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Two Particles Interactions in the One-dimensional Hubbard Model

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Abstract: The electron pairing problem is studied by means of the Hubbard Model. An exact solution is obtained and this is compared to the results obtained using the Rayleigh – Schrodinger perturbation method. The two electrons were considered to be on a 2 lattice sites. The ground state energy obtained is $\frac{1}{2}\left(u - (16t^2 + u^2)^{\frac{1}{2}}\right)$.

Key words: Hubbard model, ground State, anti ferromagnetic and exact diagonalizab.

INTRODUCTION

An understanding of the mechanism of superconductivity in the copper oxides based high temperature superconductors will require an understanding of their electronic properties. The Hubbard Model (Hubbard, J., 1963) plays a central role in the theoretical study of strongly correlated systems. The model is simple but its exact solutions are available only for very low or very high dimensions (Lieb, E.H. and F.Y. Wu, 1968). However, Quantum Monte Carlo (QMC) simulations are believed to be the most powerful and accurate method to study the Hubbard Model (White, S.R., D.J. Scalapino, 1989). It is, however, restricted to finite lattices, finite temperatures and very large computers.

One of the common techniques used to study the Hubbard Model is the Mean Field Approximation (MFA) (Micnas, R., 1990). However, the MFA is not sufficient to describe electronic correlations. Another technique is the slave-boson formalism (Caprara, S., M. Avignon, 2000). The renormalization group method is another technique (Hirsch, J.E., 1980). A variational ground state is constructed in this method. The results are sometimes unreliable. Finally, the exact diagonalization method is most desirable. It can, however, be applied to small systems because the dimension of the Hamiltonian matrix increases rapidly with the number of sites and the number of particles (Lopez-Urias, F. and G.M. Pastor, 1999).

In section 2, a brief description of the Hamiltonian is given and the diagonalization technique is explained. The Rayleigh-Schrodinger perturbention method is also applied to our system. The results are summarized in section 3.

2. *The Hubbard Hamiltonian:*

The Hubbard Hamiltonian takes the form

$$H = -t\sum_{\langle ij\rangle\sigma} C^{+}_{i\sigma} C_{j\sigma} + u\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

It describes electrons on a lattice (Peter Fulde, 1995) with one orbital per site. There is a hopping element between different sites. Interactions occur between electrons located on the same site. Strong correlations are present when the Coulomb interaction u is large compared with the band width of the system. In the limit of large u the case of half filling is special. There is one electron per site. The correlations is antiferromagnatic (Peter Fulde, 1995).

For 2 electrons on 2 sites, there are 6 possible configurations:

$$|\psi_1\rangle = |\uparrow\uparrow\rangle, \quad |\psi_2\rangle = |\downarrow\downarrow\rangle, \quad |\psi_3\rangle = |\uparrow\ \downarrow\rangle$$

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$$|\psi_4\rangle = |\downarrow\uparrow\rangle, \quad |\psi_5\rangle = |\downarrow\uparrow \ 0\rangle \ , \quad |\psi_6\rangle = |0 \uparrow\downarrow\rangle$$

The Hamiltonian is a four-by-four matrix and we need to solve the eigen value equation.

$$\begin{bmatrix} u & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & u \end{bmatrix} \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix} = E \begin{bmatrix} a \\ b \\ c \\ d \end{bmatrix}$$

The eigen values are:

$$E_1 = 0, \quad E_2 = u, \quad E_3 = \frac{1}{2}\left(u - \left(16t^2 + u^2\right)^{\frac{1}{2}}\right),$$

$$E_4 = \frac{1}{2}\left(u + (16t^2 + u^2)^{\frac{1}{2}}\right)$$

The corresponding eigenvectors are:

$$|1\rangle = -|\downarrow\uparrow\rangle + |\downarrow\uparrow \ 0\rangle$$

$$|2\rangle = -|\uparrow\downarrow\rangle + |0 \uparrow\downarrow\rangle$$

$$|3\rangle = -|\uparrow\downarrow\rangle + \frac{(u + (16t^2 + u^2)^{\frac{1}{2}})}{4t}\left\{|\downarrow\uparrow\rangle + |\downarrow\uparrow 0\rangle\right\} + |0 \uparrow\downarrow\rangle$$

$$|4\rangle = -|\uparrow\downarrow\rangle + \frac{(u + (16t^2 + u^2)^{\frac{1}{2}})}{4t}\left\{|\downarrow\uparrow\rangle + |\downarrow\uparrow 0\rangle\right\} + |0 \uparrow\downarrow\rangle$$

The ground state energy is thus E_3 and the corresponding ground state eigenvector is $|3\rangle$.

The lowest energy state has one electron up and one down compared to the state with two electrons of the same spin. This occurs because the electrons have the ability to hop back and forth. This effect causes an antiferromagnetic tendency. Hence it is agreed generally that the Hubbard model with one electron per site should be an antiferromagnet at low enough temperatures.

For the purpose of comparing the results of the exact diagonalization with that obtained using the Rayleigh-Schroduger perturbation method, the Hubbard Hamiltonian is written as;

$$H = H_0 + H_1$$

Where $H_0 = -t\sum_{\langle ij\rangle\sigma} C^{+}_{i\sigma} C_{j\sigma}$

$$H_1 = u\sum_{i} n_{i\uparrow} n_{i\downarrow}$$

$$H_0 = \begin{bmatrix} 0 & -t & -t & 0 \\ -t & 0 & 0 & -t \\ -t & 0 & 0 & -t \\ 0 & -t & -t & 0 \end{bmatrix}$$

The eigenvalues are:

$$E_1 = E_2 = 0, \quad E_3 = -2t, \quad E_4 = 2t$$

The corresponding eigenvectors are;

$$|1\rangle = |\uparrow\downarrow 0\rangle - |\downarrow\uparrow\rangle$$

$$|2\rangle = |0 \uparrow\downarrow\rangle - |\uparrow\downarrow\rangle$$

$$|3\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\uparrow 0\rangle + |0 \uparrow\downarrow\rangle$$

$$|4\rangle = |\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle - |\downarrow\uparrow 0\rangle + |0 \uparrow\downarrow\rangle$$

The ground state energy is $E_g = -2t$ and the ground state wavefunction is

$$|\psi_g\rangle = |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\uparrow 0\rangle + |0 \uparrow\downarrow\rangle$$

The first order (Peter Fulde, 1995) perturbed energy is

$$= \langle\psi_g|\ H_1\ |\psi_g\rangle = 8u$$

$$\int E_0^{(1)} = 8u$$

The result of the perturbation method shows that to a first order of perturbation, the ground state energy of the 2 electrons on 2 sites system has an energy of $8u - 2t$ compared to the result of the exact diagonalization of $\frac{1}{2}\left(u - \left(16t^2 + u^2\right)^{1/2}\right)$.

Conclusions:

The result shows that the lowest energy state is antiferromagnet in agreement with the general belief among theories. The weakness of first order perturbation is also apparent, from the non-agreement of its result with that of the exact solution.
(Hubbard, J., 1963)

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