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Transformation of the Hubbard Hamiltonian to the t-J Hamiltonian using the Raleigh-Schrodinger Perturbation Expansion

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Abstract

The t-J model is deduced from the Hubbard model using Rayleigh-Schrodinger perturbation theory. The exchange is antiferromagnetic as found by other workers.

1.0 Introduction

The Hubbard model is used to study interacting electrons in narrow-band systems. The t-J model has been studied extensively in order to understand the various properties of the cuprate superconductors [1]. In the t-J model, u is much larger than the band width. The energy states will be either empty or occupied by a spin up or a spin down electron. Double occupation of states will be negligible.

To obtain the t-J model, one can use canonical transformation or degenerate perturbation theory. Both methods lead to the same result [2]. A vast amount of literature is dedicated to studying the properties of the Hubbard model by means of a canonical transformation [3,4,5]. In perturbation theory, one must look for a Hamiltonian which resembles but is not identical to the Hamiltonian of interest. Usually the Hamiltonian of interest cannot be solved exactly but the Hamiltonian that resembles it can be solved exactly. Generally, the full Hilbert space is divided into two: a model space and the remaining space [6]. A projection operator p is to be defined which projects onto the model space. Another projection operator Q = 1 – P, projects onto the remaining space. An effective Hamiltonian H_{eff} must also be defined, which acts on the model space only but which leads to the exact ground state energy E_o.

This is

$$Heff = PHP + PHQ\frac{1}{E_o - QHQ}QHP \tag{1}$$

2.0 Hubbard model and its effective t-J model.

The one band Hubbard model is [7]

$$H = -t\sum_{\langle ij\rangle\sigma}\left(c^{+}_{i\sigma}c_{j\sigma} + h.c\right) + u\sum_{i} n_{i\uparrow}n_{i\downarrow} \tag{2}$$

where $c^{+}_{i\sigma}$ creates an electron at site i and $\langle i, j\rangle$ are nearest neighbour. This model leads to the free particle, tight binding model when u = o. When t = 0, the system is fully localized and the ground state is an insulator. At half-filling, the model has one electron per site, and by increasing the on-site coulomb repulsion u, the ground state moves from a metal to a Mott-insulator. Starting from the Hubbard model, one can obtain an effective t-J model by using the Rayleigh – Schrodinger perturbation expansion of the effective Hamiltonian H_{eff}.

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$$Heff = PHP + PH_1 R_s H_1 P + PH_1 R_s (H_1 - \delta E_o) H_1 P + \ldots \quad (3)$$

where $H = H_o + H_1$, and

$$R_s = Q \frac{1}{E_o - H_o}$$
$$H_o = \sum_i n_{i\uparrow} n_{i\downarrow}$$
$$H_1 = -t \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma}$$

It means, therefore, that the point of view here is that the unperturbed part of the Hamiltonian is the potential energy. If there is no hopping, the ground state has no double occupancy.

$$R_s = Q \frac{1}{E_o - H_o}, Q = 1 - P \quad (4)$$

$\delta E_o = \varepsilon_o - E_o$ is the energy shift in the ground state as a result of H_1. And E_o is the energy of the perturbed system.

The first term of the affective Hamiltonian contains only hopping between states. The potential energy in those states vanish as a result of the projection operator P.

$$PHP \equiv PH_1 P$$
$$= P \sum_{\langle ij \rangle \sigma} c_{i\sigma}^{+} c_{j\sigma} P \quad (5)$$

The next term

$$PH_1 R_s H_1 P = PH_1 \frac{Q}{E_o - H_o} H_1 P$$

But $Q = 1 - P$, hence

$$PH_1 Q \frac{1}{E_o - H_o} H_1 P = PH_1 (1 - P) \frac{1}{E_o - H_o} H_1 P$$
$$= \frac{PH_1 H_1 P}{E_o - H_o} - \frac{PH_1 PH_1 P}{E_o - H_o} \quad (6)$$

H_o will act on states that are singly occupied as a result of the action of P and create a double occupied state and give a contribution u which is large compared to E_o. Hence $E_o - U \approx -U$.

Hence we have, $= \frac{PH_1 H_1 P}{E_o - H_o} - \frac{PH_1 PH_1 P}{E_o - H_o}$

$$\approx -\frac{1}{u} PH_1 H_1 P + \frac{1}{u} PH_1 PH_1 P \quad (7)$$

For only nearest neighbours

$$-\frac{1}{u} H_1 H_1$$

$$= -\frac{t^2}{u} \sum_{\langle ij\rangle\sigma}\sum_{\langle klj\rangle\sigma'} \left(c_{i\sigma}^{+} c_{j\sigma} + h.c\right)\left(c_{k\sigma'}^{+} c_{j\sigma'} + h.c\right) \quad (8)$$

Each nearest neighbour bond $\langle ij \rangle$ is counted only once in the sum; since we start from a state with singly occupied sites and come back to a state with single occupied sites $\langle kl \rangle \equiv \langle ij \rangle$ survives.

Terms from $-\frac{1}{u} H_1 H_1$ that destroy two particles on the same site are left out as they have zero matrix elements, we are therefore left with

$-\frac{t^2}{u} \sum_{\langle ij\rangle\sigma\sigma'} \left(c_{i\sigma}^{+} c_{j\sigma}\ c_{i\sigma'}^{+} c_{j\sigma'} + c_{j\sigma}^{+} c_{i\sigma}\ c_{i\sigma'}^{+} c_{j\sigma'}\right)$ in Eqn. (8).

We consider four spin configurations for the neighbouring sites *i* and *j*. $\left|\uparrow i \uparrow j\right\rangle$ *and* $\left|\downarrow i \downarrow j\right\rangle$ do not contribute as the intermediate states and are prohibited by the Pauli exclusion principle. The spin configurations $\left|\uparrow i \downarrow j\right\rangle$ *and* $\left|\downarrow i \uparrow j\right\rangle$ are acceptable as they produce non-vanishing matrix elements for the surviving terms in H_1H_1. The following are the configurations left to be considered:

$$\left\langle i\uparrow j\downarrow \left| H_1 H_1 \right| i\uparrow j\downarrow \right\rangle \quad (9)$$

$$\left\langle i\uparrow j\downarrow \left| H_1 H_1 \right| i\downarrow j\uparrow \right\rangle \quad (10)$$

$$\left\langle i\downarrow j\uparrow \left| H_1 H_1 \right| i\uparrow j\downarrow \right\rangle \quad (11)$$

$$\left\langle i\downarrow j\uparrow \left| H_1 H_1 \right| i\downarrow j\uparrow \right\rangle \quad (12)$$

The configurations (10) and (11) are non vanishing, the matrix elements in (10) and (11) have the values $-2t^2/u$ respectively. The sum gives $-4t^2/u$.

We have considered only the spins. The spin operators that have exactly the same matrix elements are [2].

$$\frac{4t^2}{u} \sum_{\langle ij\rangle} \left(\vec{s}_i \cdot \vec{s}_i - \frac{n_i n_j}{4} \right)$$

The spin operators $\vec{S}_i$ and $\vec{S}_j$ can be shown to have the same matrix elements as $H_1 H_1 / u$.

$\vec{S}_i = \frac{1}{2} c_i^{+}, \alpha\, \vec{\sigma}_{\alpha,\beta}\ c_{i,\beta}$, *and* $\vec{\sigma}$ is the vector of Pauli matrices

Thus the t – J model is

$$Heff\ = H_{t-J} = -\sum_{\langle ij\rangle\sigma} t\ c_{i\sigma}^{+} c_{j\sigma} + h.c\ -\ \frac{4t^2}{u} \sum_{\langle ij\rangle} \left(\vec{s}_i \cdot \vec{s}_i - \frac{n_i n_j}{4} \right) \quad (13)$$

The first term represents the nearest neighbour hopping between sites of the lattice allowing the electrons to delocalize while the second term represents the nearest neighbour exchange interaction between the spins of the electrons. Due to the fact that, the non vanishing interaction is between antiparallel neighbouring spins, the exchange interactions is antiferromagnetic.

Conclusion

The t-J model describes electrons hopping with an amplitude of t and interacting with an antiferromagnetic exchange term $\left(\frac{4t^2}{u}\right) = J$. When t = 0, the t-J model is equivalent to the Heigenberg model.

A simple and transparent process has been presented with clear assumptions in the run up to the derivation of the model. The Rayleigh-Schrodinger perturbation theory is size consistent that is to say that the energy increases with size of the system and it has been taken to the second order. It can easily be estimated that the energy of the t-J model is E_{t-J}

$\langle H_1 \rangle + \langle H_1 R_s H_1 \rangle + \cdots$

upto second order, where $\langle \cdots \rangle = \langle \phi_o | \cdots | \phi_o \rangle$.

The wave function upto second order can be estimated also to be

$$|\psi_o\rangle = \left(P + R_s \left(H_1 - \delta E_o\right) P\right) |\psi_o\rangle + \cdots$$

In conclusion, we have deduced the t-J model from the one-band Hubbard model by a Rayleigh – Schrodinger perturbation expansion. The exchange is antiferromagnetic because the non-vanishing nearest neighbour interaction is that between antiparallel spins. We saw that the exchange coupling is antiferromagnetic in agreement with the findings in the literature. [7].

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