The two-electron Interaction in the ground state of the Hubbard-Hirsch Hamiltonian

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Abstract.

A single-band tight-binding model with on-site repulsion U and nearest-neighbour exchange interaction J (the so called Hubbard-Hirsch Hamiltonian) is studied with the help of a correlated variational approach. Two finite-sized lattices with periodic boundary conditions are considered and the criteria for the occurrence of a transition from an antiferromagnetic phase to a ferromagnetic phase are discussed.

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1.0 Introduction

Ferromagnetism is a quantum mechanical many body phenomenon caused by electronic interactions. Since the direct spin-spin interaction between electrons is very weak, ferromagnetism in itinerant electronic systems, e.g., in transition metals, must be due to a combination of the electrostatic coulomb interaction and the Pauli principle. In spite of this basic understanding, it has not been possible till date to work out exact, detailed theoretical conditions for the occurrence of ferromagnetism in itinerant electronic systems. Such conditions must be derived from a microscopic band model of itinerant electrons.

The Hubbard model, where all electronic interactions but the on site term U are neglected, was originally proposed as a simple model to describe the physics of metallic ferromagnetism [1]. Early studies provided the conclusion that the Hubbard model gives rise to ferromagnetism for large values of the on site Coulomb repulsion U within the mean-field approximation [2] (where it is equivalent to the stoner model [3]), as well as within other approximations. There are three criticisms of this conclusion:

(i) subsequent work has shown that an on-site Coulomb repulsion U by itself will not give rise to metallic ferromagnetism except in special situations or special lattice geometries [4]. Antiferromagnetism, rather than ferromagnetism, is then the normal situation with the Hubbard model.

(ii) some of the approximations used to obtain ferromagnetic phases may not be realistic models for electrons in metals.

(iii) the stability of the ferromagnetic phases obtained is uncertain [5].

Hence, it appears that in general, electrons of antiparallel spin can more easily avoid paying the price of on-site Coulomb repulsion by developing spatial correlations rather than by spin polarizing, contrary to the predictions of mean-field theory. The question then arises: What is the simplest model that contains the essential physics of metallic ferromagnetism?

The importance of the neglected nearest neighbour exchange interaction J for the stabilization of ferromagnetism has been stressed by Hirsch and co-workers [6, 7]. The restoration of this term leads us beyond the Hubbard Hamiltonian (*t-U* model) to the Hubbard-Hirsch Hamiltonian (*t-U-J* model) which is studied in this paper with the help of the variational analytic approach of Chem and Mei [8].

Any variational approach is an approximation to an exact treatment. An important advantage of the variational method, however, is that the explicit form of the variational trial wave function allows us to keep track of the physics and hence one can identify clearly which part of the wave function is relevant to any given situation. Despite this obvious advantage, our literature search so far appears to reveal that the variational method has not been used to study the Hubbard-Hirsch Hamiltonian.

In this paper, we shall focus on a system of two electrons interacting in the ground state of the Hubbard-Hirsch Hamiltonian in a finite-sized lattice containing N lattice sites. Periodic boundary conditions have been adopted throughout in order to ensure that all lattice sites are equivalent.

The organization of this paper is as follows: After introducing the Hubbard-Hirsch Hamiltonian in

Section 2, the problem of two electrons interacting under this Hamiltonian in a one-dimensional two-site lattice is solved exactly in Section 3. A variational wave function patterned after this exact solution is then employed in Section 4 to study a similar problem of two interacting electrons in a two-dimensional 3 x 3 square lattice. Results emerging from this variational calculation are presented and discussed in Section 5 while concluding remarks are given in Section 6.

2.0 Model Hamiltonian

The single-band Hubbard-Hirsch Hamiltonian may be written as [6, 7, and 9].

$$H = -t\left\{\sum_{\langle i,j\rangle,\theta} c^{+}_{i\theta}c_{j\theta} + H\cdot C\right\} + U\sum_{i}\eta_{i\uparrow}\eta_{i\downarrow} + J\sum_{\langle i,j\rangle,\theta,\theta'} c^{+}_{i\theta}c^{+}_{j\theta'}c_{i\theta'}c_{j\theta} \tag{2.1}$$

where $c^{+}_{i\theta}$, $c_{i\theta}$ and $\eta_{i\theta}$ are the creation, annihilation, and number operators respectively, for an electron of spin θ in the Wannier state on the i^{th} lattice site. The notation $\langle i,j\rangle$ means nearest neighbours, while t is the electronic hopping parameter between nearest neighbour sites i and j. *H.C.* denotes Hermitian Conjugation and its inclusion in the Hamiltonian guarantees that the expectation values of the dynamical quantities will be real.

Clearly, if J is set equal to zero in equation (2.1), we recover the $t-U$ model which is precisely the Hubbard Hamiltonian. In the following we will concentrate on the problem of two electrons interacting under the Hubbard-Hirsch Hamiltonian in finite-sized lattices.

3.0 Two electrons in a two-site lattice: Exact calculation

Let us now consider a one-dimensional lattice with only two lattice sites. Such a lattice can accommodate a maximum of four electrons. But, with only two electrons in a two-site lattice (the so called half-filling case), one can see that there is a total of six possible electronic states, which are

$$|1\uparrow,1\downarrow\rangle, |2\uparrow,2\downarrow\rangle, |1\uparrow,2\uparrow\rangle, |1\uparrow,2\downarrow\rangle, |1\downarrow,2\uparrow\rangle, |1\downarrow,2\downarrow\rangle$$

The notation $|i\theta, j\theta'\rangle$ denotes the electronic state where there is an electron at site i with spin θ and the second electron is at site j with spin θ'

With these six electronic states as basis states, the Hamiltonian matrix form of (2.1) is

$$H = \begin{pmatrix} u & 0 & -t & t & 0 & 0 \\ 0 & u & -t & t & 0 & 0 \\ -t & -t & 0 & -J & 0 & 0 \\ t & t & -J & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -J & 0 \\ 0 & 0 & 0 & 0 & 0 & -J \end{pmatrix} \tag{3.1}$$

One can easily show that the eigen energies E_s and E_t respectively, of the lowest singlet and triplet states of (3.1) are

$$E_s = \frac{(U+J)}{2} - \frac{1}{2}\sqrt{(U-J)^2+16t^2} \tag{3.2}$$

and

$$E_t = J \tag{3.3}$$

with the corresponding eigen vectors

$$|\psi\rangle_s = \frac{1}{2}\left\{\frac{\sqrt{(U-J)^2+16t^2}-(U-J)}{\sqrt{(U-J)^2+16t^2}}\right\}^{\frac{1}{2}}\left[|1\uparrow,1\downarrow\rangle + |2\uparrow,2\downarrow\rangle\right] + \frac{1}{2}\left\{\frac{\sqrt{(U-J)^2+16t^2}+(U-J)}{\sqrt{(U-J)^2+16t^2}}\right\}^{\frac{1}{2}}\left[|1\uparrow,2\downarrow\rangle - |1\downarrow,2\uparrow\rangle\right] \tag{3.4}$$

and

$$|\psi\rangle_t = |1\uparrow,2\uparrow\rangle \tag{3.5}$$

Trivial algebra shows that the triplet energy E_t is three fold degenerate, and the other two triplet states are $|1\downarrow,2\downarrow\rangle$ and $\frac{1}{\sqrt{2}}\{|1\uparrow,2\downarrow\rangle+|1\downarrow,2\uparrow\rangle\}$. In the absence of J the singlet energy E_s is always lower than the triplet energy E_t. However, if J is non-vanishing, the situation is different. Taking into account (3.2) and (3.3), the condition for "ferromagnetism", $E_t \prec E_s$ in this half-filled band system yields

$$J \succ \sqrt{\left(\frac{u}{2}\right)^2 + 2t^2} - \frac{u}{2} \tag{3.6}$$

which can be cast in the form

$$\frac{J}{4t} \succ \left\{\frac{1}{2}\sqrt{\left(\frac{u}{4t}\right)^2 + \frac{1}{2}} - \frac{u}{4t}\right\} \tag{3.7}$$

Che and Mei [8] in their variational study of the Hubbard model, constructed a correlated variational trial wave function in the form

$$|\psi\rangle = \sum_{i\neq j} X_{|i-j|}\{|i\uparrow,j\downarrow\rangle - |i\downarrow,j\uparrow\rangle\} + \sum_i X_0\{|i\uparrow,i\downarrow\rangle\} \tag{3.8}$$

patterned after the singlet state (3.4), with J = 0, and where $X_0, X_1, \cdots$, and so on are variational parameters.

We extend the work of Chen and Mei [8] in this study by constructing a correlated variational trial wave function for the Hubbard-Hirsch Hamiltonian in the form

$$|\psi\rangle = \sum_i X_0\{|i\uparrow,i\downarrow\rangle\} + \sum_{i\neq j} X_{|i-j|}\{|i\uparrow,j\downarrow\rangle - |i\downarrow,j\uparrow\rangle\} + \sum_{i\neq j} Y_{|i-j|}\{|i\uparrow,j\uparrow\rangle\} \tag{3.9}$$

patterned after the singlet and triplet states (3.4) and (3.5) respectively. Equation (3.9 will be utilized in the next section.

4.0 Two Electrons in a 3 x 3 square lattice: Variational Calculation

Figure 1 shows a sketch of the two dimensional 3 x 3 square lattice with periodic boundary conditions taken into account. Relevant information derived from the geometry of the square lattice and needed for the variational calculation are summarized in Table 1.

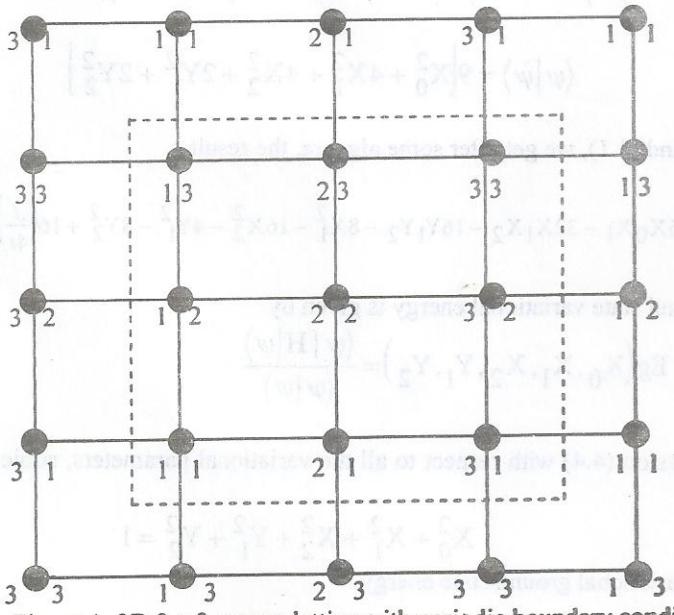

Figure 1: 2D 3 x 3 square lattice with periodic boundary conditions.

The inner dashed-lines map out the actual lattice size of the study while the numbers represent Cartesian coordinates of lattice sites.

Table 1: Relevant information derived from the geometry of the 2D 3 x 3 square lattice

Lattice separation parameter (l) between the two electrons and actual separation distance		Pair wave function $\lvert\psi_l\rangle$	Number of different pair electronic states at lattice separation parameter l	Representative pair electronic state $\lvert i\theta, j\theta'\rangle$
l	Separation distance			
0	0	$\lvert\psi_0\rangle$	9	$\lvert 11\uparrow,11\downarrow\rangle$
1	a	$\lvert\psi_1\rangle$	36	$\lvert 11\uparrow,12\downarrow\rangle$
2	$\sqrt{2}a$	$\lvert\psi_2\rangle$	36	$\lvert 11\uparrow,22\downarrow\rangle$
3	a	$\lvert\psi_3\rangle$	18	$\lvert 11\uparrow,12\uparrow\rangle$
4	$\sqrt{2}a$	$\lvert\psi_4\rangle$	18	$\lvert 11\uparrow,22\uparrow\rangle$

On the basis of the information provided in Table 1, the trial wave function given by (3.8) may be written out more fully for the 2D 3 x 3 square lattice as

$$\begin{aligned}\lvert\psi\rangle = {} & X_0\{\lvert 11\uparrow,11\downarrow\rangle+\lvert 12\uparrow,12\downarrow\rangle+\lvert 13\uparrow,13\downarrow\rangle+\cdots+\lvert 33\uparrow,33\downarrow\rangle\}+\\ & X_1\{\lvert 11\uparrow,12\downarrow\rangle-\lvert 11\downarrow,12\uparrow\rangle+\lvert 11\uparrow,21\downarrow\rangle-\lvert 11\downarrow,21\uparrow\rangle+\cdots+\lvert 32\uparrow,33\downarrow\rangle-\lvert 32\downarrow,33\uparrow\rangle\}+\\ & X_2\{\lvert 11\uparrow,22\downarrow\rangle-\lvert 11\downarrow,22\uparrow\rangle+\lvert 11\uparrow,23\downarrow\rangle-\lvert 11\downarrow,23\uparrow\rangle+\cdots+\lvert 23\uparrow,31\downarrow\rangle-\lvert 23\downarrow,31\uparrow\rangle\}+\\ & Y_1\{\lvert 11\uparrow,12\uparrow\rangle+\lvert 11\uparrow,21\uparrow\rangle+\lvert 11\uparrow,13\uparrow\rangle+\cdots+\lvert 32\uparrow,33\uparrow\rangle\}+\\ & Y_2\{\lvert 11\uparrow,22\uparrow\rangle+\lvert 11\uparrow,23\uparrow\rangle+\lvert 11\uparrow,33\uparrow\rangle+\cdots+\lvert 23\uparrow,31\uparrow\rangle\}\end{aligned}$$

and hence

$$\langle\psi\lvert\psi\rangle = 9\left[X_0^2+4X_1^2+4X_2^2+2Y_1^2+2Y_2^2\right] \tag{4.2}$$

Taking into account (2.1) and (4.1), we get after some algebra, the result

$$\langle\psi\lvert H\rvert\psi\rangle = 9t\left\{4\left(\frac{u}{4t}\right)X_0^2-16X_0X_1-32X_1X_2-16Y_1Y_2-8X_1^2-16X_2^2-4Y_1^2-8Y_2^2+16\left(\frac{J}{4t}\right)X_1^2-8\left(\frac{J}{4t}\right)Y_1^2\right\} \tag{4.3}$$

As is well known, the ground state variational energy is given by

$$Eg\left(X_0,X_1,X_2,Y_1,Y_2\right)=\frac{\langle\psi\lvert H\rvert\psi\rangle}{\langle\psi\lvert\psi\rangle} \tag{4.4}$$

Minimization of the expression (4.4) with respect to all the variational parameters, subject to the normalization constraint

$$X_0^2+X_1^2+X_2^2+Y_1^2+Y_2^2=1 \tag{4.5}$$

leads immediately to the variational ground state energy.

5.0 Numerical Results and Discussion

As a check on our method, we show in Tables 2 and 3 results obtained from the application of the variational method to the problem of two electrons interacting under the Hubbard-Hirsch Hamiltonian in a two-site lattice. This problem, which can be solved exactly, was discussed in Section 3. From equation (3.7), the transition from a ferromagnetic phase to an antiferromagnetic phase occurs at

$$\frac{J}{4t} = 2\cdot 06 \text{ and } 0\cdot 06 \text{ if } \frac{U}{4t} = -2 \text{ and } = 2,$$

Table 2: Total Energy and Variational parameters for the ID (N = 2) lattice when $\frac{U}{4t} = -2$

Exchange interaction parameter $\frac{J}{4t}$	On-site interaction parameter $\frac{U}{4t}$	Total Energy $E = \frac{Eg}{t}$	Variational parameters		
			X_0	X_1	Y_1
2.10	-2	-8.4000	0	0	1
2.09	-2	-8.3600	0	0	1
2.08	-2	-8.3200	0	0	1
2.07	-2	-8.2800	0	0	1
2.06	-2	-8.2427	0.0027	0.1205	0
2.05	-2	-8.2433	0.9927	0.1207	0
2.04	-2	-8l2438	0.9926	0.1210	0
2.03	-2	-8.2444	0.9926	0.1213	0

Table 3: Total Energy and Variational parameters for the ID (N = 2) lattice when $\frac{U}{4t} = 2$

Exchange interaction parameter $\frac{J}{4t}$	On-site interaction parameter $\frac{U}{4t}$	Total Energy $E = \frac{Eg}{t}$	Variational parameters		
			X_0	X_1	Y_1
0.5	2	-2.0000	0	0	1
0.1	2	-4.4000	0	0	1
0.08	2	-0.3200	0	0	1
0.07	2	-0.2800	0	0	1
0.06	2	-0.2451	0.2357	0.9718	0
0.05	2	-0.2829	0.2347	0.9721	0
0.02	2	-0.3964	0.2317	0.9728	0
0.01	2	-0.4343	0.2307	0.9730	0

Table 4: Total Energy and Variational parameters for the 2D 3 x 3 square lattice when $\frac{U}{4t} = -2$

Exchange interaction parameter $\frac{J}{4t}$	On-site interaction parameter $\frac{U}{4t}$	Total Energy $E = \frac{Eg}{t}$	Variational parameters				
			X_0	X_1	X_2	Y_1	Y_2
1.24	-2	-9.7450	0	0	0	0.8207	0.5714
1.23	-2	-9.7181	0	0	0	0.8194	0.5732
1.22	-2	-9.6913	0	0	0	0.8181	0.5750
1.21	-2	-9.6646	0	0	0	0.8169	0.5768
1.20	-2	-9.6607	0.9692	0.2012	0.1422	0	0
1.19	-2	-9.6662	0.9690	0.2018	0.1425	0	0
1.18	-2	-916718	0.9688	0.2025	0.1428	0	0
1.17	-2	-9.6773	0.9686	0,2031	0.1431	0	0

Table 5: Total Energy and Variational parameters for the 2D 3 x 3 square lattice when $\frac{U}{4t} = 2$

Exchange interaction parameter $\frac{J}{4t}$	On-site interaction parameter $\frac{U}{4t}$	Total Energy $E = \frac{Eg}{t}$	Variational parameters				
			X_0	X_1	X_2	Y_1	Y_2
0.17	2	-7.3941	0	0	0	0.6470	0.7625
0.16	2	-7.3774	0	0	0	0.6451	0.7641
0.15	2	-7.3608	0	0	0	0.6433	0.7656
0.14	2	-7.3443	0	0	0	0.6414	0.7672
0.13	2	-7.3294	0.3167	0.6068	0.7290	0	0
0.12	2	-7.3454	0.3172	0.6084	0.7275	0	0
0.11	2	-7.3614	0.3177	0.6100	0.7259	0	0
0.10	2	-7.3776	0.3182	0.6116	0.7243	0	0

respectively. This is clearly confirmed by Tables 2 and 3. While the physics of antiferromagnetism resides in the variational parameters, X_0, X_1 and X_2, that of ferromagnetism resides in Y_1 and Y_2. Tables 2 and 3 then show very clearly the phase transition from ferromagnetism to antiferromagnetism as the parameter $\frac{J}{4t}$ is varied. This attests to the power of the variational method, as earlier stated.

In Tables 4 and 5, we display the results obtained from the application of the variational method to the problem of two electrons interacting under the Hubbard-Hirsch Hamiltonian in a two-dimensional 3 x 3 square lattice. From these two tables, the transition from a ferromagnetic phase to an antiferromagnetic phase occurs at $\frac{J}{4t} = 1 \cdot 205$ and $0 \cdot 135$ if $\frac{U}{4t} = -2$ and $+2$, respectively. Thus, as U increases, the value of J at which the transition occurs decreases. Also, at constant on-site interaction strength U, the total energy of the two interacting electrons was always found to decrease as J increases. These trends are in agreement with the work of Amadon and Hirsch [7].

6.0 Conclusion

We have studied in this paper the effect of two interaction parameters U and J on the tendency to ferromagnetism in a single-band Hubbard-Hirsch model. The purpose of this study was to demonstrate the power of the variational method. Attention was focused on the parameter region where the transition to ferromagnetism occurs as we move away from half-filling. On the whole it was found that as U increases positively, the value of J at which the transition occurs, decreases. This study can also be seen as an extension to two dimensions of the work of Amadon and Hirsch [7] which was limited to one dimension.

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