The Hubbard model and its properties

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The Hubbard model

Electrons on a lattice with a screened interaction

Hamiltonian:

$$\begin{aligned} H &= H_{\mathrm{kin}} + H_{\mathrm{int}} \\ &= \sum_{x,y\in V,\sigma} t_{xy} c^\dagger_{x,\sigma} c_{y,\sigma} + \sum_x U_x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} c_{x\uparrow} \end{aligned}$$

V is the set of vertices (lattice sites).

$T = (t_{xy})_{x,y\in V}$ describes the hopping, t_{xy} may be complex, but T should be self adjoint. In this talk we assume t_{xy} to be real.

Often nearest neighbour hopping: $t_{xy} = t$ for nearest neighbours, 0 otherwise.

U_x is a local (repulsive) interaction. Often $U_x = U$ independent of x.

Historical remarks

- Pariser, Parr and independently Pople formulated and used the model 1953 in quantum chemistry.
- Hubbard formulated the model in 1963 to understand electron correlations in narrow energy bands.
- Kanamori independently introduced the model in 1963 to describe itinerant ferromagnetism.
- Gutzwiller independently introduced the model in 1963 to understand the metal-insulator transition.
- $\sim$ 1.400 papers on the Hubbard model before 1980.
- $\sim$ 14.000 papers on the Hubbard model before 2000.
- $\sim$ 55.000 papers on the Hubbard model till today.
  (numbers from Google Scholar)

Symmetries of the Hubbard model

Gauge symmetry:

$$c^\dagger_{x\sigma} \to \exp(i\alpha) c^\dagger_{x\sigma}, \quad c_{x\sigma} \to \exp(-i\alpha) c_{x\sigma}$$

The Hamiltonian

$$H = \sum_{x,y \in V,\sigma} t_{xy} c^\dagger_{x,\sigma} c_{y,\sigma} + \sum_x U_x c^\dagger_{x\uparrow} c^\dagger_{x\downarrow} c_{x\downarrow} c_{x\uparrow}$$

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

Symmetries of the Hubbard model

Spin symmetry:

Pauli matrices

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

local spin operators: $S_{\alpha,x} = \frac{1}{2}\sum_{\sigma,\sigma'} c^\dagger_{x\sigma}(\sigma_\alpha)_{\sigma,\sigma'} c_{x\sigma'}, \quad \alpha = x, y, z, \quad \mathbf{S}_x = (S_{x,x}, S_{y,x}, S_{z,x})$

global spin operators:

$$S_\alpha = \sum_x S_{\alpha,x}, \quad \mathbf{S} = (S_x, S_y, S_z),\ S_\pm = S_x \pm iS_y, \quad S_+ = \frac{1}{2}\sum_{\vec{n}} c^\dagger_{x\uparrow} c_{x\downarrow}, \quad S_- = S_+^\dagger$$

These operators form an $SU(2)$ algebra, $[S_x, S_y] = iS_z$.
The Hamiltonian commutes with these operators, it has a $SU(2)$ -symmetry.
H, $\mathbf{S}^2$ and S_z can be diagnosed simultaneously.

Symmetries of the Hubbard model

Particle-hole transformations:

$$c^\dagger_{x\sigma} \to c_{x\sigma}, \quad c_{x\sigma} \to c^\dagger_{x\sigma}$$

the Hamiltonian becomes

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

For a bipartite lattice, *i.e.* a lattice, which decays 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:

$$c^\dagger_{x\sigma} \to c^\dagger_{x\sigma} \text{ if } x \in A, \quad c^\dagger_{x\sigma} \to -c^\dagger_{x\sigma} \text{ if } x \in B$$

This transformation changes the sign of the kinetic energy.

Symmetries of the Hubbard model

Pseudo-Spin Symmetry

For a bipartite lattice at half filling, the Hamiltonian commutes with the operators

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

This is a second $SU(2)$-symmetry.
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.

Symmetries of the Hubbard model

Further symmetries

- Lattice symmetries:
  On translationally invariant lattices, the model has the symmetries of the lattice.
- The one-dimensional case:
  - The one dimensional Hubbard model is solvable by the Bethe ansatz.
  - It has an infinite set of invariants.

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Some rigorous results

Lieb's Theorem (1989)

Let H be the Hubbard Hamiltonian in 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 $S = 0$.

Remark

- On a bipartite lattice, using a combined particle-hole and phase transformation for spin-down only 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 with the above transformation transforms to $\hat{S}_z$, one obtains a result for $\hat{S}_z = 0$, *i.e.* $N_e = |V|$, *i.e.* half filling.

Corollary (Lieb 1989)

Let H be the Hubbard Hamiltonian 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 $S = \frac{1}{2}||A| - |B||$.

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Why $S = \frac{1}{2}||A| - |B||$?

1. $T = (t_{xy})_{x,y \in V}$ has a symmetric spectrum and the rank of T is $\max(|A|, |B|)$. Therefore, the eigenvalue 0 has a degeneracy of $||A| - |B||$. Applying Hund's rule (Mielke 1993) for small U yields $S = \frac{1}{2}||A| - |B||$.
2. For large U and half filling, the Hubbard model can be mapped to an antiferromagnetic Heisenberg model

$$H_{\mathrm{eff}} = \sum_{x,y} \frac{2t_{xy}^2}{U} \mathbf{S}_x \cdot \mathbf{S}_y$$

Lieb’s Theorem

- proves long range order – ferrimagnetism – on bipartite lattices with $|A| = \alpha|B|$, $\alpha \neq 1$.
- does not prove anti-ferromagnetism, i.e.long range order for $|A| = |B|$.
- There is no proof for long range anti-ferromagnetic order in the Hubbard model.

Some rigorous results

The Mermin-Wagner Theorem
(no long range order in one or two dimensions at finite temperature)

Theorem (Koma, Tasaki 1992) For a Hubbard model in one and two dimensions with finite range 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

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

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

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

Some rigorous results

The Mermin-Wagner Theorem, remarks

- Originally, Mermin and Wagner showed the absence of long range order at finite temperate and $d = 1$ or $d = 2$ for the Heisenberg ,model in 1966.
- Walker and Ruijgrok (1968) and Gosh (1971) extended the result to the Hubbard model.
- The result can be extended to many lattice models with a continuous symmetry.
- The proof by Koma and Tasaki is very general, it only needs a $U(1)$ symmetry.
- The algebraic decay $|x - y|^{-\alpha f(\beta)}$ is not optimal for large temperature, one expects an exponential decay.

Some rigorous results

Nagaoka’s Theorem (ferromagnetic ground state at hard-core interactions and one hole in a half-filled band)

Theorem (Tasaki 1989) The Hubbard model 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.

Some rigorous results

Nagaoka's Theorem, some remarks

- Original proofs by Thouless 1965, and Nagaoka 1966.
- The proof makes use of the Perron-Frobenius theorem, stating that an irreducible matrix with non-negative entries has non degenerate largest eigenvalue and the corresponding eigenstate has positive entries.
- Variational results by many people show that the result breaks down for $N_e < |V| - 1$ or not too large U.
- Especially on bipartite lattice, the Nagaoka ferromagnet seems to be a singular result.

Some rigorous results

Flat-band ferromagnetism, preliminary remarks

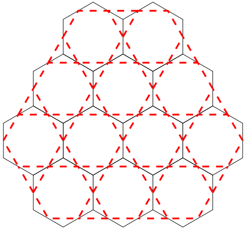
- Hund's rule favours ferromagnetism if there are degenerate single-particle eigenstates.
- For a lowest flat band, the existence of a ferromagnetic ground state is trivial.
- The main question is: When is the ferromagnetic ground state unique?
- An important quantity to answer this question is the single particle density matrix ρ_{xy}, i.e. the lattice representation of the projector onto the single particle eigenstates forming the flat band, $\rho_{xy} = \sum_i \psi_i^*(x)\psi_i(y)$, where $\psi_i(x)$ form an orthonormal basis of the degenerate single particle states forming the flat band.

25 years of flat bands

- First result by E. Lieb 1989, ferrimagnetism on bipartite lattices with a flat band.
- Ferromagnetism on line graphs, example Kagomé lattice: A. Mielke 1991ff.
- Decorated lattices: H. Tasaki (partially with A. Mielke) 1992ff.
- Complete description for fermions with irreducible $(\rho_{xy})_{x,y\in V}$: A. Mielke 1999.
- First examples with highly reducible $(\rho_{xy})_{x,y\in V}$ by Batista and Shastry 2003.
- Topologically flat bands, various authors, starting around 2008.
- First paper with correlated Bosons in flat bands: Huber and Altman 2010.
- First experimental realisation of the Kagomé lattice as an optical lattice: Jo et al. (Stamper-Kurn group, Berkeley) 2011.
- Complete description for fermions with highly reducible $(\rho_{xy})_{x,y\in V}$: A. Mielke 2012.
- Complete description for bosons and 2d line graphs below the critical density: J. Motruk, A. Mielke 2013.
- Pair formation has been observed in 1d Bose-Hubbard models by Takayoshi et al (2013), Phillips et al (2014).

Lattices with flat bands

- The Lieb lattice (a decorated square lattice, one additional vertex on each edge).
- Kagomé lattice, line graph of the hexagonal lattice.



- Pyrochlore lattice, line graph of the diamond lattice.

Fermions, ρ_{xy} irreducible

Theorem (1)

The Hubbard model with a N_d fold degenerate single particle ground state 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 proof has two steps:

Theorem (2)

The Hubbard model with a N_d fold degenerate single particle ground state 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 $S = N_e/2 - 1$.

and

Theorem (3)

The Hubbard model with a N_d fold degenerate single particle ground state and $N_e = N_d$ electrons has a multi-particle ground state with $S = N_d/2 - 1$ if and only if ρ_{xy} is reducible.

Examples of lattices with irreducible ρ_{xy}

- All complete graphs, see e.g. Mielke, Tasaki: cond-mat/9606115.
- All line graphs of bipartite, 2-connected graphs with positive nearest neighbour hopping.

  Prominent examples:

  - Kagomé lattice, line graph of the hexagonal lattice.
  - Pyrochlore lattice, line graph of the diamond lattice.
- All decorated graphs of Tasaki-type.
- Several topologically flat bands, see e.g. H. Katsura et al, EPL 91, 57007 (2010).

Fermions, ρ_{xy} highly reducible

ρ should have the following properties:

1. ρ is reducible. It can be decomposed into N_r irreducible blocks ρ_k, $k = 1, \ldots, N_r$. 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 states $\psi_i(x)$ 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.

Fermions, ρ_{xy} highly reducible

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 on the previous slide, 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 $c^{\dagger}_{x\sigma}$ 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, $S(c) = O(N_e)$. 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.

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Five steps towards renormalisation

1. Rewrite the Hubbard model in momentum space in a field theoretic form using Grassmann fields.
2. Find a generating function of correlation functions.
3. Show that the generating function is equivalent to the effective action.
4. Derive an exact renormalisation equation for the effective action.
5. Solve that equation or obtain rigorous results from it.

Field theoretic representation

Hubbard model in momentum space

$$H = \sum_{\vec{k},\sigma} \epsilon_{\vec{k}} c^{\dagger}_{\vec{k},\sigma} c_{\vec{k},\sigma} + \frac{1}{2} \sum_{k_1 \dots k_4, \sigma_1 \dots \sigma_4} V_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} c^{\dagger}_{\vec{k}_1 \sigma_1} c^{\dagger}_{\vec{k}_2,\sigma_2} c_{\vec{k}_4,\sigma_4} c_{\vec{k}_3,\sigma_3}$$

The partition function can be written as

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

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

where ϕ_K are Grassman fields, $K = (\omega_n, \vec{k}, \sigma)$ is a multi index, which contains the wave vector, the Matsubara frequencies $\omega_n = \frac{(2n+1)\pi}{\beta}$, and the spin.The interaction is still a generic interaction.

Generating function and effective action

There are several ways to do that. A generating function which yields all connected propagators is

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

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

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

The effective action

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

is related to the generating function W via

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

where

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

Renormalisation group equation

The main idea of renormalisation is simple:

- Introduce a cut-off Λ
- Perform all integrals in the expression for $G_{\rm eff}$ or W over fields ϕ_K and ϕ_K^* for which $|i\omega_n - \epsilon_{\vec{k}} + \mu| > \Lambda$.
- Derive an equation which determines how $G_{\rm eff}$ depends on Λ.

Let us introduce the modified propagator

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

The resulting equation is

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

Solutions

- In general, it is not possible to solve the renormalisation equation exactly.
- The results may diverge.
- It is well known that for sufficiently low temperatures, a divergence occurs which leads to a superconducting instability. The Fermi liquid becomes a superconductor. This effect is called Kohn-Luttinger effect.
- The exact flow equation is the basis of various approximations.
- Even approximations often need additional numerical solutions, using various discretisation and truncation schemes.

Some results

1. On the square lattice with nearest neighbour hopping t, next nearest neighbour hopping t', and (if not stated otherwise) a repulsive interaction $U > 0$
   1. Anti-ferromagnetism at or close to half filling ($\mu = 0$) for $t' = 0$.
   2. $d_{x^2-y^2}$-wave Cooper pairing at small negative values of t' and and away from half filling.
   3. A Pomeranchuk instability (an an-isotropic deformation of the Fermi surface) leading to orientational symmetry breaking, at sufficiently large $|t'|$.
   4. A ferromagnetic instability, which may occur if one varies t' and μ simultaneously so that the system stays at the van Hove singularity.
   5. s-wave Cooper pairing at negative U.
2. On other two-dimensional lattices
   1. Unconventional superconductivity or non-magnetic insulating states on the triangular lattice.
   2. On the hexagonal (honeycomb) lattice at half filling and at stronger interactions, various instabilities have been found, including a spin liquid and f-wave Cooper pairing.

Contents

Summary

The Hubbard model

1. Describes interacting itinerant fermions on a lattice.
2. Magnetic ordering:
    1. Anti-ferromagnetic or ferrimagnetic order at half filling on bipartite lattices.
    2. Ferromagnetism at large or infinite density of states at the Fermi level.
3. Superconductivity:
    1. s-wave pairing for attractive $U < 0$.
    2. $d_{x^2-y^2}$ wave-pairing for small repulsive $U > 0$ and not too close to half filling.
    3. f-wave or higher pairing for special lattices.
4. Other phenomena:
    1. Pomeranchuk instability.
    2. Metall insulator transition (Mott transition).
    3. . . .

Thank you!