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Variational Study of Bound States of two electrons Described by the *t-U-J* model

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Abstract

We study in this contribution the behavior of two electrons in a lattice by extending the work of Chen and Mei[1] and Enaibe and Idiodi[2] using the variational method. The dynamics of the electronic pair is described by the t-U-J and t-U- J $^{\prime}$ model. The energy spectra are obtained and criterion for the transition from an antiferromagnetic phase to a ferromagnetic phase is discussed.

Keywords: Superexchange, ferromagnetic state, triplet state and variational parameter.

1.0 Introduction

Hubbard model [3] and its variants constitute an important research topic in theoretical condensed matter physics, particularly in the context of strongly correlated electron systems. Most of the many-body techniques commonly used in condensed matter physics can be learnt in this context. Also there are some theoretical tools and concepts which apply to this model only. Most of the effort has been concentrated on one- and two-band Hubbard models where electrons interact through an on-site Coulomb repulsion of strength *U*. Experimental results suggest that this model should be analyzed in the strong coupling region ($U/t \gg 1$). In this limit the problem can be further simplified by replacing the Hubbard model by the *t-J* model[4], which includes a hopping term *t* for holes at nearest neighbor sites and an antiferromagnetic superexchange interaction *J* among nearest neighbour spins, while the possibility of double occupancy is explicitly excluded. The relationship of this model and the two-band Hubbard model of Emery[5] was also established by Zhang and Rice[6].

In spite of the relatively simple appearance of the *t-J* model, only few properties of the model have been elucidated in the past years. There are some rigorous results for the one-dimensional system[7,8,9], exact calculations for small clusters[10,11,12,13], variational studies of the phase diagram[14] and studies of the electron-momentum distribution[15]. In relation to the examination of cuprates, Neudert *et al* [16] extended the standard one-band Hubbard Hamiltonian to study a one-dimensional model of the cuprate Sr_2CuO_3. Cuprates are ceramic materials in which certain elements (in this example strontium) are 'sandwiched' between layers of copper and oxygen atoms[17]. Many cuprates are frequently found to exhibit superconducting properties, which is not predicted by any single-electron approximation. However, the Hubbard Model is found to describe these properties.

There is an obvious interest on this dilute limit that is related to some results pointing towards phase separation in the framework of the *t-J* model[18, 19]. According to these results, the homogeneous phase is unstable after moderate hole doping; phase separation into two regions is predicted, one hole-rich phase and a second almost purely antiferromagnetic region.

The behavior of electrons in the hole-rich phase is described by the dilute limit of the *t-J* model. In this phase, electrons can form a low density superfluid if some tendency to electron pairing takes place. This problem has been analyzed[20,21] by exactly diagonalizing *t-J* , *t-t´-J*, and Hubbard models on small clusters. This work employs the variational method to study the *t-U-J* model in what can be considered an extension of the work of Chen and Mei[1], and Enaibe and Idiodi[2]. How this is done is discussed in the following sections

2.0 Antiferromagnetic Case.

The original *t-U-J* model[22] is represented by the Hamiltonian:

$$\begin{aligned}\mathcal{H} &= \hat{T} + \hat{U} + \hat{J} \\ &= -t\sum_{\langle ij\rangle,\sigma}\left(a_{i\sigma}^{\dagger}a_{j\sigma} + h.c\right) + U\sum_i n_{i\uparrow}n_{i\downarrow} + J\sum_{\langle ij\rangle}\left[S_i^z S_j^z - \frac{n_i n_j}{4} + \frac{1}{2}\left(S_i^+ S_j^- + S_i^- S_j^+\right)\right]\end{aligned} \qquad (2.1)$$

where the spin operators are defined by $S_i^z = \frac{1}{2}\left(n_{i\uparrow} - n_{j\downarrow}\right)$. $S_i^+ = a_{i\uparrow}^{\dagger}a_{i\downarrow}$. $S_i^- = a_{i\downarrow}^{\dagger}a_{i\uparrow}$ and $\langle ij\rangle$ implies only nearest neighbours, σ is the electronic spin, $a_{i\sigma}^{\dagger}(a_{i\sigma})$ creates(annihilates) an electron at site i with spin σ and $n_i\ (= n_{i\uparrow} + n_{i\downarrow})$ is the number operator at site i with $n_{i\uparrow} = a_{i\uparrow}^{\dagger}a_{i\uparrow}$.

To give a brief illustration of our treatment, let us solve a simple two-site problem for the two electron-case. Here, there are a total of six states viz:

$|\phi_1\rangle = |1\uparrow 1\downarrow, 0\rangle$, $|\phi_2\rangle = |0, 2\uparrow 2\downarrow\rangle$, $|\phi_3\rangle = |1\uparrow, 2\downarrow\rangle$, $|\phi_4\rangle = |1\downarrow, 2\uparrow\rangle$, $|\phi_5\rangle = |1\uparrow, 2\uparrow\rangle$, $|\phi_6\rangle = |1\downarrow, 2\downarrow\rangle$.

The ground state wave function is easily obtained through exact diagonalization as

$$\psi_G = \frac{1}{2}\left[\frac{\sqrt{(J+U)^2+16t^2}+J+U}{\sqrt{(J+U)^2+16t^2}}\right]^{\frac{1}{2}}\left(|\phi_1\rangle + |\phi_2\rangle\right) + \frac{1}{2}\left[\frac{\sqrt{(J+U)^2+16t^2}-(J+U)}{\sqrt{(J+U)^2+16t^2}}\right]^{\frac{1}{2}}\left(|\phi_3\rangle - |\phi_4\rangle\right) \qquad (2.2)$$

with corresponding energy $E_G = -\frac{1}{2}\left(J - U + \sqrt{(J+U)^2 + 16t^2}\right)$. (2.3)

The other energy eigenvalues are 0, U and $-\frac{1}{2}\left(J - U - \sqrt{(J+U)^2 + 16t^2}\right)$.

As can be seen, the ground state is a spin-singlet. This is used in the following sections to construct a correlated variational ground-state wave function.

3.0 One-Dimensional Ring

Defining the variational ground-state wave function as

$$|\psi\rangle = \sum_{i\neq j}\chi_{|i-j|}\{|i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle\} + \sum_i \chi_0(i,i)|i\uparrow, i\downarrow\rangle \qquad (3.1)$$

where the $\chi(i,j)$ are variational parameters[1], we obtain for two electrons on the two-site ring,

$$\langle\psi|\psi\rangle = 2\chi_0^2 + 2\chi_1^2 \qquad (3.2a)$$

$$\begin{aligned}\langle\psi|\mathcal{H}|\psi\rangle &= -2t(4\chi_0\chi_1) + 2U\chi_0^2 - 2J\chi_1^2 \\ &= -8t\chi_0\chi_1 + 2U\chi_0^2 - 2J\chi_1^2 \qquad (3.2b)\end{aligned}$$

$$E_g = \frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} \qquad (3.3)$$

By minimizing Eq. (3.3) with respect to all the variational parameters, the ground state energy Eq. (2.3) is recovered. We can now extend this variational method to a two-dimensional lattice with periodic boundary conditions.

4.0 Two-dimensional torus of 4 × 4 square lattice

The first step in the variational study of a system of two electrons on a 4×4 square lattice is to classify the structure of the correlated ground-state wave function as we did in Eq. (3.1). For further details, the reader is referred to Reference [1]. Hence:

$$\langle\psi|\psi\rangle = 16\chi_0^2 + 64\chi_1^2 + 64\chi_2^2 + 32\chi_3^2 + 64\chi_4^2 + 16\chi_5^2 \qquad (4.1)$$

$$\langle\psi|\mathcal{H}|\psi\rangle = 16U\chi_0^2 - 256t\chi_0\chi_1 - 512t\chi_1\chi_2 - 256t\chi_1\chi_3 - 512t\chi_2\chi_4 - 256t\chi_3\chi_4 - 64J\chi_1^2$$

$$\frac{E_g}{t} = \frac{\frac{U}{t}\chi_0^2 - 16\chi_0\chi_1 - 32\chi_1\chi_2 - 16\chi_1\chi_3 - 32\chi_2\chi_4 - 16\chi_3\chi_4 - 4\frac{J}{t}\chi_1^2}{\chi_0^2 + 4\chi_1^2 + 4\chi_2^2 + 2\chi_3^2 + \chi_4^2 + \chi_5^2} \qquad (4.2)$$

Minimization of Eq. (4.2) with respect to the variational parameters and granted that $E_g/t = E$, we have,

$$\begin{bmatrix} \frac{U}{t}-E & -8 & 0 & 0 & 0 & 0 \\ -2 & -\frac{J}{t}-E & -4 & -2 & 0 & 0 \\ 0 & -4 & -E & 0 & -4 & 0 \\ 0 & -4 & 0 & -E & -4 & 0 \\ 0 & 0 & -4 & -2 & -E & -2 \\ 0 & 0 & 0 & 0 & -8 & -E \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \qquad (4.3)$$

Results obtained from the numerical solution of Eq. (4.3) will be discussed in Section 8.

5.0 FERROMAGNETIC CASE

The relevance of the *t-J* model with a negative exchange parameter *J* lies on the investigations of spin-splitting states with non-zero spin currents. Let us consider a Hamiltonian similar to that of Eq. (2.1) but with the exchange term slightly modified[22] to be

$$\hat{J}' = -J\sum_{\langle ij\rangle}\left(S_i^+ S_j^- + S_i^- S_j^+\right). \qquad (5.1)$$

With this modification, the $t-U-J'$ model becomes

$$\mathcal{H} = -t\sum_{\substack{\langle ij\rangle \\ \sigma}}\left(a_{i\sigma}^{\dagger}a_{j\sigma} + h.c\right) + U\sum_i n_{i\uparrow}n_{i\downarrow} - J\sum_{\langle ij\rangle}\left(S_i^+ S_j^- + S_i^- S_j^+\right). \qquad (5.2)$$

Assuming there are only two electrons in our system, we can classify basis states into singlet and triplet states as was done in Section 3.0 . Hence, the full correlated ground wave state function is

$$|\psi\rangle = \sum_{i\neq j}\chi(i,j)\{|i\uparrow,j\downarrow\rangle - |i\downarrow,j\uparrow\rangle\} + \sum_i \chi(i,i)|i\uparrow,i\downarrow\rangle + \sum_{i\neq j}Y(i,j)\{|i\uparrow,j\downarrow\rangle + |i\downarrow,j\uparrow\rangle\} + \sum_{i\neq j}Z(i,j)|i\uparrow,j\uparrow\rangle \qquad (5.3)$$

The $\chi(i,j)$ in Eq. (5.3) are variational parameters patterned after Chen and Mei[1] but with the triplet states *Y* and *Z* added. While the variational wave function of Chen and Mei[1] contained only singlet states, the wave function used by Enaibe and Idiodi[2] included the Z-triplet state but not the Y-triplet state.

6.0 ONE-DIMENSIONAL CASE (TWO ELECTRONS ON TWO SITES)

For a system of two electrons on two sites, Eq(5.3) written out explicitly becomes

$$|\psi_0\rangle = \chi_0\sum_{i=1}^{N}|i\uparrow,i\downarrow\rangle = \chi_0(|1\uparrow,1\downarrow\rangle + |2\uparrow,2\downarrow\rangle) \qquad (6.1)$$

Where here and henceforth, we shall adopt the simpler notation of replacing $\chi(i,j)$, $Y(i,j)$ and $Z(i,j)$ respectively by $\chi_{|i-j|}$, $Y_{|i-j|}$ and $Z_{|i-j|}$. Hence,

$$|\psi_1\rangle = \chi_1(|1\uparrow,2\downarrow\rangle - |1\downarrow,2\uparrow\rangle) \qquad (6.2)$$

$$|\psi_2\rangle = Y_1(|1\uparrow,2\downarrow\rangle + |1\downarrow,2\uparrow\rangle) \qquad (6.3)$$

$$|\psi_3\rangle = Z_1(|1\uparrow,2\uparrow\rangle). \tag{6.4}$$

$$|\psi\rangle = \chi_0(|1\uparrow,1\downarrow\rangle + |2\uparrow,2\downarrow\rangle) + \chi_1(|1\uparrow,2\downarrow\rangle - |1\downarrow,2\uparrow\rangle) + Y_1(|1\uparrow,2\downarrow\rangle + |1\downarrow,2\uparrow\rangle) + Z_1(|1\uparrow,2\uparrow\rangle). \tag{6.5}$$

$$\langle\psi|\mathcal{H}|\psi\rangle = 2U\chi_0^2 - 8t\chi_0\chi_1 + 2J\chi_1^2 - 2JY_1^2 - JZ_1^2 \tag{6.6}$$

$$\langle\psi|\psi\rangle = 2\chi_0^2 + 2\chi_1^2 + 2Y_1^2 + Z_1^2 \tag{6.7}$$

But the variational ground state energy is

$$\frac{E_g(\chi_0,\chi_1,Y_1,Z_1)}{t} = \frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle} \tag{6.8}$$

Hence $$\frac{E_g}{t}(2\chi_0^2 + 2\chi_1^2 + 2Y_1^2 + Z_1^2) = 2\frac{U}{t}\chi_0^2 - 8\chi_0\chi_1 + 2\frac{J}{t}\chi_1^2 - 2\frac{J}{t}Y_1^2 - \frac{J}{t}Z_1^2 \tag{6.9}$$

The solution of Eq. (6.9) after minimization and subject to the normalization constraint $\chi_0^2 + \chi_1^2 + Y_1^2 + Z_1^2 = 1$ is

$$E_G = E_1 = -\frac{J}{t} \tag{6.10}$$

the other energy eigenvalues are $E_2 = \frac{1}{2}\left(\frac{J}{t} + \frac{U}{t} - \sqrt{\left(\frac{J}{t} - \frac{U}{t}\right)^2 + 16}\right)$ (6.11)

$$E_3 = \frac{1}{2}\left(\frac{J}{t} + \frac{U}{t} + \sqrt{\left(\frac{J}{t} - \frac{U}{t}\right)^2 + 16}\right). \tag{6.12}$$

The ground state wave function is either

$$|\psi_G\rangle = (0 \quad 0 \quad 1 \quad 0)^T = |1\uparrow 2\downarrow\rangle + |1\downarrow 2\uparrow\rangle \tag{6.13}$$

or

$$|\psi_G\rangle = (0 \quad 0 \quad 0 \quad 1)^T = |1\uparrow 2\uparrow\rangle. \tag{6.14}$$

The energy is assumed to be ordered such that $E_G < E_2 < E_3$. The ground state energy is thus $E_G = -J/t$, with eigen function $|\psi_G\rangle$. For ferromagnetic interaction $J > 0$. In the absence of J, E_2 is the ground state. Numerical solution of Eq. (6.9) reveals that the ground state is actually a triplet state and is ferromagnetic in nature as discussed further in Section 8.

7 Two-dimensional case (two electrons on a 4×4 square lattice)

Having constructed the correlated ground-state wave function using Eq. (5.3), it is easy to show that

$$\langle\psi|\psi\rangle = 16\chi_0^2 + 64\chi_1^2 + 64\chi_2^2 + 32\chi_3^2 + 64\chi_4^2 + 16\chi_5^2 + 64Y_1^2 + 64Y_2^2 + 32Y_3^2 + 64Y_4^2 + 16Y_5^2 + 32Z_1^2 + 32Z_2^2 + 16Z_3^2 + 32Z_4^2 + 8Z_5^2. \tag{7.1}$$

With the modified Hamiltonian (see Eq.(5.2)) operating on Eq. (5.3), we get

$$\langle\psi|\mathcal{H}|\psi\rangle = 16U\chi_0^2 - 256t\chi_0\chi_1 - 512t\chi_1\chi_2 - 256t\chi_1\chi_3 - 512t\chi_2\chi_4 - 256t\chi_3\chi_4 - 256t\chi_4\chi_5 + 64J\chi_1^2 - 264tY_1Y_2 - 128tY_1Y_3 - 382tY_2Y_4 - 128tY_3Y_4 - 192tY_4Y_5 - 64JY_1^2 - 64tZ_1Z_2 - 4tZ_1Z_3 - 64tZ_2Z_4 - 32tZ_3Z_4 - 64tZ_4Z_5 - 32JZ_1^2. \tag{7.2}$$

From Eq. (7.1) and Eq. (7.2) the ground state energy can easily be calculated. The detailed results obtained are discussed in Section 8.

8.0 Results

8.1 Antiferromagnetic Case

We set $J = 4t^2/U$ in Eq. (3) and obtained the plot in Fig. 1a below. Observe that for $U/t \gg 1$, E_g approaches zero. But as $U/t \ll 1$, $E_g \cong -J$. At $U/t = 0$, there is a discontinuity.

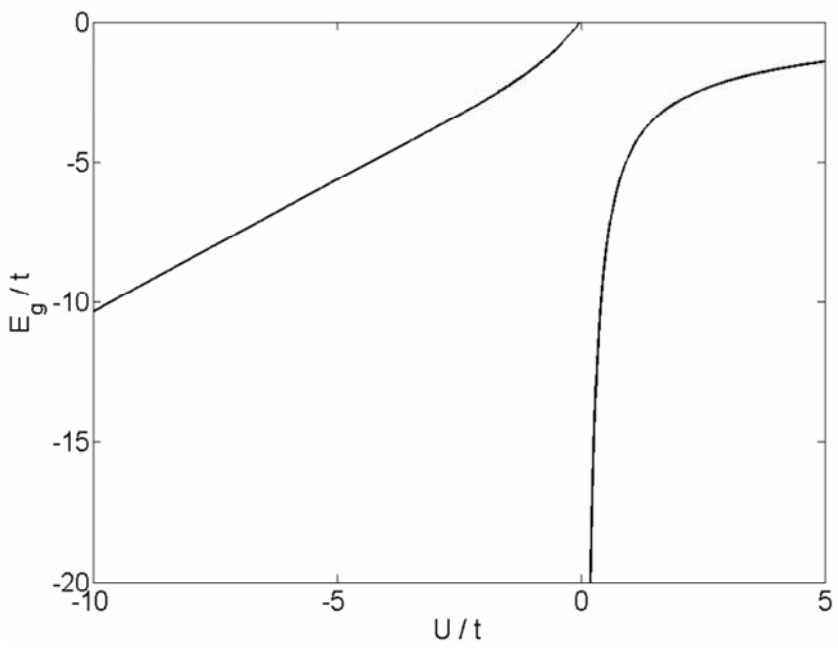

Fig. 1a Plot of E_g/t against U/t for a 1D lattice of two electrons on two sites ($J = 4t^2/U$).

If J/t = 0 in Eq. (9), the Hubbard model [3] is recovered and numerical solutions at U = 0 gives the eigenvalues as $E_0 = -8$, $E_1 = -4$, $E_2 = E_3 = 0$, $E_4 = 4$, $E_5 = 8$. The ground state energy value of -8 was also obtained by Petukhov *et al* [22]. Numerical result of the Hubbard (*t-U)* model and the *t-U-J* model are presented in Table 1 and plotted in Fig. 1(b).

We looked at the solution of the *t-U-J'* model in one-dimension and present the results in Table 2, Table 3 and Fig. 2.

Table 1: Table of U/t and the corresponding energies E ($J = 4t^2/U$) for the *t-U-J* and Hubbard (*t-U*) models for two electrons on a 4×4 square lattice with periodic boundary conditions considered everywhere.

$E = E_g/t$		
U/t	$t-U-J$	$t-U$
0	–	−8.00000000
1.00	−9.37990031	−7.94495434
1.25	−8.99507127	−7.93320535
2.00	−8.48192560	−7.90180152
5.00	−8.00802910	−7.81542522
6.00	−7.95128202	−7.79560960
7.00	−7.90886406	−7.77869214
10.00	−7.82655032	−7.74018437
15.00	−7.75447323	−7.69993150
20.00	−7.71452877	−7.67496762
25.00	−7.68893279	−7.65799873
30.00	−7.67107621	−7.64572309
40.00	−7.64775000	−7.62916062
50.00	−7.63316291	−7.61850823
60.00	−7.62317066	−7.61108363
75.00	−7.61295148	−7.60338525
80.00	−7.61035986	−7.60141625
90.00	−7.60600683	−7.59809398
100.00	−7.60249359	−7.59539901

Observe the agreement between the results in Fig. 1b in the large U/t (≥ 50) limit. While the result in [22] seems to contradict what is available in literature in the region $U/t < 50$, our result is in better agreement in this region (i.e. Hubbard *t-U* and *t-U-J* models are non-equivalent).

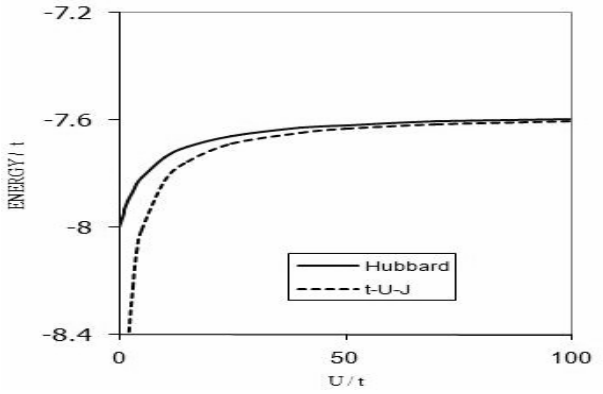

Figure 1b: Comparison between Hubbard and *t-U-J* models for two electrons on a 4×4 cluster. Observe that the two models are quite different at small values of U/t but agree greatly at very large values.

8.2 1D Ferromagnetic Case

Table 2(a): Table of the Transition from ferromagnetism (FM) to antiferromagnetism (AFM) for 1D lattice of two electrons. Observe that at $J/t = 0.2400$, $E_g/t \neq -J/t$. At this point there is transition to antiferromagnetism, Eq.(21b) becomes the ground state with $U/t = 8.0$.

J/t	E_g/t
8.0500	-8.05000
8.0250	-8.02500
8.0125	-8.01250
5.0000	-5.00000
3.0000	-3.00000
1.0000	-1.00000
0.5000	-0.50000
0.3000	-0.30000
0.2500	-0.25000
0.2450	-0.24500
0.2400	-0.24510
0.2000	-0.28290
0.1500	-0.33020
0.1300	-0.34910
0.1000	-0.37750
0.0000	-0.47210
-8.000	-8.24621

Table 2: (b) Table of the ground state energy and Variational parameters for 1D (N = 2) lattice at U/t = 8 with Y_i set to zero in Eq. (11).

J/t	E_g/t	X_0	X_1	Y_1	Z_1
8.6000	−8.6000	0	0	0	1
8.5500	−8.5500	0	0	0	1
8.5000	−8.5000	0	0	0	1
8.4500	−8.4500	0	0	0	1
8.4000	−8.4000	0	0	0	1
8.3000	−8.3000	0	0	0	1
8.2500	−8.2500	0	0	0	1
8.2000	−8.2000	0	0	0	1
8.1500	−8.1500	0	0	0	1
8.1000	−8.1000	0	0	0	1
8.0500	−8.0500	0	0	0	1
8.0250	−8.0250	0	0	0	1
8.0125	−8.0125	0	0	0	1
0.2500	−0.2500	0	0	0	1
0.2450	−0.2450	0	0	0	1
0.2400	−0.2451	0.23573	0.97182	0	0
0.0000	−0.4721	0.22975	0.97324	0	0
−8.0000	−8.2462	0.12218	0.99251	0	0
−10.0000	−10.0436	0.02172	0.99976	0	0

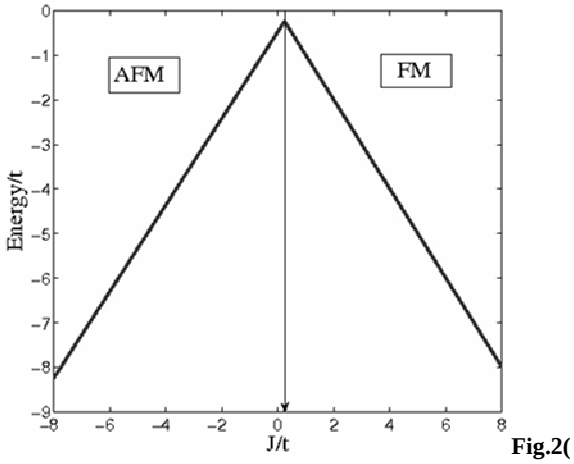

Fig.2(a): Transition from ferromagnetism (FM) to antiferromagnetism (AFM) for 1D lattice of two electrons as J/t is reduced from to -8 and $U/t = 8$. The transition occurred at $J/t = 0.24$.

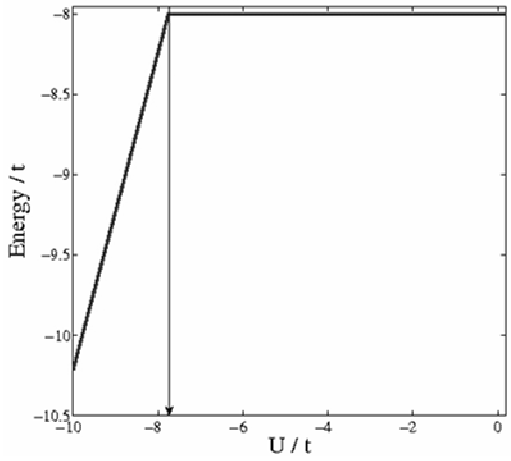

Figure 2(b): Transition from ferromagnetism to antiferromagnetism for 1D lattice with two electrons (N = 2) as U/t is gradually decreased at $J/t = 8$. Observe that the transition occurred at $U/t = -7.75$.

Analysis of the *t-U-J'* model for two electrons on two sites problem in the positive *J* region reveals that the ground state is purely ferromagnetic but a transition to antiferromagnetism was observed when $J \cong 0.24t$ and $U = 8t$.

Table 2 (c): Table of the ground state energy and Variational parameters for 1D (N = 2) lattice with U/t = 8 and both Y_i and Z_i present in Eq. (11).

J/t	E_g/t	X_0	X_1	Y_1	Z_1
8.6000	−8.6000	0	0	1	0
8.5500	−8.5500	0	0	1	0
8.5000	−8.5000	0	0	1	0
8.4500	−8.4500	0	0	1	0
8.4000	−8.4000	0	0	1	0
8.3000	−8.3000	0	0	1	0
8.2500	−8.2500	0	0	1	0
8.2000	−8.2000	0	0	1	0
8.1500	−8.1500	0	0	1	0
8.1000	−8.1000	0	0	1	0
8.0500	−8.0500	0	0	1	0
8.0250	−8.0250	0	0	1	0
8.0125	−8.0125	0	0	1	0
5.0000	−5.0000	0	0	1	0
3.0000	−3.0000	0	0	1	0
1.0000	−1.0000	0	0	1	0
0.5000	−0.5000	0	0	1	0
0.3000	−0.3000	0	0	1	0
0.2500	−0.2500	0	0	1	0
0.2450	−0.2450	0	0	1	0
0.2400	−0.2451	0.23573	0.97182	0	0
0.2000	−0.2829	0.23472	0.97206	0	0
0.1500	−0.3302	0.23346	0.97237	0	0
0.1300	−0.3491	0.23296	0.97249	0	0
0.1000	−0.3775	0.23221	0.97267	0	0
0.0000	−0.4721	0.22975	0.97324	0	0
−8.0000	−8.2462	0.12218	0.99251	0	0
−10.0000	−10.0436	0.02172	0.99976	0	0

Table 3(a): Table of the ground state energy and Variational parameters for 1D (N = 2) lattice showing the degeneracy at $U/t = -7.750$ and $J/t = 8.000$. E_s, E_{T1} and E_{T2} are respectively the singlet, triplet 1 and triplet 2 energies.

U/t	E_s	E_{T1}	E_{T2}
−7.000	−7.262087	−8.00000	−8.00000
−7.500	−7.753905	−8.00000	−8.00000
−7.700	−7.950772	−8.00000	−8.00000
−7.750	−8.000000	−8.00000	−8.00000
−7.751	−8.000985	−8.00000	−8.00000

Table 3(a) shows the three-fold degeneracy that at U/t = −7.750, the ground state became three-fold degenerate with an energy $E/t = -8.00$.

Table 3(b): Table of the ground state energy and Variational parameters for 1D (N = 2) lattice. Here we gradually reduce the interaction strength U/t and kept the exchange term constant at $J/t = 8.0$. This is plotted in fig.2(b).

U/t	E_g/t	X_0	X_1	Y_1	Z_1
0.500	−8.00000	0	0	0	1
0.200	−8.00000	0	0	0	1
0.100	−8.00000	0	0	0	1
0.000	−8.00000	0	0	0	1
−0.100	−8.00000	0	0	0	1
−0.200	−8.00000	0	0	0	1
−0.500	−8.00000	0	0	0	1
−1.000	−8.00000	0	0	0	1
−5.000	−8.00000	0	0	0	1
−7.750	−8.00000	0	0	0	1
−7.751	−8.00098	0.99228	0.12403	0	0
−8.000	−8.24621	0.99251	0.12218	0	0
−10.000	−10.21954	0.99402	0.10911	0	0

8.3 2D FERROMAGNETIC CASE

Lastly, Table 4 illustrates the situation where we set all the state functions Y_i's to zero in Eq. (11) and obtained a transition from antiferromagnetic phase to ferromagnetic phase at $J/t = 6.803$. Table 5, on the other hand, shows the result when all the states are present. A transition from an antiferromagnetic phase to ferromagnetic phase is clearly seen to occur at $J/t = 6.59$. Fig. 3 shows the result of the plot of all the energies. Observe that as the singlet state energy increases, the triplet energies decrease with both tending towards the same value as the exchange energy J/t becomes very large. The triplet 2 transition was obtained when the Y_i state was switched off in Eq. (11). Meanwhile, when all the three states are present in Eq. (11), the observed ground state is the state ($|i\uparrow j\downarrow\rangle + |i\downarrow j\uparrow\rangle$). This is shown in Table 5.

Table 4: J/t and corresponding E_g/t evaluated at $U/t = 8.0$ on a 4×4 square lattice with periodic boundary conditions considered everywhere and state Y_i set to zero in Eq. (11).

J/t	E_g/t	χ_0	χ_1	χ_2	χ_3	χ_4	χ_5	$Y_1 - Y_5$	Z_1	Z_2	Z_3	Z_4	Z_5
5.000	−7.1101	0.11904	0.22483	0.41411	0.41411	0.51126	0.57525	0	0	0	0	0	0
5.500	−7.0732	0.11395	0.21471	0.41194	0.41194	0.51373	0.58104	0	0	0	0	0	0
6.000	−7.0393	0.10923	0.20534	0.40985	0.40985	0.51592	0.58633	0	0	0	0	0	0
6.500	−7.0082	0.10483	0.19667	0.40784	0.40784	0.51787	0.59117	0	0	0	0	0	0
6.600	−7.0022	0.10399	0.19502	0.40744	0.40744	0.51824	0.59208	0	0	0	0	0	0
6.700	−6.9964	0.10316	0.19338	0.40705	0.40705	0.51860	0.59298	0	0	0	0	0	0
6.800	−6.9906	0.10234	0.19177	0.40667	0.40667	0.51894	0.59387	0	0	0	0	0	0
6.802	−6.9905	0.10232	0.19174	0.40666	0.40666	0.51895	0.59389	0	0	0	0	0	0
6.803	−6.9907	0	0	0	0	0	0	0	0.97504	0.18046	0.04072	0.09648	0.07690
6.805	−6.9926	0	0	0	0	0	0	0	0.97507	0.18037	0.04069	0.09640	0.07582
6.810	−6.9973	0	0	0	0	0	0	0	0.97515	0.18017	0.04062	0.09620	0.07561
6.820	−7.0069	0	0	0	0	0	0	0	0.97530	0.17978	0.04047	0.09580	0.07520
6.900	−7.0835	0	0	0	0	0	0	0	0.97645	0.17671	0.03932	0.09272	0.07199
7.000	−7.1793	0	0	0	0	0	0	0	0.97777	0.17303	0.03796	0.08908	0.06824
7.500	−7.6617	0	0	0	0	0	0	0	0.98289	0.15691	0.03231	0.07387	0.05303
8.000	−8.1476	0	0	0	0	0	0	0	0.98634	0.14380	0.02806	0.06241	0.04213
8.500	−8.6359	0	0	0	0	0	0	0	0.98878	0.13290	0.02477	0.05353	0.03409
9.000	−9.1262	0	0	0	0	0	0	0	0.99059	0.12367	0.02217	0.04650	0.02802
9.500	−9.6179	0	0	0	0	0	0	0	0.99196	0.11574	0.02005	0.04082	0.02334
10.000	−10.1107	0	0	0	0	0	0	0	0.99304	0.10883	0.01831	0.03616	0.01967
15.000	−15.0698	0	0	0	0	0	0	0	0.99744	0.06907	0.00991	0.01465	0.00535

Table 5: J/t and corresponding E_g/t evaluated at $U/t = 8.0$ on a 4×4 square lattice with periodic boundary conditions considered everywhere.

J/t	E_g/t	χ_0	χ_1	χ_2	χ_3	χ_4	χ_5	Y_1	Y_2	Y_3	Y_4	Y_5	$Z_1 - Z_5$
5.00	−7.1101	0.11904	0.22483	0.41411	0.41411	0.51128	0.57525	0	0	0	0	0	0
5.50	−7.0732	0.11395	0.21471	0.41194	0.41194	0.51373	0.58104	0	0	0	0	0	0
5.58	−7.0492	0.11061	0.20808	0.41047	0.41047	0.51529	0.58479	0	0	0	0	0	0
5.59	−7.0540	0	0	0	0	0	0	0.85133	0.33054	0.30073	0.20936	0.17808	0
6.00	−7.1323	0	0	0	0	0	0	0.85697	0.32628	0.29737	0.20350	0.17120	0
6.50	−7.5345	0	0	0	0	0	0	0.88116	0.30579	0.28087	0.17694	0.14090	0
6.60	−7.6169	0	0	0	0	0	0	0.88530	0.30187	0.27766	0.17214	0.13560	0
6.90	−7.8675	0	0	0	0	0	0	0.89655	0.29051	0.26826	0.15871	0.12104	0
7.00	−7.9521	0	0	0	0	0	0	0.89994	0.28686	0.26521	0.15455	0.11661	0
7.50	−8.3820	0	0	0	0	0	0	0.91467	0.26960	0.25064	0.13574	0.09716	0
8.00	−8.8215	0	0	0	0	0	0	0.92638	0.25398	0.23722	0.11993	0.08158	0
8.50	−9.2690	0	0	0	0	0	0	0.93582	0.23986	0.22492	0.10660	0.06900	0
9.00	−9.7229	0	0	0	0	0	0	0.94352	0.22710	0.21368	0.09528	0.05880	0
9.50	−10.1820	0	0	0	0	0	0	0.94989	0.21553	0.20340	0.08562	0.05045	0
10.00	−10.6458	0	0	0	0	0	0	0.95522	0.20504	0.19398	0.07733	0.04358	0
15.00	−15.4229	0	0	0	0	0	0	0.98105	0.13731	0.13167	0.03432	0.01335	0

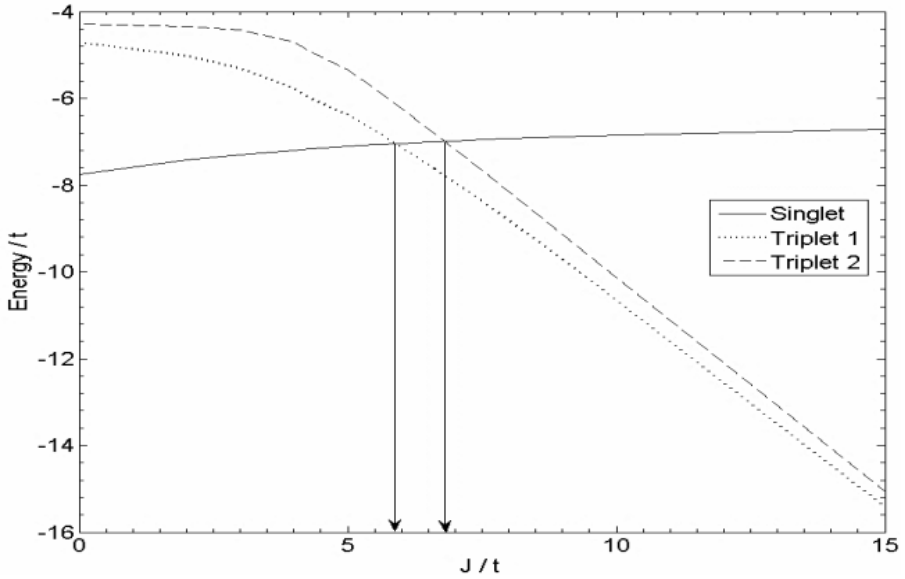

Figure 3: Plot of the ground state energies of the three states showing the singlet and the triplet states; triplet 1 is the $\{|i\uparrow, j\downarrow\rangle + |i\downarrow, j\uparrow\rangle\}$ state while triplet 2 is the $|i\uparrow, j\uparrow\rangle$ state. Observe that for $J/t \leq 6.00$, the ground state is purely antiferromagnetic.

9.0 Conclusion

We have looked at the solution of the *t-U-J* model for two electrons both in the positive and negative *J* cases. It has also been shown that on-site *s* wave pairing is strongly suppressed by the positive *U* and that in the dilute limit, *t-U-J* and Hubbard models are only equivalent for very large *U* values ($U > 50$) as observed in Table 1 and Fig. 1(b). Our result agrees with the result of Reference [22] in the large *U* limit but slightly disagrees in the $U < 50$ limit.

It has been shown that the ground state of the *t-U-J* model in the 1D case is a ferromagnetic degenerate triplet state. But for the 2D 4×4 square lattice, the triplet state ($|i\uparrow, j\downarrow\rangle + |i\downarrow, j\uparrow\rangle$) was found to be the ground state rather than the triplet state ($|i\uparrow, j\uparrow\rangle$). This study can also be viewed as a generalization of the variational technique employed in [2].

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