Hubbard Model: An Overview

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Abstract

This is a brief overview of Hubbard model. Section 1 is brief history and an overview of the power of Hubbard model. Formulation of Hubbard model is discuss in section 2 and the solution of the model is derived in section 3. Special cases as our first interpretation of Hubbard model, where $t = 0$ or $U = 0$, is discuss in section 4. As a conclusion, an intriguing interplay of the wave and particle aspect of Hubbard model is covered on the last section 5.

1 Introduction

Hubbard model is a paradigm in condensed matter physics, reducing many-body interactions to an effective one-body descriptions.[1]

The Hubbard model is named after John Hubbard following the submission of his 1963 paper. Hubbard continued to refine his model, which would eventually led to six installments.

This papers launched the field of strongly correlated systems and its variants constitute an important research topic in theoretical condensed matter physics.

Technically, Hubbard model is just an extension of the so-called tight-binding model where in electron can hop between lattices without feeling each other. Qualitatively, Hubbard model gives a different result from tight-binding model for strong interactions. For instance, Hubbard model at half filling - one electron per lattice site - is capable of reproducing Mott transition.

Analytical methods of solving the Hubbard model are all approximate, except in 1D, where the so called Bethe ansatz provides an exact solution.

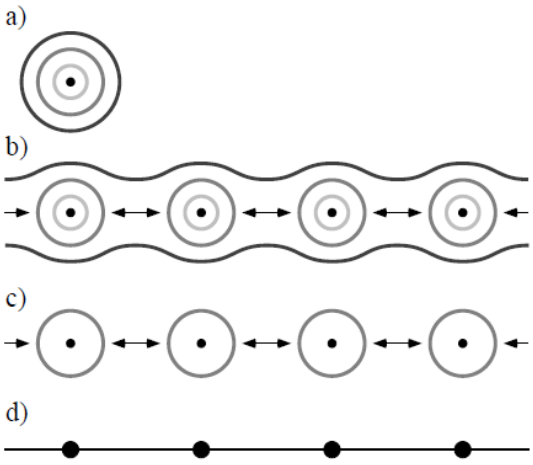

Figure 1: Hubbard Model lattice sites

Our focus on this report is the one dimensional Hubbard model for it is integrable, which means that many physical properties can be determined exactly. One dimensional Hubbard model solution serves as a benchmark of other approximate and numerical methods. This allows us to study many-body physics beyond the restrictions of perturbation theory or intuitive non-systematic approximations.

2 Formulation of Hubbard Model

Hubbard model consists of lattice sites, and a set of electrons that hop around from site to neighboring site in the lattice. Figure 1 is the best transformation of an (a) atomic orbits in a (b) crystal that is (c) non-degenerate into a (d) lattice site. An electron has a property called spin that can either be spin up or spin down.

A particular lattice site can accommodate zero, one, or two electrons, but if two electrons are on the same site they must have opposite spin to obey the Pauli exclusion principle. A configuration with two electrons of opposite spin on the same site has an increased energy, because electrons repel each other electrically. That energy cost is denoted U.

It is also assumed that an electron can hop from one site to a neighboring site; when it does so, its spin doesn't change. The change of hopping to

another neighboring site is based on the variable conventionally denoted by -t.

Certain refinements can be added to the model. One can add a magnetic field h. If h is positive, it will favor configurations that have more electrons with spin up. Another refinement could be the addition of chemical potentials. A positive chemical potential increases the energy of configurations that have more electrons.

For this study, we'll focus on the Hubbard model bare, without any form of refinement. To start with, we need to be introduced to tight-binding model.

2.1 Extension of tight-binding model

Hubbard model is based on tight-binding approximation. In tight-binding approximation, electrons are viewed as occupying the standard orbitals of their constituent atoms, and then "hopping" between atoms during conduction. Tigh-binding model consider the interaction of a single electron with the potential of nuclei and other electrons in an average way only. Using second quantization formalism, the Hamiltonian operator in tight-binding framework is given as,

$$H = -t \sum_{(i,j,\sigma)} (c^{\dagger}_{(i,\sigma)} c_{(j,\sigma)}) + h.c. \tag{1}$$

Hubbard model formulates the conduction in terms of the hopping integral to include the so-called "on-site repulsion", which stems from the Coulomb repulsion between electrons at the same atomic orbitals.

The Hamiltonian is now made up of two components: H_{hop} and H_{int}. The H_{hop} describes quantum mechanical hopping of electrons while H_{int} describes nonlinear repulsive interactions.

$$H = \underbrace{-t \sum_{(i,j,\sigma)} (c^{\dagger}_{(i,\sigma)} c_{(j,\sigma)})}_{H_{hop}} \underbrace{- U \sum_{(i=1)}^{N} (n_{(i,\uparrow)} n_{(i,\downarrow)})}_{H_{int}} \tag{2}$$

The hopping amplitude t is assumed to be real, representing the quantum amplitude that an electron hops from site i to j. The U is assumed to be real as well. Both t and U are treated as constant.

3 1D Hubbard Model Solution

For 1D Hubbard Model, an exact solution is provided by using the Bethe ansatz method. Bethe ansatz was invented to solve Heisenberg spin models, which is essentially a model of lattice bosons.

For one-dimensional Hubbard model we are interested in the ground state solution of the Schrodinger equation:

$$H\left|\psi\right\rangle = E\left|\psi\right\rangle \tag{3}$$

where H is given by equation (2).

The Hamiltonian, H, is found to commute with $\sum_{(i=1)}^{N} n_{(i,\uparrow)}$ and $\sum_{(i=1)}^{N} n_{(i,\downarrow)}$.

$$[\sum n_{(i,\uparrow)}, H] = [\sum n_{(i,\downarrow)}, H] = 0 \tag{4}$$

We can, then, look for energy eigenstate from the spin-down and spin-up fixed numbers M and M', where N = M + M' is the total number of electrons.

The fixed numbers M and M' are good quantum numbers for our eigenstate $|M, M'\rangle$. Therefore we characterize the Hamiltonian eigenstate by M and M', and rewrite the Schrodinger equation (3) as,

$$H\left|M, M'\right\rangle = E(M, M')\left|M, M'\right\rangle \tag{5}$$

The energy eigenstate can be recast as a linear combination of state of electron at specific sites.

$$\left|M, M'\right\rangle = \sum \underbrace{f(x_1, x_2, ..., x_N)}_{\text{amplitude of the state } |X\rangle} \quad \left|x_1, x_2, ..., x_N\right\rangle \tag{6}$$

For convenience we can write the N-tuple $x_1, x_2, ..., x_N$ as X,

$$\left|M, M'\right\rangle = \sum f(X)\left|X\right\rangle \tag{7}$$

Substituting this eigenstate to equation (5), we have

$$H\left|M, M'\right\rangle = E(M, M')\left|M, M'\right\rangle$$
$$H\sum f(X)\left|X\right\rangle = E(M, M')\sum f(X)\left|X\right\rangle$$

Using Hubbard hamiltonian, equation above we have,

$$T\sum_{i=1}^{N} f(x_1,...,x_i+1,...,x_N)+f(x_1,...,x_i-1,...,x_N) \\ +U\Big[\sum_{i<j}\delta(x_i-x_j)\Big]f(X)=Ef(X) \quad (8)$$

In equation (8), we have to solve for f and E. This is where Bethe ansatz is needed.

We can write the function $f(X)$ using Bethe ansatz as,

$$f(X)=\sum_{P}[Q,P]exp(i(k_{P1}x_{Q1},...,k_{PN}x_{QN})) \quad (9)$$

where $[Q,P]$ is a set of $N!\times N!$ coefficients indexed by a pair of permutations, Q,P, all yet to be determined. $Q=\{Q1,Q2,...,QN\}$ is the permutations that maps the indexed set $\{1,2,...,N\}$ into $Q1,Q2,...,QN$.

Substituting equation (9) to equation (8), we have

$$E=E(M,M')=-2T\sum_{j=1}cos(k_j) \quad (10)$$

4 Hubbard Model First Interpretation

Special cases of Hubbard model provides some insights about the model without doing difficult mathematics. This serves as the first test of the validity of the model. For Hubbard model, the cases of $t=0$ or $U=0$ can be diagonalized and understood by elementary means.[2]

4.1 Non-hopping system: $t=0$

For non-hopping system, our Hubbard model's Hamiltonian given by eq. (2) is reduced to $H_{t=0}=H_{int}=UD$, where

$$H_{t=0}=U\bigg(\sum n_{(j,\uparrow)}n_{(j,\downarrow)}\bigg) \quad (11)$$

This Hamiltonian is already a diagonalized form. A general eigenstate is given in terms of Wannier state,

$$|\mathbf{x}, \sigma\rangle = \left(\prod_{x \in X} c^{\dagger}_{x,\uparrow} \right) \left(\prod_{x \in Y} c^{\dagger}_{x,\downarrow} \right) |0\rangle \tag{12}$$

where X and Y represent lattice sites occupied by up-spin and down-spin electrons respectively. The total number of electrons is N = M + M' such that $|X| = M$ and $|Y| = M'$.

Using equation (12) our Hamiltonian is given now as,

$$H_{t=0} |\mathbf{x}, \sigma\rangle = E(M, M') |\mathbf{x}, \sigma\rangle \tag{13}$$

has an energy eigenvalues given by,

$$E(M, M') = \sum U_x = U \tag{14}$$

The limit $t \to 0$ of the Hubbard Hamiltonian (2) is called the atomic limit, because the eigenstate describes electrons localized at the sites.[2]

4.2 Non-interacting system: $U = 0$

Our Hamiltonian for non-interacting system is reduced to $H_{U=0} = H_{hop}$, the tight-binding Hamiltonian similar to equation (1) (including its conjugate of course).

$$H_{U=0} = -t \sum_{j} c^{\dagger}_{j,\sigma} c_{j,\sigma} + h.c. \tag{15}$$

This Hamiltonian is not diagonal since it is a quadratic form in fermion operators. This can be diagonalized by discrete Fourier transformation defined as,

$$c^{\dagger}_{j,\sigma} = \frac{1}{L} \sum_{k=0}^{L-1} \widetilde{c}^{\dagger}_{k,\sigma} e^{-i\phi jk} \tag{16}$$

Inserting equation (16) to equation (15) leads to,

$$
\begin{aligned}
H_{U=0} &= -t\sum_j c^\dagger_{j,\sigma}c_{j,\sigma} + h.c \\
&= -\frac{t}{L}\sum_j\sum_{k=0}^{L-1}\widetilde{c}^\dagger_{k,\sigma}e^{-i\phi jk}\widetilde{c}_{k,\sigma}e^{i\phi(j+1)k} + h.c \\
&= -\frac{t}{L}\sum_j\sum_{k=0}^{L-1}\widetilde{c}^\dagger_{k,\sigma}\widetilde{c}_{k,\sigma}e^{-i\phi jk}e^{i\phi jk}e^{i\phi k} + h.c \\
&= -\frac{t}{L}\sum_j\sum_{k=0}^{L-1}\widetilde{c}^\dagger_{k,\sigma}\widetilde{c}_{k,\sigma}(2cos(\phi k)) \\
&= -\frac{t}{L}\sum_{k=0}^{L-1}\widetilde{c}^\dagger_{k,\sigma}\widetilde{c}_{k,\sigma}(2Lcos(\phi k)) \\
&= -2t\sum_{k=0}^{L-1}cos(\phi k)\widetilde{n}_{k,\sigma}
\end{aligned}
$$

where $\widetilde{n}_{k,\sigma} = \widetilde{c}^\dagger_{k,\sigma}\widetilde{c}_{k,\sigma}$.

Now that it is diagonalize, we obtain an alternative basis. We introduce what is called the Bloch basis.

$$
|\mathbf{q},\sigma\rangle = \Big(\prod_{k\in K}\widetilde{c}^\dagger_{k,\uparrow}\Big)\Big(\prod_{k\in K'}\widetilde{c}^\dagger_{k,\downarrow}\Big)|0\rangle \tag{17}
$$

The row vector $\mathbf{q} = (q_1, ..., q_N)$ are the momenta of the electrons which are delocalized.

Using this Bloch basis for our Hamiltonian, we have

$$
H_{U=0}\,|\mathbf{q},\sigma\rangle = -2t\sum_{j=1}^{N}cos(q_j)\,|\mathbf{q},\sigma\rangle \tag{18}
$$

5 Physics of Hubbard Model

The physics of the Hubbard model maybe understood as arising from the competition between the two contributions, H_0 and D to the Hamiltonian.[2]

This is analogous to the competition of the minimization of energy and maximization of entropy.

It is also observe that wave-particle dualism plays a role in the competition between hopping tendency and the interaction of the electrons. In H_{hop}, electrons behave like "waves", note the cosine part of the eigenvalue, while H_{int} behave more as a "particle".

Technically, the tight binding Hamiltonian H_{hop} do not commute with the operator D which counts the number of doubly occupied sites.[2] Therefore the Hubbard Hamiltonian is not diagonal both in Bloch and Wannier basis.

An interesting aspect of the Hubbard model, aside from the mathematical difficulty, is the idea that even though the Hamiltonian H_{hop} and H_{int} gives us trivial order, their sum $H = H_{hop} + H_{int}$ is believed to generate various nontrivial order.

This interplay explains the transition from metal to insulator, antiferromagnetism, ferrimagnetism, ferromagnetism, Tomonaga-Luttinger liquid, and superconductivity.

References

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[2] Fabian H. L. Essier, Holger Frahm, Frank Gohmann, Andreas Klumper, Vladimir E. Korepin, *The One-dimensional Hubbard Model* Cambridge University Press, August 2009

[3] Hal Tasaki, *The Hubbard Model - Introduction and Selected Rigorous Results* arXiv:cond-mat/9512169v4

[4] Hubbard Model: `https://en.wikipedia.org/wiki/Hubbard_model`

[5] Tight-binding Model: `https://en.wikipedia.org/wiki/Tight_binding`