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EFFECT OF MOVING AWAY FROM HALF FILLING ON THE VARIATIONAL TWO ELECTRON t-U-J INTERACTIONS ON ONE DIMENSIONAL EVEN LATTICES

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ABSTRACT

In this study, the two electron interactions on one dimensional (1D) lattices is investigated in a t-U-J model where the t is the kinetic term, the U is the onsite Coulombic term and J is the nearest neighbour (NN) exchange term. Specifically, the effect of moving away from half filling (i.e. when the number of electrons N_e equals the number of sites N) will be investigated by studying N = 4, 6, 8 and 10 in addition to N = 2. The mathematical method to be used is the simplified formulation of the correlated variational approach, (CVA) recently developed by us. The ground state energies and the transition points from antiferromagntism to ferromagnetism are obtained for the various sites (N = 2,4,6 8 and 10) and at different values of the onsite interaction strength U/4t and the exchange interaction strength J/4t. It is observed that the energies decrease as one moves away from half filling. The implication of these results is then discussed.

KEYWORDS: Ferromagnetism, t-U-J model, variational approach, lattices, half filling.

INTRODUCTION

The origin of ferromagnetism in transition metals has been a controversial issue for quite a very long time. This controversy stems from the apparent dual character, itinerancy and localization properties (Pimenov et al.1999) of the d electrons believed to be responsible for magnetism in transition metals. Itinerant magnetism refers to the magnetic effects in a metallic system due to the interactions of the conduction electrons in motion from one atomic site to another while localized magnetism is due to the incomplete filling of electrons in the inner atomic shells so that there is a well defined magnetic moment at every fixed atomic site. J. Hubbard proposed his famous model in 1963 to study the electron correlation due to the strong Coulomb interaction. In the Hubbard model, the hopping integral (the t term in the Hamiltonian) describes the itinerancy tendency of electrons while the onsite electron correlation (the U term) describes the localization tendency. Within the Hubbard model (also known as the t-U model), the Mott-Hubbard transition (metal-insulator transition) is successfully explained (Bulla 2000) and metal magnetic properties have been discussed (Vollhardt et al.2000). However, the single-band Hubbard model exhibits antiferromagnetism rather than ferromagnetism (Hirsch 1989: Petukhov et al.1992: Amadon and Hirsch, 1996: Ulmke 2000).

As a further search for the candidate model to account for metallic ferromagnetism, the exchange interaction term J has been added to the Hubbard Hamiltonian to achieve the t-U-J model (Hirsch, 1989). In a recent study, Enaibe and Idiodi (2003) showed that the model contains both ferromagnetism and antiferromagnetism in agreement with the suggestion of Hirsch (1989). Their work however, is restricted to only two electrons on 1D two sites (N=2) and 2D nine sites (3 x 3) lattices.

The two sites, two electrons case means half filling (i.e equal number of sites N and electrons N_e) and the 3 x 3 case is an investigation of the model in 2D. It cannot, therefore, be used to account for the effect of moving away from half filling, that is, increasing the number of sites more than two but still using only two electrons. The purpose of the present study is to investigate the effect of moving away from half filling. So in addition to N = 2, four other 1D even lattices (N = 4, 6. 8 and 10) will be studied.

The mathematical approach to be used is the simplified formulation (Akpojotor and Idiodi, 2004) of the correlated variational approach (CVA) first introduced in 1989 by Chen and Mei. This approach usually lead to the expression of the Hamiltonian of a given lattices in matrix form. This is then solved to obtain the eigenvalues which is the energy spectrum of that lattice system while the eigenvectors becomes the variational parameters needed to express its wave function. In their study, Enaibe and Idiodi (2003) had used the Chen and Mei formulation. So in addition to investigating the effect of moving away from half filling, this current study is an extension of our simplified formulation of the CVA to the t-U-J model.

The plan of this study is as follows. In sec.II, we will show how to use the simplified CVA to obtain the matrix forms of the t-U-J Hamiltonian of the various sites. These matrices will then be solved numerically and the results obtained will be discussed in sec.III. This will be followed by a conclusion.

II. THE VARIATIONAL APPROACH

The variational approach is an approximation technique used when the model Hamiltonian is time independent. The variational ground state energy is given by (Chen and Mei, 1989)

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$$E_g = \frac{\langle \psi_g / H / \psi \rangle}{\langle \psi / \psi \rangle} \tag{2.1}$$

where the ket in the Hilbert space is the trial wave function defined as

$$/\psi> = \sum_{L=0}^{S-1} X_L /\psi_L> + \sum_{L=1}^{S-1} Y_L /\psi_L> . \tag{2.2}$$

In Eq. (2.2), the X and Y are the variational parameters, the L is the lattice separation between the two electrons and the S denotes the total number of such separations possible in a given lattice. It is given by

$$S = \left(\frac{N+2}{2}\right) \text{ for even lattices.} \tag{2.3}$$

A single lattice separation is denoted by a and all other separations are written in terms of a. Owing to the convention introduced in Akpojotor et al.(2002), L takes values from

$$L_{CX} = 0.1.2,\ldots.S-1 \tag{2.4}$$

for states in which the two electrons have opposite spins (i.e singlet states) while for states in which both electrons have spins up (i.e. triplet states),

$$L_{CY} = 1.2.3,\ldots,S-1 \tag{2.5}$$

The H in Eq.(2.1) is the single band t-U-J Hamiltonian which can be expressed as (Hirsch,1989)

$$H = -t\left[\sum_{<i,j>,\sigma,\sigma^1} C^+_{i\sigma} C_{j\sigma} + H.C.\right] + U\sum_i n_{i\uparrow} n_{i\downarrow} + J \sum_{<i,j>\sigma,\sigma^1} C^+_{i\sigma} C^+_{j\sigma^1} C_{i\sigma^1} C_{j\sigma} \ , \tag{2.6}$$

where t is the hopping term, U is the Coulomb term and J is the exchange interaction while $C^+_{i\sigma}(C_{j\sigma^1})$ and $n_{i\sigma}$ are respectively the creation (annihilation) and number operators for an electron in the Wannier state on the ith (jth) lattice site with spin projection σ and H.C is the Hermitian conjugate.

A serious criticism of the Chen and Mei(1989) variational formulation is that it is tedious and prone to mistake because one has to draw the lattice diagram for every lattice site to be studied, write out all the possible states from it and then correlate the intersite states. Also, the Hamiltonian for the lattice site being studied has to be expanded in full before using it to operate on each of the correlated states. Thereafter, the inner products of both the numerator and the denominator are obtained to write equation for the variational ground state energy, which is then minimized with respect to each of the variational parameters to obtain several equations which can be expressed as the matrix form of the Hamiltonian. This whole process is very tasking especially as the number of sites is increased and as we move to higher dimensions. This was why a simplified formulation was recently developed (Akpojotor and Idiodi 2004).

The salient feature of our formulation is deriving a general formular to directly obtain the matrix form of the two electron model Hamiltonian interaction on any size lattice in all the three dimensions simply by using the Hamiltonian to operate on any of the states in each separation. This formular is

$$HR_{I_{CR}} = \left[E_{\delta I_{CR} I_R} - 4\left(\frac{U}{4t}\right)_{00} - 4\left(\frac{J}{4t}\right)_{(I_{CX}=1)(I_X=1)} + 2T_{X I_{CX} I_X} + 4\left(\frac{J}{4t}\right)_{(I_{CY}=1)(I_Y=1)} + 2T_{Y I_{CY} I_Y}\right] R_{I_{CR}} \tag{2.7}$$

where $E = E_g/t$ is the total energy, R (=X,Y,Z) are the variatinal parameters with X for states in which the electrons have opposite spins while Y and Z are for states with both electrons having spins up and spins down respectively. We are considering only Y here because it can easily be shown that using both Y and Z will yield the same results as using either Y or Z.

The L_X and L_Y in Eq.(2.7) are the respective separations of the new states obtained by operating on a selected state in each separation in Eqs. (2.4) and (2.5). The T_X and T_Y are the respective total number of states with separations L_X and L_Y All the other parameters retain their earlier definitions.

Thus the quantities to be determined before using Eq. (2.7) are S, L_C, L_X, L_Y, T_X and T_Y. The method to obtain S and L_C have been shown in Akpojotor et al.(2002). To obtain L_X, L_Y, T_X and T_Y, one have to operate on the selected state in each separation in L_C with only the particle creation and annihilation operators of the t-U-J Hamiltonian given by

$$H_I = \sum_{<i,j>} C^+_{i\uparrow} C_{j\uparrow} + C^+_{j\uparrow} C_{i\uparrow} + C^+_{i\uparrow} C_{j\uparrow} + C^+_{j\uparrow} C_{i\uparrow} \tag{2.8}$$

The selected state for the first separation (i.e. $L_{CX} = 0$) is site (i,i) where i = N/2 for even 1D lattices. The selected states for other separations greater than $L_{CX} = 0$ are then chosen sequentially as site (i,i+1), (i,i+2),....,(i,i+N/2).

For N = 2, S = 2, $L_{CX} = 0,1$ and $L_{CY} = 1$. Its activation will then be

$$H_t/\psi_0 >= H_t/1\uparrow,1\downarrow>=/2\uparrow,1\downarrow> +/1\uparrow,2\downarrow>$$

$$H_t/\psi_1 >= H_t/1\uparrow,2\downarrow>=/2\uparrow,2\downarrow> +/1\uparrow,1\downarrow>$$

$$H_t/\psi_1 >= H_t/1\uparrow,2\uparrow>=/2\uparrow,2\uparrow> +/1\uparrow,1\uparrow>$$ (These two new triplet states are rejected because of the Pauli exclusion principle)

Thus a table showing L_{CX}, L_{CY}, L_X, L_Y, T_X and T_Y can now be prepared.

Table 2.1: A table showing L_{CX}, L_{CY}, L_X, L_Y, T_X and T_Y for N=2

L_{CX}	L_X	T_X
0	1	2
1	0	2
L_{CY}	L_Y	T_Y
1	0	0

Using Eq.(2.7) and Table 2.1, the matrix representation of the two electron interaction on two sites is obtained as shown in Eq.(2.9).

$$\begin{bmatrix} E-4(U/4t) & 2 & 0 \\ 2 & E-4(J/4t) & 0 \\ 0 & 0 & E+4(J/4t) \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ Y_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \qquad (2.9)$$

The same procedure is used to obtain the matrix representation of the two electron t-U-J Hamiltonian on N = 4,6,8 and 10. All these matrices which are in the form of an eigenvalue problem (Harper, 1989) are then solved to obtain their eigenvalues which yield the energy spectrum of the various lattice systems while the eigenvectors becomes the variational parameters needed to express their wave functions. The results are discussed in the next section.

III DISCUSSION OF RESULTS

The lowest value of the energy spectrum is the ground state energy of that system. The implication is that the state, antiferromagnetic or ferromagnetic, which provides this total energy, will be the state of the system. If singlet states provide the lowest energy, then the system will be antiferromagnetic while it will be ferromagnetic if the triplet states provide the total energy. The values of the exchange interaction strength J/4t and onsite interaction strength U/4t at which there is transition from antiferromagnetic to ferromagnetic will be called the transition point.

Tables 4.1 and 4.2. show the total energies and variational parameters for N = 2 lattice as the onsite interaction strength U/4t is decreased from 2 to –2. These were the same results obtained by Enaibe and Idiodi (2003) using the more complex Chen and Mei formulation (1989). We observe that in each table, the total energy increases as the J/4t is increased till there is a transition from antiferromagnetism to ferromagnetism. Thereafter, it began to decrease as J/4t is increased.

Further, we observe that in Table 4.1 and 4.2, as U/4t is decrease from 2 to –2, the exchange interaction strength increases. Thus the transition point for U/4t =2 is J/4t = 0.0606, for U/4t = 0 is J/4t = 0.3536 and that for U/4t = -2 is J/4t = 2.0600. Observe also that the total energy decreases as U/4t is decreased from 2 to –2. It is E = -0.2429 at the transition point U/4t = 2, E = -1.4143 at U/4t = 0 and E = -8.2427 at U/4t = -2.

Now for the larger sites (N = 4,6,8 and 10), we observe from our computation the same trend for the total energy at constant values of the U/4t: it increases as the J/4t is increased till there is a transition from antiferromagnetism to ferromagnetism. Thereafter, it began to decrease as J/4t is increased. The physical implication is that the interaction favouring antiferromagnetism gets weaker as the exchange interaction strength is increased. This goes on until the interaction favouring ferromagnetism begins to dominate and this domination is enhanced as J/4t is increased hence the total energy decreases.

TABLE 4.1 Total energies and variational parameters for the 1D (N = 2) lattice when U/4t = 2

Exchange Interaction Parameter J/4t	Onsite Interaction Parameter U/4t	Total energy $E = E_g/t$	Variational parameters		
			X_0	X_1	Y_1
0.0601	2	-0.2448	0.2357	0.9718	0
0.0602	2	-0.2444	0.2358	0.9718	0
0.0603	2	-0.2440	0.2358	0.9718	0
0.0604	2	-0.2436	0.2358	0.9718	0
0.0605	2	-0.2432	0.2358	0.9718	0
0.0606	2	-0.2429	0.2358	0.9718	0
0.0607	2	-0.2428	0	0	1.0000
0.0608	2	-0.2432	0	0	1.0000
0.0609	2	-0.2436	0	0	1.0000
0.0610	2	-0.2440	0	0	1.0000

TABLE 4.2. Total energy and variational parameters for the 1D (N = 2) lattice when U /4t = -2

Exchange Interaction Parameter J/4t	Onsite Interaction Parameter U/4t	Total energy $E=E_g/t$	Variational parameters		
			X_0	X_1	Y_1
2.0100	-2	-8.2456	0.9925	0.1219	0
2.0200	-2	-8.2450	0.9926	0.1216	0
2.0300	-2	-8.2444	0.9926	0.1213	0
2.0400	-2	-8.2438	0.9926	0.1210	0
2.0500	-2	-8.2433	0.9927	0.1207	0
2.0600	-2	-8.2427	0.9927	0.1205	0
2.0700	-2	-8.2800	0	0	1.0000
2.0800	-2	-8.3200	0	0	1.0000
2.0900	-2	-8.3600	0	0	1.0000
2.1000	-2	-8.4000	0	0	1.0000

TABLE 4.3: A table showing the total energy and exchange interaction strength as the onsite interaction strength is varied from 2 to –2 for N = 2,4,6,8 and 10.

No. of sites N	Onsite Interaction Parameter U/4t	Exchange Interaction Parameter J/4t	Total energy $E = E_g/t$
2	2	0.0606	-0.2429
	0	0.3535	-1.4143
	-2	2.0600	-8.2427
4	2	0.0907	-3.0160
	0	0.2885	-3.4642
	-2	1.8972	-8.5271
6	2	0.0860	-3.5271
	0	0.2705	-3.6956
	-2	1.9930	-8.5017
8	2	0.0851	-3.7233
	0	0.2628	-3.8043
	-2	1.9995	-8.5001
10	2	0.0844	-3.8188
	0	0.2586	-3.8638
	-2	2.0000	-8.5000

Similarly, the observation made for N = 2 that as the U/4t is decreased from 2 to –2, the exchange interaction strength increases, is consisfent in the larger sites (See Table 4.3). The implication is that U/4t enhances the transition from antiferromagnetism to ferromagnetism since its increase will decrease the value of J/4t needed to induce the transition. It is pertinent to point out that though U/4t enhances the transition, it cannot by itself induce it even for very large values i.e U/4t→ ∞.

Finally, we observe in Table 4.3 that the interaction is enhanced as we move away from half filling. This is because the total energy decrease from E = -0.2429 for N = 2 to E = -3.8188 for N = 10 at U/4t = 2, E = -1.4142 for N = 2 to E = -3.8638 for N = 10 at U/4t = 0 and E = -8.2427 for N = 2 to E = -8.5000 for N = 10 at U/4t = -2.

CONCLUSION

This study has shown that the observations made at half filling are consistent even as one moves away from half-filling. However, it is observed further that the tendency to transit from antiferromagnetism to ferromagnetism is enhanced as one moves away from half filling. This means increasing the lattice sites enhances ferromagnetism. It follows therefore that to apply the model to real materials, large sites have to be used. This seems to agree with the general opinion in the literature that finite lattice sizes often suppress the results of electron correlations (Chen and Mei 1989: Amadon and Hirsch 1996). The Chen and Mei correlated variational approach was an attempt to overcome this finite size effect. But as stated above, their formulation is complex, tedious and prone to mistake as one moves to larger sites and higher dimensions. For example, to study an N x N x N = 11 x 11 x 11 lattice, one has to draw the lattice diagram to write out all the 1,771,561 states, correlate the interstates, expand the full Hamiltonian for all the states and use same to operate on all the correlated states. Thus its use is often restricted to small lattices too and the need to go beyond it resulted our simplified formulation (Akpojotor and Idiodi 2004). The successful application of this formulation here means we can now study any number of sites in any of the dimensions and thereby have completely overcome the finite size effect.

REFERENCES

Akpojotor G. E and Idiodi J.O., 2004. A highly simplified variational formulation of the two electron t-U and t-t^1-U models. Zuma J. Pure and Applied Sc. 6(1): 124 - 128

Akpojotor, G. E, Idiodi J. O., Enaibe E.A. and Enukpere E., 2002 A method to determine the states in two electron lattice system. Nig. J.Phys. 14 (2): 117-121.

Amadon J. C and Hirsch J.E.C., 1996. Metallic ferromagnetism in a single-band model: Effect of band filling and Coulomb interactions. Phys. Rev B54: 6364-6375.

Bulla R., 2000. Progress Report (September 1996-December 1999) of the Center of Electronic Correlation and Magnetism, Institute of Physics, University of Augsburg, Germany: pp126-130. First published in Phys. Rev. Lett. 83: p136.

Chen L. and Mei C., 1989. Exact calculation of the two electron interaction in the ground states of the Hubbard model. Phys. Rev. B39: 9006-9011.

Enaibe, E. A. and Idiodi, J.O.A., 2003. The two-electron interaction in the ground state of the Hubbard-Hirsch Hamiltonian. J. of the Nig. Assoc. of Math. Phys. 7: 275-280.

Harper, C., 1989. Introduction to Mathematical Physics Prentice-Hall of India Private Limited, New Delhi, 58pp.

Hirsch, J.E., 1989. Metallic ferromagnetism in a single-band model. Phys. Rev. B40: pp2354-2361.

Hubbard J., 1963. Electrons correlations in narrow energy bands. Proc. Roy. Soc. London, Series A276: 238-257.

Petukhov A.G., Galan J. and Verges J.A .,1992. Bound states of two electrons described by the t-J model. Phys. Rev. B46: 6212-6216.

Pimenov A., Hartinger Ch., Loidl A., Mukhin A.A., Ivanov V.Yu. and Balbashov A. M., 1999. Itinerant versus localized transport in $La_{1-x}Sr_xMnO_3$ for $x < 0.175$. Phys.Rev. B59: 12419-12424.

Ulmke M., 2000. Ferromagnetism in the Hubbard model on fcc-type lattices. Progress Report (September 1996-December 1999) of the Center of Electronic Correlation and Magnetism, Institute of Physics, University of Augsburg, Germany: pp121-125. First published (1998) in Eur. Phys. J. B1: p301.

Vollhardt D., Blumer N., Held K., Koller M., Schlipf J and Ulmke M., 1997. Non-pertubative approaches to magnetism in strongly correlated electrons systems. Progress Report (September 1996-December 1999) of the Center of Electronic Correlation and Magnetism, Institute of Physics, University of Augsburg, Germany: pp93-104. First published (1997) in Z. Phys. B103: p238.