xy}^2 c_{x,\sigma}^\dagger c_{y,\sigma} c_{y,\sigma'}^\dagger c_{x,\sigma'} P_0 \\ &= \frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t_{xy}^2 c_{x,\sigma}^\dagger c_{y,\sigma'} c_{y,\sigma'}^\dagger c_{x,\sigma} P_0 - \frac{1}{U} \sum_{x,y} t_{xy}^2 \\ &= \sum_{x,y} \frac{2t_{xy}^2}{U} \mathbf{S}_x \cdot \mathbf{S}_y P_0 + \frac{1}{U} P_0 \sum_{x,y,\sigma,\sigma'} t_{xy}^2 c_{x,\sigma}^\dagger c_{x,\sigma} c_{y,\sigma'}^\dagger c_{y,\sigma'} P_0 - \frac{1}{U} \sum_{x,y} t_{xy}^2 \\ &= \sum_{x,y} \frac{2t_{xy}^2}{U} \mathbf{S}_x \cdot \mathbf{S}_y P_0 \end{aligned} \quad (20)$$

This transformation is of importance on its own. It shows that the Hubbard model at half filling and for large U can be mapped to the anti-ferromagnetic Heisenberg model. For the corollary above it has the consequence that the total spin of the Hubbard model at half filling and for large U is the same as for the Heisenberg model, therefore $S = \frac{1}{2}||A| - |B||$.

Since the ground state is unique for all U , it is sufficient to know the total spin S for small or large U : due to uniqueness it cannot change.

Lieb's theorem suggests anti-ferromagnetism or ferrimagnetism (depending on whether the two sub-lattices A and B have the same size or not) for the Hubbard model at half filling. But, whereas for the anti-ferromagnetic Heisenberg model long-range order was proven in two dimensions in the ground state and in three dimensions for sufficiently low temperatures, there is no proof for long-range order for the Hubbard model up to now. The methods to prove long-range order for the Heisenberg model cannot be applied to the Hubbard model. The simple reason is that the Hubbard model is much more complicated and allows for a wider variety of phenomena. Nevertheless, many results including those from renormalization (see Sect. 4) indicate the existence of long range order for large U .

Lieb's proof uses the fact that for an even number of fermions, there is always a ground state with $S_z = 0$ due to the $SU(2)$ spin symmetry. This means that the ground state can be written in the form $\psi = \sum_{\alpha,\beta} W_{\alpha\beta} \psi_{\alpha,\uparrow} \psi_{\beta,\downarrow}$ where $\psi_{\alpha,\sigma}$ form an orthonormal basis of multi-particle states

with $N_e/2$ particles with spin σ . Since t_{xy} and U_x are real, one can assume that the matrix W is self adjoint. The expectation value of the Hamiltonian in the state ψ can be written in a quadratic form $E(W)$ in W and it can be shown that for non-positive interactions $E(W) \geq E(|W|)$. $|W|$ is the positive semi-definite matrix satisfying $W^2 = |W|^2$. It is then easy to see that the ground state corresponding to $|W|$ has $S = 0$. Uniqueness is shown by assuming that a second ground state with some W exists. Then, $R = |W| - W$ is a ground state as well. A lengthy but easy to understand argument that uses the fact that the graph of T is connected then shows that $W = \pm|W|$ and therefore that the ground state is unique. Compared to many other proofs, Lieb's proof is very elegant and compact, only somewhat more than one page in a letter. I recommend that everyone read it.

3.2 The Mermin-Wagner theorem

The term Mermin-Wagner Theorem is usually used for a huge class of theorems that state that for lattice models in one or two spacial dimensions with a continuous symmetry, like an $SU(2)$ symmetry, there is no long range order at finite temperature. Originally, Mermin and Wagner [17] showed in 1966 that in the one- or two-dimensional Heisenberg model there is no long-range order, neither anti-ferromagnetic nor ferromagnetic. This result was extended to the Hubbard model by Walker and Ruijgrok in 1968 [18] and by Ghosh in 1971 [19]. Further, Hohenberg [20] showed in 1967 that there cannot be superconductivity or long range crystalline order in one or two dimensions. The proof for the Hubbard model was considerably simplified and somewhat extended by Koma and Tasaki [21].

Theorem (Koma, Tasaki 1992) For a Hubbard model in one and two dimensions with finite-ranged hopping (*i.e.* $t_{xy} = 0$ if the distance $|x - y|$ lies above some finite value) in the thermodynamic limit, the following bounds hold for the correlation functions

$$|\langle c_{x\uparrow}^\dagger c_{x\downarrow}^\dagger c_{y\downarrow} c_{y\uparrow} \rangle| \leq \begin{cases} |x - y|^{-\alpha f(\beta)} & \text{for } d = 2 \\ \exp(-\gamma f(\beta)|x - y|) & \text{for } d = 1 \end{cases} \quad (21)$$

$$|\langle \mathbf{S}_x \cdot \mathbf{S}_y \rangle| \leq \begin{cases} |x - y|^{-\alpha f(\beta)} & \text{for } d = 2 \\ \exp(-\gamma f(\beta)|x - y|) & \text{for } d = 1 \end{cases} \quad (22)$$

for some $\alpha > 0$, $\gamma > 0$, $f(\beta) > 0$ where $\langle \dots \rangle$ denotes the expectation value at inverse temperature β and $f(\beta)$ is a decreasing function of β that behaves like $f(\beta) \approx 1/\beta$ for $\beta \gg \beta_0$ and $f(\beta) \approx (2/\beta_0)|\ln(\beta)|$ for $\beta \ll \beta_0$, where β_0 is some constant.

This result rules out long-range spin-order or superconductivity at finite temperatures in one or two dimensions. The power laws for $d = 2$ are certainly not optimal for high temperatures, where one expects an exponential decay of correlation functions. But they are sufficient to exclude long-range order. This means that a Kosterlitz-Thouless transition may occur [22].

The interesting point of the proof is that it only needs a $U(1)$ symmetry. Thus, any lattice model with a $U(1)$ symmetry in one or two dimensions cannot have superconducting or magnetic long-range order at finite temperature in one or two dimensions.

The older proof of Ghosh [19] uses the $SU(2)$ spin symmetry and the Bogoliubov inequality and is easy to understand.

The result by Koma and Tasaki is more general; their proof uses a method developed by McBryan and Spencer [22] for classical spin systems and its extension to quantum spin systems developed by Ito [23]. The proof uses the fact that for an arbitrary observable A one has $\text{Tr}(A \exp(-\beta H)) = \text{Tr}(G(\theta) A G(\theta)^{-1} \exp(-\beta G(\theta) H G(\theta)^{-1}))$. $G(\theta)$ is a local transformation. The right-hand side can be bounded using some Schwartz inequality stating that for hermitian matrices O and P one has $\text{Tr}(OP) \leq (\text{Tr}(O^*O)\text{Tr}(P^*P))^{1/2}$, and the Golden-Symanzik-Thompson inequality $\text{Tr} \exp(O + P) \leq \text{Tr}(\exp(O) \exp(P))$. Suitable choices for A and $G(\theta)$ then yield the bounds.

In one dimension, with nearest-neighbor hopping only, and for finite U_x , the Lieb-Mattis theorem [24] says that the minimal energy in the subspace with fixed spin S is strictly lower than the minimal energy in the subspace with $S + 1$. This clearly rules out ferromagnetism in one dimension in the ground state.

3.3 Nagaoka's theorem

The so called Nagaoka Theorem was actually first proven by Thouless [25] 1965 for some special bipartite lattices. The proof of Nagaoka [26], only one year later, is more general and applies to non-bipartite lattices as well. Therefore, the result is called the Nagaoka theorem today. The most general proof is due to Tasaki [27]. It states the following:

Theorem (Tasaki 1989) The Hubbard model (1) with non-negative t_{xy} , $N_e = |V| - 1$, and a hard-core repulsion $U_x = \infty$ for all $x \in V$ has a ground state with a total spin $S = \frac{1}{2}N_e$. The ground state is unique except for the usual $(2S + 1)$ -fold spin degeneracy provided a certain connectivity condition for t_{xy} holds.

This theorem is remarkable, because it states that there is a unique ferromagnetic ground state in the vicinity of half filling, where an anti-ferromagnetic spin order is assumed to be present. The proof of the theorem uses the Schwarz inequality to show that a ferromagnetic ground state exists. To show uniqueness, it uses the Perron-Frobenius theorem, which states that for a matrix with only non-negative entries and for which the graph is connected (the matrix is irreducible), the eigenstate with the largest eigenvalue is unique and has non-negative entries. The theorem can be applied here by finding a suitable basis for the multi-particle Hilbert space of the Hubbard model. The connectivity condition in the theorem ensures that the graph of the Hamiltonian in that basis obeys the irreducibility needed in the Perron-Frobenius theorem. Essentially it states that through the hopping of particles, arbitrary permutations of the particles can be realized. This holds for almost any lattice except the one-dimensional chain.

The Nagaoka theorem made people believe that for many lattices, *e.g.*, also for hyper-cubic lattices, a large region in the parameter space (U large and a density close to but not at half filling) exists where the Hubbard model has ferromagnetic ground states. But any attempt to prove that has failed so far. Instead, many variational calculations by various groups mainly

in the early '90s showed that the Nagaoka state is not very stable. Changing the conditions a bit, either putting more than one hole in the system or lowering U causes the Nagaoka state to become unstable against single spin flips, *i.e.*, $E(S = N_e/2 - 1) < E(S = N_e/2)$ (for details see *e.g.* [28]). Exact diagonalization of small systems yields the same result. On the other hand, for some special non-bipartite lattices, these calculations indicate that the Nagaoka state may be more stable and that a larger region in the parameter space exists where the ground state is ferromagnetic.

3.4 Flat-band systems

A first example of a lattice having a flat band is a bipartite lattice with $|A| = n|B|$. A simple example which Lieb [10] used as an illustration for his theorem is the quadratic lattice with additional lattice sites on each edge. If there is only nearest-neighbor hopping, the original lattice sites of the quadratic lattice form one of the sub-lattices, say B and the new lattice sites form the second sub-lattice A . There are twice as many lattice sites on A as on B . Each elementary cell contains one lattice site from B and two from A , in total three. We have thus a three-band model. Since the lattice is bipartite, the single-particle spectrum is symmetric with respect to 0. There is one energy band in the center, which is completely flat. The flat band causes the extensive magnetization $S = \frac{1}{2}||A| - |B|| = \frac{1}{2}|B|$, as we pointed out already in Sect. 3.1. Since this magnetization is related to the existence of two sub-lattices, the system is ferrimagnetic.

Two years after Lieb, first examples of lattices with a flat band at the bottom of the spectrum were published [29–33]. One class of such lattices are line graphs, the other are decorated lattices. Since the construction of a line graph is elementary and since we need it later, we give a more detailed description here.

Let $G = (V, E)$ be a graph with a vertex set V and an edge set E . Any lattice can be regarded as a graph. The lattice sites are the vertices and there are edges between two vertices if there is a non-vanishing hopping matrix element connecting the two. If we allow only for nearest neighbor hopping, the hopping matrix is (up to a factor t) the adjacency matrix $A(G) = (a_{xy})_{xy \in V}$ of the graph. $a_{xy} = 1$ if $\{x, y\} = e \in E$ is an edge of the graph, 0 otherwise.

The line graph $L(G)$ of a graph G is constructed as follows: The vertex set $V(L(G))$ of the line graph is the edge set $E(G)$ of the original graph and two vertices of the line graph are connected, if the corresponding edges in G have a vertex in common.

Figure (1) shows an illustration of the construction of a line graph. Let G be a part of the hexagonal lattice, as shown in black. Now we put a new vertex in the middle of each edge and connect two new vertices if the edges of the original hexagonal lattice have a vertex in common. This procedure yields a new lattice built of hexagons surrounded by triangles, shown in red. The new lattice constructed that way is the line graph of the hexagonal lattice, it is called the kagome lattice. You may take any lattice or even any graph G and construct the line graph in that way.

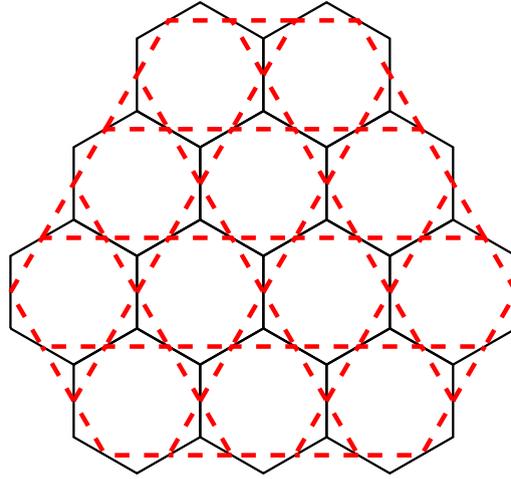


Fig. 1: The kagome lattice (red, dashed) as the line graph of the hexagonal lattice (black).

Let us now investigate the spectral properties of the adjacency matrix $A(L(G))$ of a line graph. To do this, we first introduce a new matrix $B(G) = (b_{xe})_{x \in V, e \in E}$, the so called edge vertex incidence matrix. The matrix elements $b_{xe} = 1$ if the edge e connects to the vertex x , $b_{xe} = 0$ otherwise. Note that B has $|V|$ columns and $|E|$ rows. Except for a graph without loops or with only one loop, $|E| > |V|$ and the kernel of B has a dimension $\geq |E| - |V|$. The adjacency matrix of the line graph and the incidence matrix of the original graph are related via $A(L(G)) = B(G)^T B(G) - 2$. As a consequence, -2 is a lower bound of the spectrum of $A(L(G))$ and becomes the lowest eigenvalue with degeneracy at least $|E| - |V|$ if $|E| > |V|$. In fact, one can show that the degeneracy is $N_d = |E| - |V| + 1$ if G is bipartite and connected, $N_d = |E| - |V|$ if G is not bipartite and connected.

This fact can now be applied to a lattice. If G is a translationally invariant lattice with one or more energy bands, $L(G)$ is a lattice as well and the lowest energy band lies at energy $-2t$ and is completely flat. A lattice that is a line graph, *e.g.* the kagome lattice, has a lowest flat band. This makes it easy to construct ground states of the Hubbard model, at least for $N_e \leq N_d$. In that case, any state with all electrons having the same spin is a ground state, since this state minimizes both the kinetic energy and the interaction. This construction is indeed trivial. The interesting question is whether there are other ground states and whether they can be characterized completely. This is indeed possible for $N_e = N_d$ as the following theorem shows [29, 30]:

Theorem (Mielke 1991) Let H be the Hubbard model on a line graph $L(G)$ of a two-connected bipartite graph G or a three-connected graph G and let $N_e = N_d$, and $U_x > 0$ for all x . Then the ground state has a spin $S = \frac{N_d}{2}$ and is unique up to the $(2S + 1)$ -fold degeneracy due to the $SU(2)$ spin symmetry.

The kagome lattice is obviously an example for this theorem.

The original proof of the theorem uses some graph theoretical notions. We will not present it here since later a more general and simpler result has been shown which does not use the notion of a line graph.

On the other hand, let us discuss the single-particle ground states with energy $-2t$ a bit further since they serve for many easy illustrations we may need later. Let p be a self-avoiding closed path (x_1, x_2, \dots, x_n) of even length n on G . It obviously translates to an even path on $L(G)$. Let us now construct the single-particle state $\psi_p(e)$ as follows. $\psi_p(e) = 0$ if e lies not on p . On p , $\psi_p(e) = \pm 1$ with alternating sign for subsequent edges of G . It is easy to see that $B\psi_p = 0$. ψ_p is therefore a ground state of $A(L(G))$ with eigenvalue -2 . It can be shown that these states form an over-complete basis of the eigenspace of the eigenvalue -2 .

If G is a bipartite plane graph, like the hexagonal lattice, each face f is surrounded by a self-avoiding path, let us call it f as well. Let F be the set of faces. Due to Euler's theorem, $|F| = |E| - |V| + 2$. One of the faces is the outer face of the graph, there are exactly $|E| - |V| + 1$ inner faces. It is easy to see that the states ψ_f corresponding to the inner faces f are linearly independent. They thus form a basis (not orthonormal) of the eigenspace of the ground state energy. Using this construction, it is possible to construct all ground states for $N_e \leq N_d$.

One year later, 1992, Tasaki [32] published a class of decorated lattices with lowest flat bands, for which he proved a similar result. In 1993 [33], we investigated these lattices further and showed how one can construct all ground states with $N_e \leq N_d$ for these decorated lattices. We further showed that for these lattices the characterization of the ground states can be mapped to a percolation problem. This allows us to show that the system remains ferromagnetic with an extensive but not saturated total spin S up to some critical density. Below that density the system is paramagnetic.

This construction is most easily understood for line graphs of planar bipartite graphs, see the kagome lattice in Fig. 1 as an example. For these graphs, the faces yield the single-particle ground state. The inner faces form a basis (not orthogonal). Neighboring faces of G have an edge in common. Therefore, putting electrons with different spin on neighboring faces may produce a double occupancy on that edge. This yields a higher energy. To obtain a ground state, electrons on neighboring faces should have the same spin. But if $N_e < N_d$ not all faces are occupied and one may form non-touching clusters with total spins pointing in different directions. Constructing non-touching clusters of faces is a percolation problem on the dual graph of G . This percolation problem has a percolation threshold, above which one large extended cluster is formed. This cluster has an extensive spin, whereas all other finite clusters have a finite spin. Therefore, above the percolation threshold the system is ferromagnetic. The percolation problem is not the classical percolation problem since each cluster with a spin S has a $2S + 1$ -fold degeneracy.

Since 1993, more classes of lattices with flat bands have been found and investigated. A general result, which covers all these cases, is available as well. It needs a condition on the projector $\rho = (\rho_{xy})_{x,y \in V}$ onto the space of single-particle ground-states [16, 34, 35].

Theorem (Mielke 1993, 1999) The Hubbard model with an N_d -fold degenerate single-particle ground state, $U_x > 0$, and $N_e \leq N_d$ electrons has a unique $(2S + 1)$ -fold degenerate ferromagnetic ground state with $S = N_d/2$ if and only if $N_e = N_d$ and ρ_{xy} is irreducible.

The original proof of this theorem was complicated and used a special construction for a non-orthonormal basis of single-particle ground-states. The later proof is simpler. First, the following result is shown:

Theorem (Mielke 1999) The Hubbard model with an N_d -fold degenerate single-particle ground-state, $U_x > 0$, and $N_e \leq N_d$ electrons has a multi-particle ground state with $S < N_e/2 - 1$ if it has a single spin-flip ground state with $S = N_e/2 - 1$.

In other words: To prove stability of ferromagnetism, it is sufficient to show that there is no single spin-flip ground state. This is indeed easy if $N_e = N_d$ and ρ_{xy} is irreducible. Therefore, the first theorem is a consequence of the second. Note that the second theorem is not trivial at all. For other lattices, you may easily construct cases where a ferromagnetic state is stable with respect to single spin flips but where it nevertheless is not the ground state of the system.

The last two results are very general; they hold for arbitrary lattices and arbitrary, even complex, hopping matrix elements t_{xy} . This is important because the flat band physics started to attract much attention in the past few years for mainly two reasons. First, using optical lattices it is now possible to investigate these systems experimentally. For instance the kagome lattice was build using that technique by Jo *et al.* in 2012 [36]. Second, people became interested recently in so-called topological flat bands. Here, the flat (often quasi flat) band arises from special choices for the phases of complex t_{xy} .

In 2003, Tanaka and Ueda [37] showed that for the special case of the kagome lattice, the ferromagnetic ground states remains stable if one introduces a special perturbation that yields a small dispersion to the lowest flat band, provided U is not too small. Similarly, Tasaki [38] showed in 1996 that for some decorated lattices the ferromagnetic ground state remains stable. These results are important because they indicate that flat band ferromagnetism is not something exotic like the Nagaoka ferromagnet.

Another interesting question is what happens if ρ_{xy} is not irreducible. Batista and Shastry [39] were the first to investigate an example for such a lattice; today many examples are known. One can show the following general results [40]:

Let ρ have the following properties:

1. ρ is reducible. It can be decomposed into N_r irreducible blocks ρ_k , $k = 1, \dots, N_r$. N_r should be an extensive quantity, *i.e.*, $N_r \propto N_d \propto |V|$, so that in the thermodynamic limit the density of degenerate single-particle ground states and the density of irreducible blocks are both finite.
2. Let V_k be the support of ρ_k , *i.e.*, the set of vertices for which at least one element of ρ_k does not vanish. $\rho_{k,xy} = 0$ if $x \notin V_k$ or $y \notin V_k$. One has $V_k \cap V_{k'} = \emptyset$ if $k \neq k'$ because of the fact that ρ_k are irreducible blocks of the reducible matrix ρ and $\bigcup_k V_k \subseteq V$.
3. We choose the basis B such that the support of each basis state $\psi_i(x) \in B$ is a subset of exactly one V_k . We denote the number of states belonging to the cluster V_k as ν_k . One has $\sum_k \nu_k = N_d$.
4. $\nu_{\max} = \max_k \{\nu_k\}$ is $O(1)$, *i.e.*, not an extensive quantity.

With these properties one can show

Theorem (Mielke 2012) For Hubbard models with a lowest single-particle eigenenergy 0 which is N_d -fold degenerate and for which the projector onto the eigenspace of 0 fulfils the properties listed above, the following results hold for $N_e \leq N_d$:

1. The ground state energy is 0.
2. Let A_x be an arbitrary local operator, *i.e.*, an arbitrary combination of the four creation and annihilation operators $c_{x\sigma}^\dagger$ and $c_{x\sigma}$. The correlation function $\rho_{A,xy} = \langle A_x A_y \rangle - \langle A_x \rangle \langle A_y \rangle$ has a finite support for any fixed x and vanishes if x and y are out of different clusters V_k . The system has no long-range order.
3. The system is paramagnetic.
4. The entropy at zero temperature $S(c)$ is an extensive quantity, $S(c) = \mathcal{O}(N_e)$. It increases as a function of $c = N_e/N_d$ from 0 for $c = 0$ to some maximal value $S_{\max} \geq \sum_k [(\nu_k - 1) \ln 2 + \ln(\nu_k + 2)]$ and then decays to $S(1) = \sum_k \ln(\nu_k + 1)$.

These models have therefore no long-range order. The most interesting aspect is the finite entropy at zero temperature.

3.5 Uniform density theorem

The uniform density theorem [41–43] is valid on a bipartite lattice and at half filling. The proof makes use of the particle-hole symmetry which is valid in that case. It states

Theorem (MacLachlan 1959, 1961; Lieb, Loss, McCann 1993) For the Hubbard model on a bipartite lattice and at half filling, either in a canonical ensemble with $N_e = |V|$ at $T > 0$ or in the ground state at $T = 0$ or in a grand canonical ensemble with $\mu = 0$, the density matrix $\rho_{\sigma,xy} = \langle c_{x\sigma}^\dagger c_{y\sigma} \rangle$ has the property

$$\rho_{\sigma,xy} = \frac{1}{2} \delta_{xy} \quad \text{if } x, y \in A \text{ or } x, y \in B \quad (23)$$

The theorem may appear to be trivial if one has a translationally invariant lattice in mind. The point is, it holds for arbitrary t_{xy} and arbitrary U_x on an arbitrary bipartite graph, translational invariance is not used and not necessary. The theorem is therefore of large importance in quantum chemistry, *i.e.*, for the Pariser-Parr-Pople variant of the Hubbard model.

3.6 Further rigorous results

There are further rigorous results on the Hubbard model. Many of them deal with the absence of ferromagnetism or at least with the absence of a fully polarized ground state under certain conditions. For details I refer to [8, 9, 44].

4 (Functional) Renormalization

4.1 General idea

First ideas on renormalization were developed in the '50s and '60s, mainly in the context of field theory, especially QED. The main idea is to separate different scales, often energy scales. If one is interested in the physics at low temperature, for example, one wants to separate degrees of freedom at higher energies from those at lower energies. Typically, this is done in many discrete steps or in a continuous form, either by integrating out the higher degrees of freedom or by separating them from the lower degrees of freedom. In that way, new effective interactions between the lower degrees of freedom are generated. If one is able to control them in some way, one can derive an effective theory at low energies.

Today, two ways have been used to apply this general idea to the Hubbard model. One idea is to use continuous unitary transformations to (block-) diagonalize the Hamiltonian of the system. This approach was developed independently by Wegner [45] and by Glazek and Wilson [46] and was applied to the Hubbard model by Wegner and coworkers [47–49]. The continuous unitary transformation brings the Hamiltonian to a block-diagonal form where in each block the number of quasi-particles is conserved. The transformation creates new interactions between the quasi-particles. These interactions, if they become strong, can cause instabilities of the Fermi liquid. A stability analysis shows which kinds of long-range order may occur.

The second, older, and more popular method is to use a field theoretic formulation and to integrate out higher degrees of freedom. Here as well, effective interactions occur and a stability analysis shows which instabilities occur.

In this section, we explain briefly the field theoretic renormalization. For a detailed and mathematical introduction I refer to the book of Salmhofer [50]. For a recent review I refer to [51].

4.2 Field-theoretic representation of the Hubbard model

In the following we want to deal with a system of interacting particles. Let us assume that we have a usual two-particle interaction. The single-particle contribution typically contains the kinetic energy and some single-particle potential. We assume that this contribution can be diagonalized, and we choose the basis for the representation of the Hamiltonian such that it is diagonal. Furthermore, we assume that we have a finite system where the single-particle energies ε_i are discrete. Eventually, we may take the thermodynamic limit. Then, the Hamiltonian is of the form

$$\hat{H} = \sum_i \varepsilon_i c_i^\dagger c_i + \sum_{i,j,k,l} V_{i,j,k,l} c_i^\dagger c_j^\dagger c_l c_k \quad (24)$$

Having such a system, one typically wants to calculate expectation values of some operators $A = A(\{c_i^\dagger, c_i\})$. At finite temperatures, they are

$$\langle A(\{c_i^\dagger, c_i\}) \rangle = Z^{-1} \text{Tr} \left[A(\{c_i^\dagger, c_i\}) \exp(-\beta(\hat{H} - \mu\hat{N})) \right] \quad (25)$$

where $\beta = 1/T$ is the inverse temperature, μ is the chemical potential and

$$Z = \text{Tr} \exp(-\beta(\hat{H} - \mu\hat{N})) \quad (26)$$

is the grand canonical partition function of the system. The traces are calculated over the entire Fock space. We now use the standard way to obtain a field-theoretic representation for the grand canonical partition function. For a general introduction see the book of Negele and Orland [52]. It uses two main ingredients:

1. Coherent states for fermions, constructed with the help of Grassmann variables ξ_i . A coherent state for Fermions is defined as an eigenstate of the annihilation operators and has the form

$$|\xi\rangle = \exp\left(-\sum_i \xi_i c_i^\dagger\right) |\text{vac.}\rangle = \prod_i (1 - \xi_i c_i^\dagger) |\text{vac.}\rangle \quad (27)$$

These states form an over-complete basis with the completeness relation

$$\int D[\xi] \exp\left(-\sum_i \xi_i^* \xi_i\right) |\xi\rangle \langle \xi| = 1 \quad (28)$$

2. The representation

$$\exp\left(-\beta(\hat{H} - \mu\hat{N})\right) = \left[\exp\left(-\frac{\beta}{M}(\hat{H} - \mu\hat{N})\right)\right]^M \quad (29)$$

together with the fact that for large M , *i.e.*, small $\varepsilon = \beta/M$ one has

$$\exp\left(-\varepsilon(\hat{H} - \mu\hat{N})\right) =: \exp\left(-\varepsilon(\hat{H} - \mu\hat{N})\right) : + \mathcal{O}(\varepsilon^2) \quad (30)$$

The symbols $: \cdot :$ denote normal ordering, which means that all creation operators stand left of all annihilation operators. We need the normal ordering to calculate matrix elements of operators between two coherent states. If the operator is normal-ordered, we obtain its matrix element simply by replacing the creation and annihilation operators by the corresponding Grassmann variables.

These two ingredients are used to write the partition function in the form

$$Z = \lim_{M \rightarrow \infty} \int D[\xi] \exp\left(-S_M[\xi]\right) \quad (31)$$

$$S_M[\xi] = \varepsilon \sum_{k=1}^M \left[\sum_i \xi_{i,k}^* \left(\frac{\xi_{i,k} - \xi_{i,k-1}}{\varepsilon} - \mu \xi_{i,k} \right) + H(\{\xi_{i,k}^*, \xi_{i,k-1}\}) \right] \quad (32)$$

where $\varepsilon = \beta/M$. Typically one introduces in the limit $M \rightarrow \infty$ the function $\xi_i(\tau)$, where $\xi_{i,k} = \xi_i(\varepsilon k)$. Then we may write

$$\frac{\xi_{i,k} - \xi_{i,k-1}}{\varepsilon} = \frac{\xi_i(\varepsilon k) - \xi_i(\varepsilon k - \varepsilon)}{\varepsilon} \rightarrow \frac{\partial \xi_i(\tau)}{\partial \tau} \quad (33)$$

$$\varepsilon \sum_{k=1}^M \rightarrow \int_0^\beta d\tau \quad (34)$$

and

$$S[\xi] = \int_0^\beta d\tau \left(\sum_i \xi_i^*(\tau) \left(\frac{\partial}{\partial \tau} - \mu \right) \xi_i(\tau) + H(\{\xi_i^*(\tau), \xi_i(\tau)\}) \right) \quad (35)$$

$$Z = \int_{\xi_i(\beta) = -\xi_i(0)} D[\xi] \exp(-S[\xi]) \quad (36)$$

Here and in the following I give only a brief overview, for details I refer to standard text books like [52].

To use this method for a renormalization of the Hubbard model, we formulate the Hubbard model in momentum space

$$H = \sum_{\vec{k}, \sigma} \varepsilon_{\vec{k}} c_{\vec{k}, \sigma}^\dagger c_{\vec{k}, \sigma} + \frac{1}{2} \sum_{k_1 \dots k_4, \sigma_1 \dots \sigma_4} V_{\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4} c_{\vec{k}_1, \sigma_1}^\dagger c_{\vec{k}_2, \sigma_2}^\dagger c_{\vec{k}_4, \sigma_4} c_{\vec{k}_3, \sigma_3} \quad (37)$$

Due to translational invariance, the single-particle Hamiltonian H_{kin} is diagonal. Further, we use the fact that the functions $\xi_i(\tau)$ are anti-periodic and use a Fourier representation ϕ with Fourier frequencies ω_n . The partition function now becomes

$$Z = \int D[\phi] \exp(S[\phi^*, \phi]) \quad (38)$$

$$S[\phi^*, \phi] = \sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \phi_K^* \phi_K - V[\phi^*, \phi] \quad (39)$$

where $K = (\omega_n, \vec{k}, \sigma)$ is a multi index, which contains the wave vector, the frequencies ω_n , and the spin. The interaction is still a generic interaction.

The physics of the system can be obtained by calculating expectation values, in particular propagators. This can be done using the generating functions. There are several ways to do that. A generating function that yields all connected propagators is

$$W[J^*, J] = \ln \left\langle \exp \left(-V[\phi^*, \phi] + \sum_K (J_K^* \phi_K + \phi_K^* J_K) \right) \right\rangle_0 \quad (40)$$

Here $\langle \dots \rangle_0$ denotes the expectation value in the non-interacting system, *i.e.*,

$$\langle A[\phi^*, \phi] \rangle_0 = \frac{\int D[\phi] A[\phi^*, \phi] \exp \left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \phi_K^* \phi_K \right)}{\int D[\phi] \exp \left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \phi_K^* \phi_K \right)} \quad (41)$$

The main idea of renormalization is simple. We introduce a cut-off Λ and perform all integrals in the expression for W over fields ϕ_K and ϕ_K^* for which $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda$. The remaining integrals can again be written as

$$W[J^*, J] = \ln \left\langle \exp \left(-V_\Lambda[\phi^*, \phi, J^*, J] + \sum_{K: |i\omega_n - \varepsilon_{\vec{k}} + \mu| < \Lambda} (J_K^* \phi_K + \phi_K^* J_K) \right) \right\rangle_{\Lambda, 0} \quad (42)$$

The non-interacting part now depends on Λ since the integration over some of the fields introduces new quadratic contributions. Since the original system is translationally invariant, the new quadratic contributions are translationally invariant and hence diagonal. Therefore, the average depends on Λ . The new interaction $V_\Lambda[\phi^*, \phi, J^*, J]$ also depends explicitly on Λ and on the fields J_K and J_K^* with $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda$. In the new integral, divergences are shifted, since the single-particle energies $\varepsilon_{\vec{k}}$ and eventually μ as well are shifted. Since we are interested in propagators near the Fermi surface, the fields J_K and J_K^* in $V_\Lambda[\phi^*, \phi, J^*, J]$ are uninteresting. We will never calculate derivatives with respect to these fields. Therefore we may set them to 0 explicitly.

In a next step, we introduce a new cut-off Λ_1 and perform the integral over all fields ϕ_K and ϕ_K^* for which $|i\omega_n - \varepsilon_{\vec{k}} + \mu| > \Lambda_1$. This yields again a new V_{Λ_1} and shifted single-particle energies. We iterate this procedure and obtain finally an effective theory that depends only on fields with small values of $|i\omega_n - \varepsilon_{\vec{k}} + \mu|$. This is now the effective theory we are looking for. *A priori* it is not clear that the procedure converges. For special cases and for not too large interaction, one can eventually prove convergence.

Let us mention that there are various technically different variants of the procedure described above. Instead of a discrete series of steps one can vary the cut-off continuously. Instead of a hard cut-off as described above, one can introduce a soft cut-off (these notions will be explained later). Instead of W one can use a different generating function. For Fermi systems it is often easier not to use W but

$$G_{\text{eff}}[\psi^*, \psi] = \ln \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_0 \quad (43)$$

W and G_{eff} contain the same information and can be mapped to each other. To see that, we calculate

$$\begin{aligned} & Z_0 \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_0 \\ &= \int D[\phi] \exp\left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \phi_K^* \phi_K - V[\phi^* + \psi^*, \phi + \psi]\right) \\ &= \int D[\phi] \exp\left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) (\phi_K^* - \psi_K^*) (\phi_K - \psi_K) - V[\phi^*, \phi]\right) \\ &= \exp\left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \psi_K^* \psi_K\right) \\ &\quad \times \int D[\phi] \exp\left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \phi_K^* \phi_K \right. \\ &\quad \left. - V[\phi^*, \phi] - \sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) (\phi_K^* \psi_K + \psi_K^* \phi_K)\right) \\ &= Z_0 \exp\left(\sum_K (i\omega_n - \varepsilon_{\vec{k}} + \mu) \psi_K^* \psi_K + W[C(K)^{-1} \psi_K^*, C(K)^{-1} \psi_K]\right) \end{aligned} \quad (44)$$

and therefore

$$G_{\text{eff}}[\psi^*, \psi] = \sum_K \psi_K^* C(K)^{-1} \psi_K + W[C(K)^{-1} \psi_K^*, C(K)^{-1} \psi_K] \quad (45)$$

where

$$C(K) = \frac{1}{i\omega_n - \varepsilon_{\vec{k}} + \mu} \quad (46)$$

Without going into the details, let us mention that since W is the generating function for connected propagators, one can show that G_{eff} is the generating function for connected, amputated propagators. Due to the factors $C(K)^{-1}$ in the argument of W , one multiplies the final result by a factor $C(K)^{-1} = (i\omega_n - \varepsilon_{\vec{k}} + \mu)$ for each derivative one takes, so that the factors $C(K)$ for the external lines are cancelled.

4.3 Renormalization group equations for G_{eff}

In this subsection we derive the renormalization group equation for the effective action. In contrast to the above description for W we will use a continuous renormalization. For computational and mathematical details we refer to [50].

Let us introduce the modified propagator

$$C^\Lambda(K) = \frac{\Theta_\Lambda(K)}{i\omega_n - (\varepsilon_{\vec{k}} - \mu)} \quad (47)$$

Here $\Theta_\Lambda(K)$ is a cut-off function. The most simple case would be a hard cut-off, *e.g.*,

$$\Theta_\Lambda(K) = \theta(|\varepsilon_{\vec{k}} - \mu - i\omega_n| - \Lambda) \quad (48)$$

For analytic calculations, a cut-off function that is differentiable might be more suitable. This is called a weak cut-off. For $|\varepsilon_{\vec{k}} - \mu - i\omega_n| \gg \Lambda$ one has $\Theta_\Lambda(K) = 1$ and $C^\Lambda(K) = C(K)$. For $|\varepsilon_{\vec{k}} - \mu - i\omega_n| \ll \Lambda$ one has $\Theta_\Lambda(K) = 0$ and therefore $C^\Lambda(K) = 0$. I define

$$G_{\text{eff}}^\Lambda[\psi^*, \psi] = \ln \frac{\int D[\phi] \exp\left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K - V[\phi^* + \psi^*, \phi + \psi]\right)}{\int D[\phi] \exp\left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K\right)} \quad (49)$$

For values of K with $\Theta_\Lambda(K) = 0$ only $\phi_K = 0$ contributes. G_{eff}^Λ is then given by $-V$. For values of K with $\Theta_\Lambda(K) = 1$, G_{eff}^Λ is given by G_{eff} . G_{eff}^Λ interpolates between $-V$ and G_{eff} . The goal is to derive a differential equation for G_{eff}^Λ which has the initial condition $-V$ and can be solved. We start with

$$F[\psi^*, \psi] = F \left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*} \right] \exp\left(\sum_K (\eta_K^* \psi_K + \eta_K \psi_K^*)\right) \Big|_{\eta=\eta^*=0} \quad (50)$$

$$\begin{aligned} & \int D[\phi] \exp\left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K + \sum_K (\eta_K^* \phi_K + \eta_K \phi_K^*)\right) \\ &= \exp\left(\sum_K \eta_K^* C^\Lambda(K) \eta_K\right) \int D[\phi] \exp\left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K\right) \end{aligned} \quad (51)$$

The second equation can be written as

$$\begin{aligned} \left\langle \exp \left(\sum_K (\eta_K^* \phi_K + \eta_K \phi_K^*) \right) \right\rangle_{\Lambda,0} &= \frac{\int D[\phi] \exp \left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K + \sum_K (\eta_K^* \phi_K + \eta_K \phi_K^*) \right)}{\int D[\phi] \exp \left(\sum_K \phi_K^* (C^\Lambda(K))^{-1} \phi_K \right)} \\ &= \exp \left(\sum_K \eta_K^* C^\Lambda(K) \eta_K \right) \end{aligned} \quad (52)$$

This yields

$$\begin{aligned} \exp(G_{\text{eff}}^\Lambda[\psi^*, \psi]) &= \langle \exp(-V[\phi^* + \psi^*, \phi + \psi]) \rangle_{\Lambda,0} \\ &= \exp \left(-V \left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*} \right] \right) \left\langle \exp \left(\sum_K (\eta_K^* (\phi_K + \psi_K) + \eta_K (\phi_K^* + \psi_K^*)) \right) \right\rangle \Big|_{\eta=\eta^*=0} \\ &= \exp \left(-V \left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*} \right] \right) \exp \left(\sum_K \eta_K^* C^\Lambda(K) \eta_K + \sum_K (\eta_K^* \psi_K + \eta_K \psi_K^*) \right) \Big|_{\eta=\eta^*=0} \\ &= \exp \left(-V \left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*} \right] \right) \exp \left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi_K^*} \right) \exp \left(\sum_K (\eta_K^* \psi_K + \eta_K \psi_K^*) \right) \Big|_{\eta=\eta^*=0} \\ &= \exp \left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi_K^*} \right) \exp \left(-V \left[\frac{\partial}{\partial \eta}, \frac{\partial}{\partial \eta^*} \right] \right) \exp \left(\sum_K (\eta_K^* \psi_K + \eta_K \psi_K^*) \right) \Big|_{\eta=\eta^*=0} \\ &= \exp \left(\sum_K \frac{\partial}{\partial \psi_K} C^\Lambda(K) \frac{\partial}{\partial \psi_K^*} \right) \exp \left(-V[\psi_K^*, \psi_K] \right) \end{aligned} \quad (53)$$

and

$$\frac{\partial}{\partial \Lambda} \exp(G_{\text{eff}}^\Lambda[\psi^*, \psi]) = \sum_K \frac{\partial}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial}{\partial \psi_K^*} \exp(G_{\text{eff}}^\Lambda[\psi^*, \psi]) \quad (54)$$

finally

$$\frac{\partial}{\partial \Lambda} G_{\text{eff}}^\Lambda[\psi^*, \psi] = \sum_K \frac{\partial}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial G_{\text{eff}}^\Lambda[\psi^*, \psi]}{\partial \psi_K^*} + \sum_K \frac{\partial G_{\text{eff}}^\Lambda[\psi^*, \psi]}{\partial \psi_K} \frac{\partial C^\Lambda(K)}{\partial \Lambda} \frac{\partial G_{\text{eff}}^\Lambda[\psi^*, \psi]}{\partial \psi_K^*} \quad (55)$$

This is the differential equation for G_{eff}^Λ we were looking for. It is an exact renormalization group equation.

4.4 Numerical solutions

In general, it is not possible to solve the renormalization equation exactly. Furthermore, it is not at all clear that the results do not diverge. It is well known that for sufficiently low temperatures, a divergence occurs that leads to a superconducting instability. The Fermi liquid becomes a superconductor. This effect is called the Kohn-Luttinger effect. It was found by

Kohn and Luttinger [53] in a second order perturbative calculation in 1965 and can be treated in a mathematically rigorous way [50].

The exact flow equation (55) is the basis of various approximations. Approximations are mostly truncations of the effective action G_{eff} . In general, it contains arbitrary many-body terms. Most approximations truncate it to a two-particle term. Often, further truncations to special two-particle terms are used. It turns out that rather simple truncations are sufficient to describe the many-body phenomena one is interested in. Compared to other techniques, the functional renormalization group has many advantages. The most important is that it allows for a very precise description of low energy scales. For a detailed review of truncation schemes I refer to [51].

But even after a suitable truncation, the resulting equations for the expansion coefficients can often not be treated analytically. A numerical solution is possible, but needs a discretization of k -space. Often, one uses a discretization along the Fermi surface (in 2D, a line) and splits the k -space in sectors, each containing exactly one of the segments of the Fermi surface. First results applying such a truncation and discretization scheme were obtained by Halboth and Metzner [54,55]. Their approach neglected the frequency dependence. More recent approaches are more sophisticated, using a more elaborate truncation scheme or taking the frequency dependence into account.

4.5 Some results

Without going into details, we list some of the important instabilities found using renormalization theory, mainly in two dimensions. For a detailed review we refer to the article of Metzner *et al.* [51].

1. On the square lattice with nearest-neighbor hopping t , next-nearest-neighbor hopping t' , and (if not stated otherwise) a repulsive interaction $U > 0$ one finds several instabilities of the Fermi liquid:

- (a) Anti-ferromagnetism at or close to half filling ($\mu = 0$) for $t' = 0$.

This is consistent with the expectations for large U and with Lieb's theorem, see Sect. 3.1.

- (b) d -wave Cooper pairing at small negative values of t' and away from half filling.

The $d_{x^2-y^2}$ pairing is found in a large parameter region using various different truncation schemes. It is therefore now widely believed that the Hubbard model has a d -wave superconducting ground state at weak repulsive interactions $U > 0$.

The interplay between anti-ferromagnetism and d -wave Cooper pairing is interesting since it occurs as well in high-temperature cuprate superconductors.

- (c) A Pomeranchuk instability (an anisotropic deformation of the Fermi surface) leading to orientational symmetry breaking, at sufficiently large $|t'|$.

According to the uniform density theorem, there is no Pomeranchuk instability on a bipartite lattice at half filling, see Sect. 3.5

- (d) A ferromagnetic instability, which may occur if one varies t' and μ simultaneously so that the system stays at the van Hove singularity. At the van Hove singularity, the density of states is infinite. A large or infinite density of states at the Fermi level is believed to favor ferromagnetism, according to the Stoner criterion, which is a simple translationally invariant mean-field criterion.

Although there is no extensive degeneracy of states in the single-particle spectrum at the Fermi surface, this results is similar to flat-band ferromagnetism, see Sect. 3.4. Let us mention that some of the functional renormalization schemes indicate a direct competition between ferromagnetism and superconductivity.

- (e) s -wave Cooper pairing at negative U .

2. On other two-dimensional lattices

- (a) Unconventional superconductivity or non-magnetic insulating states on the triangular lattice.

On the triangular lattice, the anti-ferromagnetic order is strongly suppressed because the lattice is not bipartite and the anti-ferromagnetic spin interaction is strongly frustrated.

At weak interactions, only a superconducting instability is expected.

- (b) On the hexagonal (honeycomb) lattice at half filling, the Fermi surface consists of a set of Dirac points. The density of states vanishes. There are no instabilities at small interactions. At stronger interactions, various instabilities have been found, including a spin liquid and f -wave Cooper pairing.

A more complete summary of these results can be found in [51].

5 Summary, conclusions, and outlook

The aim of this lecture was to present an introduction to the Hubbard model and its properties so that the reader has an overview and knows the very recent advances in the field as well. I put the focus on rigorous results, since they already provide much insight into the physics of the Hubbard model and serve as landmarks, and shortly described the method of functional renormalization and the results obtained.

The reader who is interested in rigorous results can take the three short reviews of Lieb [8] and Tasaki [9, 44] as a starting point or can dive into the original proofs using the references. There are still many open questions in this field.

The reader who wants to better understand functional renormalization should consult the review of Metzner *et al.* [51], or, if he is interested in the mathematical aspects, the book of Salmhofer [50].

Many other methods have been used to study the Hubbard model. Some of them are introduced and discussed in the other lectures in this School.

The fermionic Hubbard model has been investigated during the last 50 years, but there are still lots of open questions. In the past five years, the interest in the bosonic Hubbard model has increased, mainly because it is possible now to experimentally investigate such systems using optical lattices. Much less is known for the bosonic case. Most of the proof techniques that worked well for fermions cannot be applied here, so that there are only very few rigorous results. Other techniques that have been applied to the fermionic case are difficult as well. But due to the current and increasing interest, I expect many new results in this fascinating field in the near future.

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