

A HIGHLY SIMPLIFIED CORRELATED VARIATIONAL
APPROACH TO FERROMAGNETISM AND
TRIPLET SUPERCONDUCTIVITY IN THE TWO-ELECTRON
 t - U - V - J MODEL

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ABSTRACT

The dynamics of the interacting electronic pair is examined in this work by the single band t-U-V-J model, which is hoped to provide an insight into the interaction mechanisms of ferromagnetism and triplet superconductivity. The mathematical method used is a highly simplified correlated variational approach (HSCVA) recently developed by us. The results obtained provide an insight into the behaviour of electronic correlations in the t-U-V-J potential. In particular, the parameter space for a transition from antiferromagnetism to ferromagnetism and from singlet superconductivity to triplet superconductivity are clearly delineated

MY PRESENTATION FORMAT

Motivation for the work

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MOTIVATION FOR THE WORK

- Electronic correlations in matter are largely responsible for the various interesting properties of solid materials in nature such as the chemical bonding, magnetic, electrical and optical properties.^{1,2} Electronic correlations could also lead to phase transition of the parent material such as in the Mott-Hubbard (metal-insulator) transition³, high temperature superconductivity⁴ and ferromagnetism.^{5,6} It is widely believed that these phenomena which involve strongly correlated electrons cannot be investigated with any standard perturbation theory.⁷⁻⁹ Also there is currently no proven exact and satisfactory theory to investigate the strong correlations of electrons. This is why there is still no consensus on the origin of the aforementioned phenomena. This is very challenging especially in the case of ferromagnetism in metals which is one of the oldest strong coupling phenomena observed in nature.
- In this presentation, the strong correlation of electrons and its implications will be investigated using the General lattice model. Specifically, a physically motivated truncated form of the General lattice Hamiltonian will be used for the investigation, by employing a non-perturbative approach.

METHODOLOGY

- **THE GENERAL LATTICE MODEL FOR STRONGLY CORRELATED ELECTRONS**

- The general lattice Hamiltonian model within the occupation number formalism for electrons with spin σ interacting via a spin-dependent interaction $V^{ee}(r-r^1)$ in the presence of an ionic lattice potential $V^{ion}(r)$ has the form⁶

- $$H = H_0 + H_{int} \quad (1.1)$$

- where

$$\hat{H}_0 = \sum_{\sigma} \int d^3 r \hat{\psi}_{\sigma}^{+}(r) \left[-\frac{\hbar^2}{2m} \Delta + V^{ion}(r) \right] \hat{\psi}_{\sigma}(r) \quad (1.2)$$

- $$\hat{H}_{int} = \frac{1}{2} \sum_{\sigma\sigma^1} \int d^3 r \int d^3 r^1 V^{ee}(r-r^1) \hat{n}_{\sigma}(r) \hat{n}_{\sigma^1}(r^1) \quad (1.3)$$

- In the above equation, the $\hat{\psi}_{\sigma}(r), \hat{\psi}_{\sigma}^{+}(r)$ are the usual field operators and

$$\hat{n}_{\sigma}(r) = \hat{\psi}_{\sigma}^{+}(r) \hat{\psi}_{\sigma}(r) \text{ is the local density.}$$

- After some initial assumptions (see Ref. 6) , the Hamiltonian may be written in the lattice representation as

- $$H = \sum_{\alpha ij \sigma} t_{\alpha ij} c_{\alpha i \sigma}^+ c_{\alpha j \sigma} + \frac{1}{2} \sum_{\alpha \beta \gamma \delta} \sum_{ijmn} \sum_{\sigma \sigma^1} v_{ijmn}^{\alpha \beta \gamma \delta} c_{\alpha i \sigma}^+ c_{\beta j \sigma^1}^+ c_{\delta n \sigma^1} c_{\gamma m \sigma} \quad (1.4)$$

- where α, β, γ and δ represent the bands while i, j, m and n represents the sites
- The Hamiltonian given by Eq.(1.4) is too general to be tractable in dimensions $d > 1$. Therefore, it has to be simplified using physically motivated truncations such as:
 - i. That the Fermi surface (FS) lies within a single conduction band that is well separated from other bands so that the inter band interaction is weak hence we will restrict our study to a single band ($\alpha = \beta = \gamma = \delta = 1$) which is also called tight binding (TB) band. Thus Eq. (1.4) reduces to

$$H_{1-band} = \sum_{ij \sigma} t_{ij} c_{i \sigma}^+ c_{j \sigma} + \frac{1}{2} \sum_{ijmn} \sum_{\sigma \sigma^1} v_{ijmn} c_{i \sigma}^+ c_{j \sigma^1}^+ c_{n \sigma^1} c_{m \sigma} \quad (1.5)$$

- ii. The above single band Hamiltonian is still too complicated for most purposes, as such it needs to be simplified further. Taking into account the weak overlap between neighbouring orbitals in a TB description, one expects that the overlap between nearest neighbours (NN) is important hence only NN hopping and interactions are allowed. So the site indices are restricted to only NN positions leaving us with a purely local contribution,

- $v_{iiii} = U$ (1.6)
- which is the on-site Coulombic interaction term;

- and four NN contributions:
- $v_{ijij} = V$ (1.7)
- which is the NN Coulombic interaction term,

- $v_{iijj} = \Delta t$ (1.8)
- which gives rise to an occupation dependent hopping rate,

- $v_{ijji} = J$ (1.9)
- which is the NN Heisenberg exchange term and

- $v_{iijj} = J^1$ (1.10)
- which describes the exchange hopping processes.

- Thus it is by adding the appropriate contribution from Eqs. (1.6 – 1.10), to the kinetic part in Eq.(1.5) that we will obtain the so called t-U model (commonly known as Hubbard model), t-U-V model, t-U-J model, t-U-V-J model, etc.
- It is necessary to point out that an explicit evaluation of the relative size of all these contributions was given in the original paper by Hubbard (1963) but the four NN contributions were shown to be negligibly small in the special cases of interest to Hubbard.
- Thus the choice of the NN contributions to be included to the original Hubbard model in this current work will depend on the physical situation.
- Basically, the problem of developing a theory for ferromagnetism in metals emanates from the apparent dual character, itinerancy and localization properties of the electrons in these materials.^{8,10,11} The Hubbard model¹² was developed with the hope that the kinetic part will represent the itinerancy while the Coulombic interaction will be for the localization for ferromagnetism. After more than four decades of intense study of the model, there is general consensus that it usually favours antiferromagnetism.^{13,14} It has been suggested that three natural ways to go beyond the original Hubbard model are to enhance the kinetic part in order to increase the itinerancy of the electrons, include other interaction matrix elements^{5,6,8} within the single band model or include band degeneracy¹⁵ that allows intra-atomic exchange. We take the second path here: adding other interaction terms.

The t-U-V-J Model

- It is Amadon and Hirsch⁵ who suggested that to achieve a realistic model of electrons in metals, the NN Coulombic interaction V should also be included to the t-U-J model to achieve the t-U-V-J model given by

$$H = -t \left[\sum_{\langle i,j \rangle, \sigma} C_{i\sigma}^+ C_{j\sigma} + H.C. \right] + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j \rangle} n_i n_j + J \sum_{\langle i,j \rangle, \sigma, \sigma^1} C_{i\sigma}^+ C_{j\sigma^1}^+ C_{i\sigma^1} C_{j\sigma} \quad (1.11)$$

The need to include the V term is based on the fact that its absence will make the General lattice model to be unstable towards triplet SC, as electrons of parallel spins attract each other. The attraction between the parallel spins is $V - J$, as such the instability will disappear for $V \geq J$ which is expected to be the situation for electrons in metals.

- In their study of one dimensional (1D) lattices using both the numerical exact diagonalization and mean field theory (MFT), Amadon and Hirsch⁵ showed that in the exact case, the V term suppresses the tendency to ferromagnetism particularly for small U for all band fillings while MFT predicts no effect of V . Consequently, that study suffers two setbacks: it is limited to 1D lattices and the observation made for the role of V from the exact calculation is different from that of the MFT as one moves away from half filling.
- Thus as hinted earlier, the goal of this work is to investigate the dynamic of the two-electrons interacting under the t - U - V - J model on finite-sized lattices in one dimension (1D), 2D and 3D using a highly simplified correlated variational approach (HSCVA).

THE CHOICE OF CALCULATION

- As stated earlier, the general belief in the literature is that electronic correlations is a quantum-mechanical strong coupling phenomenon which cannot be investigated by any standard perturbation theory.⁶ Since the General lattice model is time independent, the variational approach which provides an approximate calculation of the ground state energy spectrum and wave function of a time independent Hamiltonian. is a feasible candidate.

- In 1989, Chen and Mei developed a variational method for quantum systems consisting of two electrons interacting under the Hubbard Hamiltonian in 1D and 2D lattices. The method which is also known as the correlated variational approach (CVA) has been extended to three dimensional (3D) lattices.
- The Chen and Mei formulation has three shortcomings today:
- It was developed only for singlet states as such it can not be applied to both magnetism and triplet superconductivity¹⁶ which require the inclusion of triplet states.
- It is complex, tedious and time consuming and Chen and Mei have two separate expressions for the 1D and 2D ground state variational energies.
- The resulting variational energy equations have to be minimized with respect to each of the variational parameters to obtain several equations, which can then be expressed as the matrix form of the Hamiltonian. This could be tedious especially for large lattice sizes.

- Thus there is need to develop a simpler formulation of the CVA. This is another goal of this present work and there will be two steps to achieve it
- First, a very simple and general expression for the ground state variational energy applicable to all three dimensions and with triplet states included will be obtained. The inclusion of the triplet states is important as ferromagnetism is caused by parallel spins. Interestingly, the triplet superconductors are believed to have the same band mechanism as the ferromagnetic metals.¹⁶⁻¹⁸
- This expression, like that of Chen and Mei, has to be minimized with respect to the variational parameters, to obtain the matrix form of the system.
- Therefore, as a further step to simplify the formulation, the process of minimization will be avoided. This is the second step wherein a general expression will be developed to obtain directly the matrix form of the two interacting electrons on any lattice size in all three dimensions, without going through the minimization process.

EXACT CALCULATION FOR $N = 2$ SITES

- We began our calculation by obtaining expressions for the exact ground state energy and exact wave function for a quantum system of two interacting electrons on N sites ($N = 2$). The expression for the ground state energy will be obtained from the energy spectrum which is the eigenvalues of the matrix representation of the t - U - V - J Hamiltonian for $N = 2$. The eigenvector associated with this ground state energy is, of course, the exact wave function.

- The matrix form of a given Hamiltonian H , with respect to a set of basis wave functions $|\psi_i\rangle$ is given by

$$H_{ij} = \langle \psi_i | H | \psi_j \rangle \quad (1.12)$$

- where the i and j are elements taking values of $i = 1, 2, 3, \dots, N$ and $j = 1, 2, 3, \dots, N$ while the ket $|\psi\rangle$ and its bra $\langle \psi|$, are the wave functions. Suppressing for now the subscripts on the wavefunctions, they are defined respectively as

$$|\psi\rangle = \sum_{i=1, j=1}^N R_{ij} |i\sigma, j\sigma^1\rangle \quad (1.13)$$

$$\langle \psi| = \sum_{i=1, j=1}^N R_{ij} \langle i\sigma, j\sigma^1| \quad (1.14)$$

- where the electronic state $|i\sigma, j\sigma^1\rangle$ means that one electron is on lattice site i with spin σ and the other electron is on lattice site j with spin, σ^1 while the R_{ij} ($= X_{ij}, Y_{ij}, Z_{ij}$) are the expansion coefficients.

- By putting in the appropriate values, Eq. (1.13) can be expressed in full as

$$\begin{aligned}
 |\psi\rangle = & \sum_{i=1}^N X_{ii} |i \uparrow, i \downarrow\rangle + \sum_{i=1, j=1; i \neq j}^N X_{ij} [|i \uparrow, j \downarrow\rangle - |i \downarrow, j \uparrow\rangle] \\
 & + \sum_{i=1, j=1; i \neq j}^N Y_{ij} |i \uparrow, j \uparrow\rangle + \sum_{i=1, j=1; i \neq j}^N Z_{ij} |i \downarrow, j \downarrow\rangle
 \end{aligned}
 \tag{1.15}$$

- For the two electrons on two sites problem, we have a total of six states:
- $|1\rangle = |1 \uparrow, 1 \downarrow\rangle$, $|2\rangle = |2 \uparrow, 2 \downarrow\rangle$, $|3\rangle = |1 \uparrow, 2 \downarrow\rangle$, $|4\rangle = |1 \downarrow, 2 \uparrow\rangle$, $|5\rangle = |1 \uparrow, 2 \uparrow\rangle$,
 $|6\rangle = |1 \downarrow, 2 \downarrow\rangle$.

$$\tag{1.16}$$

- It can easily be shown that the Hamiltonian matrix size for the two-electron interaction on K sites will be
- $(2K^2 - K) \times (2K^2 - K)$. (1.17)
- where $K = N$ for 1D lattices with N sites,
- $K = N^2$ for 2D lattices of size $N \times N$ (1.18)
- and $K = N^3$ for 3D lattices of size $N \times N \times N$.
- Eq. (1.17) implies that we have a matrix size of 6×6 to handle for a 1D lattice of $N = 2$ sites, while for $5 \times 5 \times 5$ 3D lattice, one has the outlandish matrix size of 31125×31125 to deal with! It is this astronomical growth of the matrix size with the lattice size that restricts the application of the exact method to small lattice sizes.

- To obtain these 6 x 6 matrix, we have to use the the t-U-V-J Hamiltonian given Eq (1.11) which can be expanded for N = 2 as

$$\begin{aligned}
 \bullet H = & -t \left[C_{1\uparrow}^+ C_{2\uparrow} + C_{2\uparrow}^+ C_{1\uparrow} + C_{1\downarrow}^+ C_{2\downarrow} + C_{2\downarrow}^+ C_{1\downarrow} \right] + U [n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow}] + V [n_{1\uparrow} n_{2\downarrow}] \\
 & - J [C_{1\uparrow}^+ C_{2\downarrow}^+ C_{2\uparrow} C_{1\downarrow} + C_{1\downarrow}^+ C_{2\uparrow}^+ C_{2\downarrow} C_{1\uparrow} + C_{1\uparrow}^+ C_{2\uparrow}^+ C_{2\uparrow} C_{1\uparrow} + C_{1\downarrow}^+ C_{2\downarrow}^+ C_{2\downarrow} C_{1\downarrow}].
 \end{aligned}
 \tag{1.19}$$

- to operate on each of the six states in Eq. (1.16) to obtain the following new states, taking into account the anticommutation rule of fermions,

$$|i \uparrow, j \downarrow\rangle = - |j \downarrow, i \uparrow\rangle \quad :$$

- $H|1\rangle = -t|3\rangle + t|4\rangle + U|1\rangle$
- $H|2\rangle = -t|3\rangle + t|4\rangle + U|2\rangle$
- $H|3\rangle = -t|1\rangle + -t|2\rangle + V|3\rangle - J|4\rangle$
- $H|4\rangle = t|1\rangle + t|2\rangle - J|3\rangle + V|4\rangle$
- $H|5\rangle = V|5\rangle - J|5\rangle$
- $H|6\rangle = V|6\rangle - J|6\rangle$

(1.20)

- By using the condition that the eigen states $\{|m\rangle: m = 1, 2, \dots, 6\}$ constitute an orthonormal set, i. e.

$$\langle m | m^1 \rangle = \delta_{mm^1} \begin{cases} 1 & \text{if } m = m^1 \\ 0 & \text{if } m \neq m^1 \end{cases} \quad (1.21)$$

the real matrix form of Eq. (1.12) can now be written out as

$$E_g = \begin{bmatrix} U & 0 & -t & t & 0 & 0 \\ 0 & U & -t & t & 0 & 0 \\ -t & -t & V & -J & 0 & 0 \\ t & t & -J & V & 0 & 0 \\ 0 & 0 & 0 & 0 & V - J & 0 \\ 0 & 0 & 0 & 0 & 0 & V - J \end{bmatrix} \quad (1.22)$$

- The 6 x 6 matrix is clearly block-diagonalized into a 4 x 4 matrix and a 2 x 2 matrix.
- The 2 x 2 matrix which emerges from the triplet states, is already in diagonal form. Hence its eigenvalues are precisely the diagonal elements $V-J$. Thus the energy for the triplet states, which is doubly degenerate, is
- $E_t = E_g / t = V/t - J/t.$ (1.23)
- The first triplet energy emerges from the states with +1 unit of spin and the second is from the states with -1 unit of spin. Since both types of triplet states produce the same energy, then using any of them will be enough to represent the effect or interaction of triplet states.

- The remaining 4 x 4 matrix can be diagonalized by expressing it in form of an eigenvalue problem and solving it, will result to four eigen values of which the lowest of them is the ground state energy for the singlet states:

$$E_s = \frac{E_g}{t} = -2 \left[\sqrt{\left(\frac{U}{4t} - \frac{V}{4t} - \frac{J}{4t} \right)^2 + 1} - \left(\frac{U}{4t} + \frac{V}{4t} + \frac{J}{4t} \right) \right] \quad (1.24)$$

- The eigen vectors of this lowest energy can now be used to express the the ground state wavefunction as

$$|\psi\rangle = \sum_{i=1}^N X_{i,i} |i\uparrow, i\downarrow\rangle + \sum_{\langle i,j \rangle} X_{i,j} [|i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle] + \sum_{\langle i,j \rangle} Y_{i,j} [|i\uparrow, j\uparrow\rangle \quad (1.25)$$

- where $\langle i, j \rangle$ stands for only nearest neighbour interactions.

CHEN AND MEI VARIATIONAL FORMULATION FOR N = 2 SITES

- The variational ground state energy is given by Chen and Mei¹⁴

$$E_g = \frac{\langle \psi | H | \psi \rangle}{\langle \psi | \psi \rangle} \quad (1.26)$$

- where H is the Hamiltonian of the t-U-V-J model and $|\psi\rangle$ is the trial wave function.
- Now the Chen and Mei variational parameters are function of the lattice site separations (i.e $|i - j|$) only, hence the wavefunction is

$$|\psi\rangle = \sum_{i=1}^N X_{|i-i|} |i \uparrow, i \downarrow\rangle + \sum_{\langle i,j \rangle}^N X_{|i-j|} [|i \uparrow, j \downarrow\rangle - |i \downarrow, j \uparrow\rangle] + \sum_{\langle i,j \rangle}^N Y_{|i-j|} [|i \uparrow, j \uparrow\rangle] \quad (1.27)$$

- which for N = 2 becomes

$$|\psi\rangle = X_0 [|1 \uparrow, 1 \downarrow\rangle + |2 \uparrow, 2 \downarrow\rangle] + X_1 [|1 \uparrow, 2 \downarrow\rangle - |1 \downarrow, 2 \uparrow\rangle] + Y_1 |1 \uparrow, 2 \uparrow\rangle$$

- Consequently, it can be shown that the denominator of Eq.(1.26) is
- $\langle \psi / \psi \rangle = 2 X_0^2 + 2 X_1^2 + Y_1^2$ (1.27)

- Similarly, by using the Hamiltonian to operate on the wavefunction, we obtain a new one, that is,

- $H / \psi \rangle = / \psi^1 \rangle$

- hence the numerator in Eq. (1.26) becomes

- $\langle \psi / H / \psi \rangle = \langle \psi / \psi^1 \rangle$

- $= -8t X_0 X_1 + 2UX_0^2 + 2VX_1^2 + 2JX_1^2 + VY_1^2 - JY$ (1.28)

- Thus, Eq.(1.26) can now be expressed using Eqs (1.27) and (1.28) as

$$E_g = \frac{-8t X_0 X_1 + 2UX_0^2 + 2VX_1^2 + 2JX_1^2 + VY_1^2 - JY_1^2}{2X_0^2 + 2X_1^2 + Y_1^2} \quad (1.29)$$

- This is minimized wrt the variational parameters to obtain several equations which can be expressed in the matrix form as

$$\begin{bmatrix} E - 4(U/4t) & 2 & 0 \\ 2 & E - 4(V/4t) - 4(J/4t) & 0 \\ 0 & 0 & E - 4(V/4t) + 4(J/4t) \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ Y_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (1.30)$$

- Which is a 3 x 3 blocked matrix of 2 x 2 for the singlet part and 1 x 1 for the triplet part.

- Thus it is easy to see that the eigenvalues E_t and E_s , that will yield nontrivial eigenvectors, subject to the normalization condition

- $$X_0^2 + X_1^2 = 1; \quad Y_1^2 = 1 \quad (1.31)$$

- are

- $$E_t = 4(V / 4t) - 4(J / 4t) \quad (1.32)$$

- and

- $$E_s = -2 \left[\sqrt{\left(\frac{U}{4t} - \frac{V}{4t} - \frac{J}{4t} \right)^2 + 1} - \left(\frac{U}{4t} + \frac{V}{4t} + \frac{J}{4t} \right) \right] \quad (1.33)$$

- which agrees with the energy of the triplet states and singlet states obtained from the exact calculation.

THE HIGHLY SIMPLIFIED FORMULATION OF THE CVA

- The reduction of the matrix size in the variational calculation from 6×6 to 3×3 is because the variational wave function is expressed in terms of the various site separations of the electronic states unlike the exact formulation in which the wave function is expressed in terms of the different electronic states.
- In other words, to write the variational wave function, one has to group all the electronic states into their various site separations (Chen and Mei referred to them as classes) and then express the wavefunction in terms of these separations. This is why the variational matrix size depends on the possible separations and not on the individual states. Our highly simplified formulation is developed by taking advantage of this dependence on the separations.

- Thus we defined our trial wavefunction in terms of the separations as

$$|\psi\rangle = \sum_{L_{CX}=0}^{S-1} X_{L_{CX}} |\psi_{L_{CX}}\rangle + \sum_{L_{CY}=1}^{S-1} Y_{L_{CY}} |\psi_{L_{CY}}\rangle \quad (1.34)$$

- where the $X_{L_{CX}}$ and $Y_{L_{CY}}$ are the variational parameters, while the L_{CX} and L_{CY} are the lattice site separations between the two electrons in an electronic state and the S denotes the total number of such separations that are possible in a given lattice

- $S = \frac{1}{2}(N + 2)$ for even N sites, (1.35)

- $S = \frac{1}{2}(N + 1)$ for odd N sites, (1.36)

- $S = \frac{1}{8}(N + 4)(N + 2)$ for even $N \times N$ sites, (1.37)

- $S = \frac{1}{8}(N + 3)(N + 1)$ for odd $N \times N$ sites, (1.38)

- $S = \frac{1}{48}(N + 6)(N + 4)(N + 2)$ for even $N \times N \times N$ sites, (1.39)

- $S = \frac{1}{48}(N + 5)(N + 3)(N + 1)$ for odd $N \times N \times N$ sites, (1.39)

- It can easily be shown by mere expansion as done in the case of Chen and Mei that the inner product in the denominator of the variational ground state energy is

$$\langle \psi / \psi \rangle = \sum_{L_{CX}=0}^{S-1} n_{L_{CX}}^s X_{L_{CX}}^2 + \sum_{L_{CY}=1}^{S-1} n_{L_{CY}}^t Y_{L_{CY}}^2 \quad (1.40)$$

- where $n_{L_C} = n_{L_{CX}}^s$ and $n_{L_C} = n_{L_{CY}}^t$ are the total number of states with separation L_C for singlet and triplet states respectively.
- Similarly, it can be shown that the numerator of the variational ground state energy is

$$\begin{aligned} \langle \psi / H / \psi \rangle = & -t \left[\sum_{L_{CX}=0}^{S-1} n_{L_{CX}}^s X_{L_{CX}} X_{L_X} T_{L_X} \right] + U n_0^s X_0^2 + (V + J) n_1^s X_1^2 \\ & - t \left[\sum_{L_{CY}=1}^{S-1} n_{L_{CY}}^t Y_{L_{CY}} Y_{L_Y} T_{L_Y} \right] + (V - J) n_1^t Y_1^2 \end{aligned} \quad (1.40)^*$$

- Combining the two equations, the ground state becomes

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

$$= \frac{-t \left[\sum_{L_{CX}=0}^{S-1} n_{L_{CX}}^s X_{L_{CX}} X_{L_X} T_{L_X} \right] + U n_0^s X_0^2 + (V + J) n_1^s X_1^2 - t \left[\sum_{L_{CY}=1}^{S-1} n_{L_{CY}}^t Y_{L_{CY}} Y_{L_Y} T_{L_Y} \right] + (V - J) n_1^t Y_1^2}{\sum_{L_{CX}=0}^{S-1} n_{L_{CX}}^s X_{L_{CX}}^2 + \sum_{L_{CY}=1}^{S-1} n_{L_{CY}}^t Y_{L_{CY}}^2} \quad (1.41)$$

- which is the general expression for the variational ground state energy applicable to all the three dimensions. This is the simplified correlated variational approach (SCVA).
- It is easily observed that by making $V = J = 0$, Eq. (1.41) reduces to an expression for the t-U Hamiltonian. Thus when $V = J = Y = 0$, Eq. (1.41) will provide the same variational ground state energy equation as the more complex and separate expressions for 1D and 2D lattice obtained in Ref. (14).

- The rules to obtain S , L_C and n_{L_C} have been formulated by Akpojotor et al. To obtain L_X , L_Y , T_{L_Y} and T_{L_X} , one has to operate on a selected two-electron state with separation L_C with only the particle creation and annihilation operators of the kinetic part of the t-U-V-J Hamiltonian, given by

$$H_P = \left[C_{i\uparrow}^+ C_{j\uparrow} + C_{j\uparrow}^+ C_{i\uparrow} + C_{i\downarrow}^+ C_{j\downarrow} + C_{j\downarrow}^+ C_{i\downarrow} \right] \quad (1.42)$$

- For 1D in which a typical state is denoted by $|i\uparrow, j\downarrow\rangle$ say,

$$H_P |i\uparrow, j\downarrow\rangle = |(i\pm 1)\uparrow, j\downarrow\rangle + |i\uparrow, (j\pm 1)\downarrow\rangle, \quad (1.43)$$

- 2D in which a typical state is denoted by $|ii\uparrow, jk\downarrow\rangle$ say,

$$H_P |ii\uparrow, jk\downarrow\rangle = [|(i\pm 1)i\uparrow, jk\downarrow\rangle + |i(i\pm 1)\uparrow, jk\downarrow\rangle + |ii\uparrow, (j\pm 1)k\downarrow\rangle + |ii\uparrow, j(k\pm 1)\downarrow\rangle] \quad (1.44)$$

- and for 3D in which a typical state is denoted by $|iii\uparrow, jkl\downarrow\rangle$ say,

$$H_P |iii, jkl\rangle = [|(i\pm 1)ii\uparrow, jkl\downarrow\rangle + |i(i\pm 1)i\uparrow, jkl\downarrow\rangle + |ii(i\pm 1)\uparrow, jkl\downarrow\rangle + |iii\uparrow, (j\pm 1)kl\downarrow\rangle + |iii\uparrow, j(k\pm 1)l\downarrow\rangle + |iii\uparrow, jk(l\pm 1)\downarrow\rangle] \quad (1.45)$$

- So once the aforementioned parameters have been determined for any lattice, we can write the variational ground state energy for it. However, it has to be minimized like that of Chan and Mei to obtain the matrix representation of that lattice.
- Since this process of minimization is often laborious especially as the lattice size increases, we decided to sought for a means to avoid this process of minimization as a further simplification of the CVA.

$$H_{L_{CR}L_R} [R_{L_{CR}}] = \begin{bmatrix} E_{\delta_{L_{CR}L_R}} - 4\left(\frac{U}{4t}\right)_{\delta_{0L_{CR}}\delta_{0L_R}\delta_{RX}} - 4\left\{\left(\frac{V}{4t}\right) + \left(\frac{J}{4t}\right)\right\}_{\delta_{1L_{CR}}\delta_{1L_R}\delta_{RX}} + 2T_{L_{CR}L_R\delta_{RX}} \\ - 4\left\{\left(\frac{V}{4t}\right) - \left(\frac{J}{4t}\right)\right\}_{\delta_{1L_{CR}}\delta_{1L_R}\delta_{RY}} + 2T_{L_{CR}L_R\delta_{RY}} \end{bmatrix} [R_{L_{CR}}] = [0]$$

(1.46)

- which is the highly simplified formulation (HSCVA).

Application to the two-electron interaction on $n = 2$ sites

- For the case of two electrons on two sites, $S = 2$ from Eq. (2.47). Therefore, $L_{CX} = 0, 1$ and $L_{CY} = 1$. The selected state is $|1\uparrow, 1\downarrow\rangle$. So using Eq.(2.65), one gets

$$H_P / \psi_0 \rangle = H_P / |1\uparrow, 1\downarrow\rangle = 2 / |2\uparrow, 1\downarrow\rangle$$

- $H_P / \psi_1 \rangle = H_P / |1\uparrow, 2\downarrow\rangle = 2 / |2\uparrow, 2\downarrow\rangle$

$$H_P / \psi_2 \rangle = H_P / |1\uparrow, 2\uparrow\rangle = 2 / |2\uparrow, 2\uparrow\rangle \quad (1.47)$$

- Hence the table of $L_{CX}, L_X, T_{L_{CX} L_X}, L_{CY}, L_Y$ and $T_{L_{CY} L_Y}$

L_{CX}	L_X		L_{CY}	L_Y	
0	1	$T_{L_{CX} L_X}$	0	-	$T_{L_{CY} L_Y}$
1	0	1	1	0	0

- Taking into account the HSCVA, the matrix rep. for $N = 2$ is

- $$\begin{bmatrix} E - 4(U / 4t) & 2 & 0 \\ 2 & E - 4(V / 4t) - 4(J / 4t) & 0 \\ 0 & 0 & E - 4(V / 4t) + 4(J / 4t) \end{bmatrix} \begin{bmatrix} X_0 \\ X_1 \\ Y_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (1.48)$$

- Which is the same as the one obtained from the Chen and Mei CVA.
- This method was applied to
- $N = 3, 4, 5, 6, 7, 8, 9, 10$ and 11 for ID,
- $N \times N = 3 \times 3, 5 \times 5$ and 7×7 for 2D and
- $N \times N \times N = 3 \times 3 \times 3, 5 \times 5 \times 5$ and $7 \times 7 \times 7$ for 3D.

Presentation and Discussion of Results

- The condition to produce a ferromagnetic phase is that the lowest state energy of the triplet states E_t , must be smaller than that of the singlet states, E_s , i.e. $E_t < E_s$
- The last values of $J/4t$ at the various values of $U/4t$ and $V/4t$ at which there is transition from the antiferromagnetic phase to the ferromagnetic phase will be called the transition point T_p .

RESULTS FOR THE EVEN 1D LATTICE (N = 2 SITES)

The ground state energy for the singlet states of the two electrons on two sites problem, from the exact calculation, Chen and Mei and from the HSCVA is

$$E_s = -2 \left[\sqrt{\left(\frac{U}{4t} - \frac{V}{4t} - \frac{J}{4t} \right)^2 + 1} - \left(\frac{U}{4t} + \frac{V}{4t} + \frac{J}{4t} \right) \right] \quad (1.49)$$

while that for the triplet states

$$E_t = 4 \left(\frac{V}{4t} \right) - 4 \left(\frac{J}{4t} \right) \quad (1.50)$$

Taking them into account, then at the condition to produce ferromagnetism (i.e $E_t < E_s$), the value of the NN exchange interaction strength at the T_p will be⁵

$$\frac{J}{4t} > \frac{1}{2} \left[\sqrt{\left(\frac{U}{4t} - \frac{V}{4t} \right)^2 + \frac{1}{2}} - \left(\frac{U}{4t} + \frac{V}{4t} \right) \right] \quad (1.51)$$

Thus these three eqs can be used to obtain the analytical values of the E_s , E_t and $J/4t$ respectively at the T_p when $U/4t$ and $V/4t$ are given arbitrary values

This is done and the result is present in Table 1

Table 1 The lowest energies at the T_p of both the singlet and triplet states calculated analytically for the 1D lattice with $N = 2$ sites as the on-site interaction strength $U/4t$ and the NN interaction strength $V/4t$ are varied.

On-site interaction strength $U/4t$	NN interaction strength $V/4t$	NN exchange interaction strength $J/4t$	Lowest energy for singlet states E_s at T_p	Lowest energy for triplet states E_t at T_p
3	3	0.3535	10.5857	10.5860
	0	0.0411	-0.1644	-0.1644
	-3	0.0207	-12.0833	-12.0828
0	3	3.0411	-0.1644	-0.1644
	0	0.3535	-1.4143	-1.4140
	-3	0.0411	-12.1644	-12.1644
-3	3	6.0207	-12.0833	-12.0828
	0	3.0411	-12.1644	-12.1644
	-3	0.3535	-13.4143	-13.4140
0	0	0	-2.0000	0

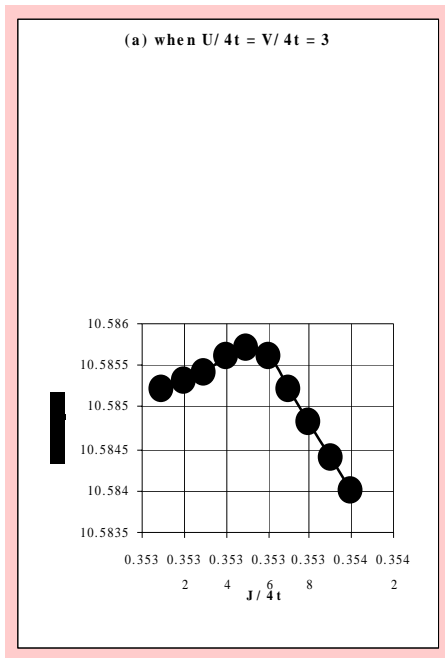
- This matrix is also solve numerical and the results are the same as that of the analytical.

On-site interaction strength $U/4t$	NN interaction strength $V/4t$	NN exchange interaction strength $J/4t$	Ground state energy	Variational parameters	
				X_0	X_1
3	3	0.3535	10.5857	0.8165	0.5773
	0	0.0411	-0.1644	0.1622	0.9868
	-3	0.0207	-12.0833	0.0828	0.9966
0	3	3.0410	-0.1644	0.9966	0.0819
	0	0.3535	-1.4143	0.8164	0.5774
	-3	0.0411	-12.1644	0.0833	0.9966
-3	3	6.0207	-12.0830	0.9991	0.0415
	0	3.0411	-12.1644	0.9966	0.0819
	-3	0.3535	-13.4143	0.8165	0.5774
0	0	0	-2.0000	0.7071	0.7071

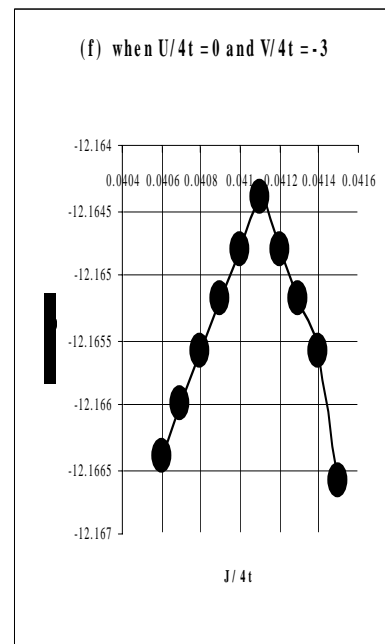
- This successful check gave us confidence to apply the numerical approach to solve the other matrices of the lattice systems considered in this work
- The following observations are made from their results
- It is observed in that if the starting value of $J/4t$ of a given value of $U/4t$ and $V/4t$ is greater than its value at the transition point so that the system is antiferromagnetic (i.e $E_t > E_s$), then as the value of $J/4t$ is increased from the starting value, the lowest energy of the singlet states will be increasing while that of the triplet states will be decreasing.
- This will go on till after the T_p at which $E_t < E_s$. Thereafter, as $J/4t$ is increased further, the E_t will continue to decrease while the E_s will also continue to increase.
- The physical implication is that at the constant values of the on-site and NN interaction strengths, the electronic correlations favouring antiferromagnetism gets weaker while that of ferromagnetism gets stronger as the NN exchange interaction strength is increased until there is a transition from antiferromagnetism to ferromagnetism.
- This trend is observed from computation to be consistent in all the lattices in 1D as well as in the higher dimensions. The trend agrees with the condition to produce ferromagnetism, which is $E_t < E_s$.

- Another trend common to all the lattices in the various dimensions is that in the antiferromagnetic phase, all the variational parameters for the singlet states have non-zero values while those for the triplet states have zero values. This trend is reversed in the ferromagnetic phase. Here lies the beauty and power of the CVA: the relative magnitude of the variational parameters reveal clearly the relative importance of the various parts of the wave function just as the ground state energy determines the favourable state of the system.
- The observations above are clearly shown graphically.

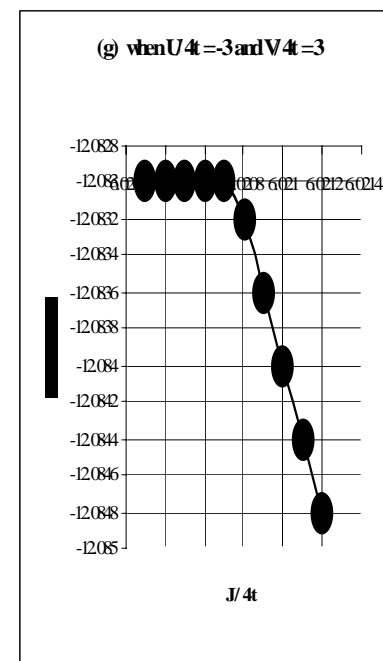
Fig. 1 below shows the ground state energy as function of the NN exchange interaction strength $J/4t$ for the 1D lattice $N = 2$ as $U/4t$, $V/4t$ and $J/4t$ are varied for (a) positive U and V , (b) positive U and negative V , (c) negative U and positive V and (d) negative U and V . Observe that at the constant values of the U and V , the electronic correlations favouring antiferromagnetism gets weaker while that of ferromagnetism gets stronger as the NN exchange interaction strength is increased until there is a transition from antiferromagnetism to ferromagnetism. This trend is consistent in all the lattices in 1D as well as in the higher dimensions. The trend agrees with the condition to produce ferromagnetism, which is $E_t < E_s$. Observe further that that V suppresses the tendency to ferromagnetism while the U enhances it. This accounts for the very small values of $J/4t$ at increasing positive values of $U/4t$ and very large values of $J/4t$ at increasing positive values of $U/4t$. For example, when $U/4t = -3$, the values of $J/4t$ required to induce the transition to the ferromagnetic phase are about twice that of the values of $V/4t$ i.e $2V < J$. These are very interesting and consistent results with the literature. For it has been argued earlier⁵ that whenever $V < J$, the system will be unstable towards triplet superconductivity..



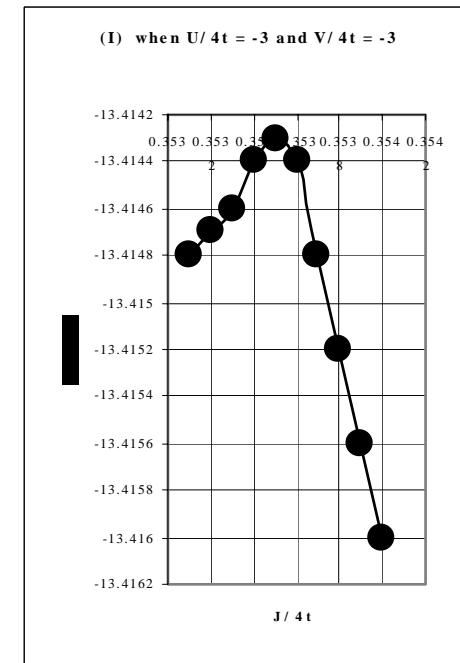
(a)



(b)

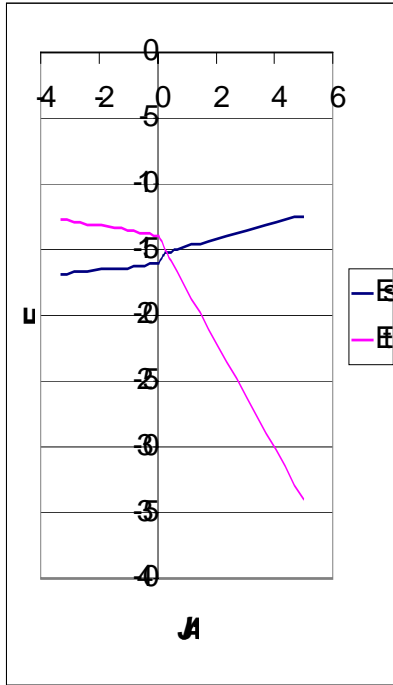


(c)

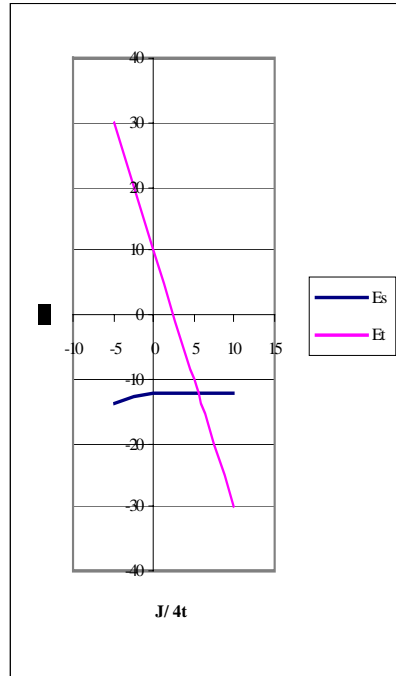


(d)

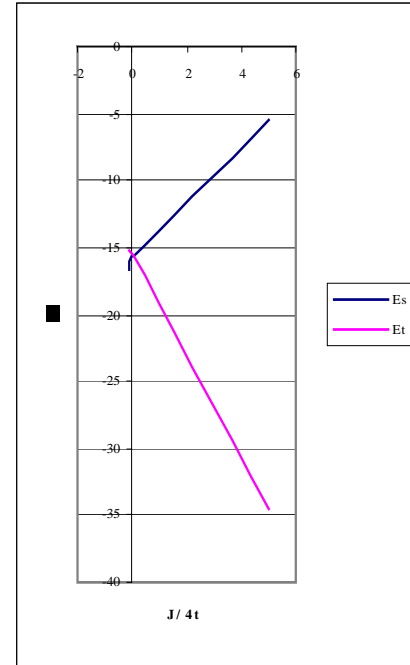
Fig. 2 below shows graphs of the lowest energies for both the singlet and triplet states (E_s and E_t) plotted against positive and negative $J/4t$ as both $U/4t$ and $V/4t$ are varied from -3 to 3 for $N \times N \times N = 3 \times 3 \times 3$. It is observed that for all values of J , the transition from AF to ferro is only when J is positive which is in agreement with the rule that J must be positive.



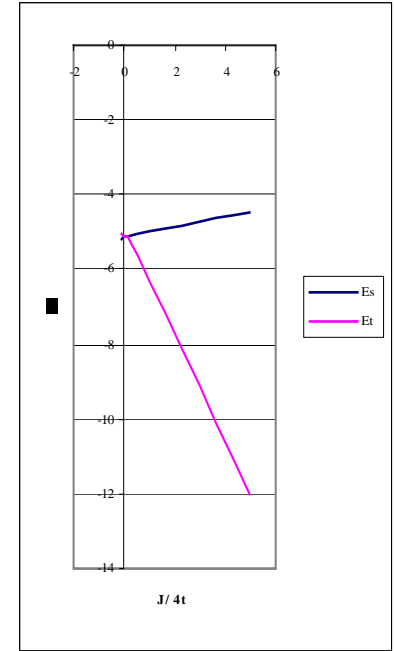
(a) $U/4t = V/4t = -3$



(b) $U/4t = -3$ and $V/4t = 3$

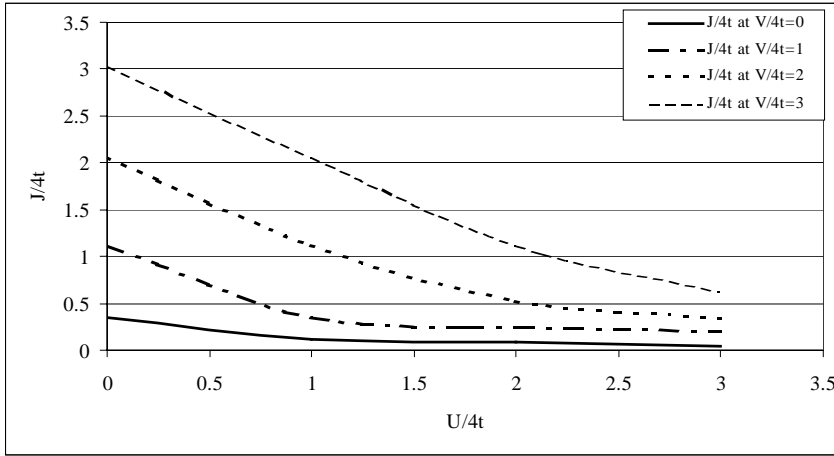


(c) $U/4t = 3$ and $V/4t = -3$

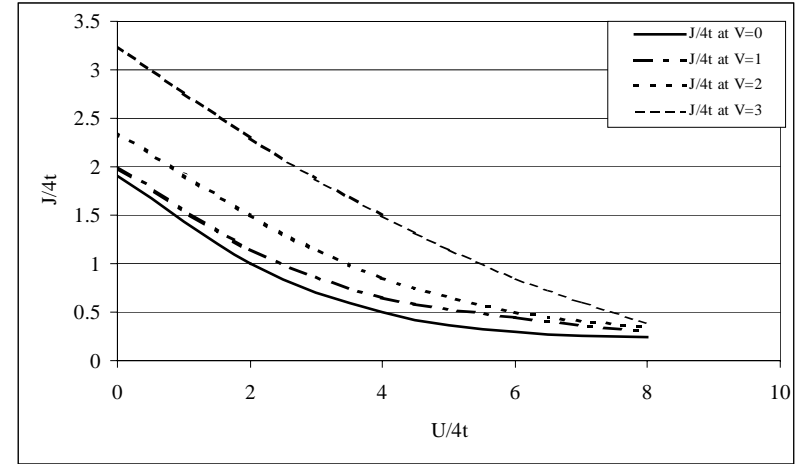


(d) $U/4t = V/4t = 3$

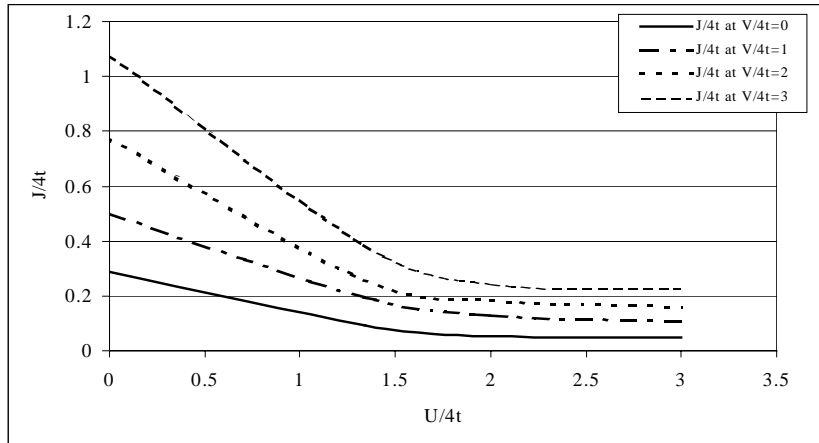
Fig. 3 below are graphs of $J/4t$ plotted against $U/4t$ at half filling (a) this work (b) Ref (5) and quarter filling (c) this work and (d) Ref(5). Observe that they compare favourably. In their ID study of the t - U - V - J model, Ref (5) observed that the exact calculation shows that V affects the parameter space for the transition away from half-filling while mean field theory shows no effect. It is obvious from Fig. 3 that the former is correct.



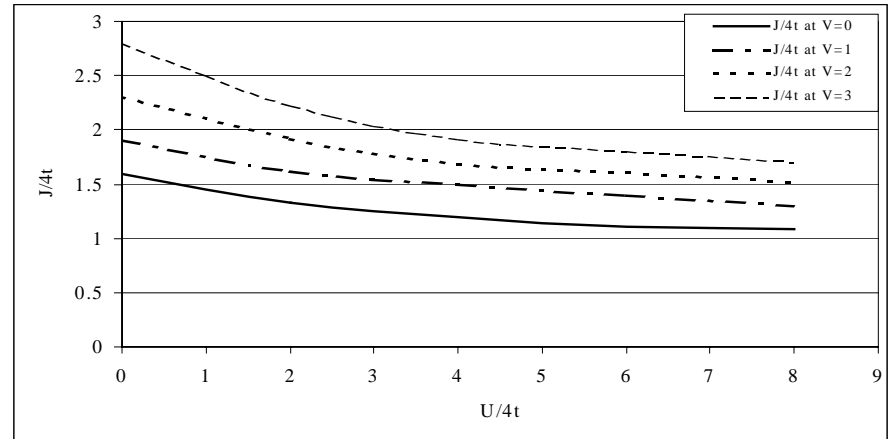
(a)



(b)



(c)



(d)

THE PARAMETER SPACE ($U/4t$, $V/4t$ AND $J/4t$) AT THE TRANSITION POINT TO FERROMAGNETISM

- It has been observed in the results that at constant values of $U/4t$, the $J/4t$ increases as $V/4t$ is increased while at constant values of $V/4t$, the $J/4t$ decreases as $U/4t$ is increased.
- The physical implication of this trend is that the NN repulsion suppresses the tendency to ferromagnetism while the on-site repulsion enhances it.
- This accounts for the very small values of $J/4t$ at increasing positive values of $U/4t$. For example, a closer study of the aforementioned tables, reveals that when $U/4t = -3$, the values of $J/4t$ required to induce the transition to the ferromagnetic phase are about twice that of the values of $V/4t$ i.e $2V < J$.

- These are very interesting and consistent results with the literature. For it has been argued in section 1.4.4 (see also Amadon and Hirsch⁵) that whenever $V < J$, the system will be unstable towards triplet superconductivity.
- Interestingly, this occurs for the negative values of U as such they confirm earlier suggestions in the literature that the negative- U Hubbard model would be useful for studying superconductivity.
- Thus the extension here is that the t - U - V - J model with negative- U would be useful for studying triplet SC.

- It was observed that for positive values of $U/4t$, J is very small. For example, when $U/4t = V/4t = 3$, $J/4t$ is always very small so that $V > J$.
- It has been stated earlier that the expected situation of the electrons in metals is that $V \geq J$.
- These results also confirm earlier suggestions in the literature that the positive- U Hubbard model would be useful for studying magnetism. Thus the extension here also, is that the t - U - V - J model with a positive- U would be useful for studying magnetism.

CONCLUSION

- The dynamics of the two interacting electrons described by the t-U-V-J model has been investigated to delineate the parameter space for the different physics accessible to the model. In particular, the parameter space for the occurrence of a transition from an anti ferromagnetic phase to a ferromagnetic phase has been obtained. Further, possible effects such as band filling, dimensionality and even-odd number of sites on the parameter space at the transition point were also investigated.
- The research findings obtained in this work which showed that the t-U-V-J model is a useful paradigm to describe the physics of ferromagnetism in materials, can be classified as follows.

- 1. The system is antiferromagnetic when $J = 0$ for any finite values of U and V and this emphasizes the domineering role of J in the crossover to ferromagnetism.
- 2. As the value of V is increased at constant value of the U , the value of J at the transition point from antiferromagnetism to ferromagnetism increases and this implies that V suppresses the tendency to ferromagnetism. This, however, does not mean negative- V can induce ferromagnetism.
- 3. As the value of U is increased at constant value of V , the value of J at the transition point from antiferromagnetism to ferromagnetism decreases and this implies that U enhances the tendency to ferromagnetism.
- 4. When U is positive and V is chosen so that $V \geq J$, the system will be stable towards ferromagnetism and when U is negative and V is chosen so that $V < J$, the system is likely to be unstable towards triplet superconductivity.
- The roles of U , V and J can be enhanced or suppressed by the number of sites and this determines effects such as band filling, dimensionality and even – odd number of sites .
- Though we have investigated these effects, we are leaving out their discussion today, because the focus today is to show that the t - U - V - J model can possibly be used to account for the physics of ferromagnetism and triplet superconductivity as well as to explain our HSCVA as a possible good mathematical tool to study the electronic correlations.

- Finally, it is pertinent to point out here that we are not naïve of the fact that in practice, we need a considerable density of state to study the strong electronic correlation systems. Further, each material have peculiar properties; for example, band degeneracy and Hund's rule exchange coupling can play a significant role¹⁵ or an insignificant role in the stability of ferromagnetism in metals.^{5,19} However, our goal here is to have an insight into the behaviour of the t-U-V-J model and this has been achieved. Thus we are now more confident to increase the density of state as well as apply the model to real materials.

THANK YOU

• REFERENCES

- 1. van Boeyan R. W. et al.(2004) Phys. Rev. Lett. 92: 2232021
- 2. Eschrig H. (2003) The particle world of condensed matter
- 3. Kehrein S. (1997) in Phys. Rev. Lett. 81: 3912
- 4. Bednorz J. G and Muller K. A. (1988) Rev. Mod. Phys. 60: 585
- 5. Amadon J. C. and Hirsch J. E. C. (1996) Phys. Rev B54: 6364
- 6. Vollhardt D. et al. (2000). Z. Phys. B 103: 283
- 7. Alexandrov A. S. and Kabanov V. V. (1996) Phys. Rev. B54: 3655.
- 8. Hirsch J. E. (1989) Phys. Rev. B40: 2354
- 9. Hirsch (1999) Phys. Rev B59: 436
- 10. Enz C. P. (1992) A course on many-body theory applied to solid-state physics. World Scientific Publishing Co., Singapore. Ch. 5: 257 - 372.
- 11. Ulmke M. (2000) Eur. Phys. J. B1: 301.
- 12. Hubbard (1963) Proc. R. Soc. London A276: 238
- 13. Bulla R. (1999) Phys. Rev. Lett. 83: 136
- 14. Chen L. and Mei C. (1989) Phys. Rev. B39: 9006
- 15. Dua and Singh (2007) J. Appl. Phys. 101: 09G5101
- 16. Aoki D. et al. (2001) Nature 413: 613; (2002) J of Phys. and Chem. of solids: 1179;
- 17. Nashioka T. (2002) Phys. Rev. Lett. 88: 2372031
- 18. Lhotel E. (2003) Phys. Rev. Lett. 91: 2097011
- 19. Barreteau et al. (2004) Phys. Rev. B 69:0644321