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A VARIATIONAL APPROACH TO THE STUDY OF STRONGLY CORRELATED ELECTRON SYSTEMS

EDISON A. ENAIBE
Department of Physics, University of Benin, Benin City, Nigeria.

and

JOHN O. A. IDIODI
Department of Physics, University of Benin, Benin City, Nigeria.
e-mail: idijohn@Uniben.edu

ABSTRACT

An investigation of the dynamic behavior of two electrons interacting under an extended Hubbard – type potential ($t - t' - U$ model) is presented, employing a variational analytic approach. The role of the next – nearest neighbour hopping parameter t' is discussed, and the results obtained from the extended Hubbard model are compared with those emerging from the usual t – u Hubbard model which contains only a nearest neighbor hopping parameter.

1. INTRODUCTION

After several years of intense experimental and theoretical studies of the copper – oxide superconductors, there is now a consensus that these materials should be described as strongly correlated electron systems [1].

The undoped parent compound such as La_2CuO_4 is understood to be a Mott-Hubbard insulator [1], with spin – ½ local moment on the copper sites which are antifeomagnetically ordered below about 200k. Upon doping with holes in the copper – oxygen plane, the long – range antiferromagnetic order is replaced by short – range order and superconductivity emerges as the ground state.

However, while there is still no quantitative microscopic theory of how superconductivity arises from doping the antiferromagnetic and insulating parent compounds, it is clear that the superconductivity state can be described in terms of a generalized pairing picture [2].

Thermodynamic considerations suggest the presence of a gap in the energy spectrum of the electrons at the fermi surface. Thus by forming the Cooper pair [3] the electrons can lower the ground state energy of the system below the original fermi energy. In the process the fermi distribution will become distorted so that the whole problem must be treated self consistently in order to arrive at the new ground state.

As a starting theoretical "parent" model, the Hubbard model has received increasing attention for its relevance for high T_c superconductivity, quantum antiferromagnetism, and ferromagnetism, thus playing a central role in the theoretical investigation of strongly correlated electron systems [4]. Several

theoretical methods have been applied to the Hubbard model in order to elucidate the parameter space of the different physics accessible to the Hubbard model. These methods [4] include amongst others Quantum Monte – Carlo methods, Lanczos algorithm, Hartree – Fock approximation, slave fermion or slave boson techniques, perturbation and variational methods.

The variational method can be used for the approximate determination of the lowest ground state energy level of a system. Any variational approach is an approximation to an exact treatment. In view of the fact that the many – body problem in condensed matter physics is quite complicated it is not unusual in the study of highly correlated electron systems to encounter approximation methods.

The variational method consist in evaluating the integral

$$E = \frac{\int \Psi\, H\, \Psi\, d\tau}{\int \Psi\, \Psi\, d\tau} = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle} \qquad (1.1)$$

using a guessed trial wave function Ψ. We thus have an explicit expression for the energy, which can be thought of as the variational ground state energy of the system.

The variational theorem then asserts that of all possible conceivable wave functions, the correct ground state wave function is the one that minimizes the ground state energy. In practice the trial wave function selected, often contains one or more variational parameters which must be chosen to minimize the energy.

An important advantage of the variational method is that the explicit form of the wave function allows us to keep track of the physics and hence identify clearly which part of the wave function is relevant to any given situation.

In this paper, we focus on a system of two electrons interacting in the ground state of the Hubbard model in a two dimensional (2D) 4X4 square lattice. The system has sixteen sites (N=16) available for the electronic motion, and as usual, an infinite – sized lattice where each lattice site has the same environment can be realized from the finite – sized lattice with the help of periodic boundary conditions. A correlated ground state wave function for performing variational calculations on such a system has been reported by Chen and Mei [5]. It must be emphasized here that since the wave function of Chen and Mei is patterned after the exact wave function for a system containing only two lattice sites (N=2), it is not obvious that this wave function is the most suitable variational wave function if N is chosen greater than 2. One of the aims of this paper is to investigate this point. We would like to verify whether the results obtained with the trail wave function of Chen and Mei [5] are in accord with reality or not.

The work of Chen and Mei [5] was limited to the standard t-U Hubbard model, which contains only a nearest neighbor (NN) electronic hopping parameter t and an on – site electronic interaction strength U. The second important aim of this paper is to apply the variational analytic approach of Chen and Mei [5] to the extended Hubbard hamiltonian (the t – t'- U model). The idea is to investigate the role of the next nearest neighbor (NNN) electronic hopping parameter t' on the total ground state energy and the pair correlated function (PCF) of the two electrons.

The organization of this paper is as follows: section 2 contains the theoretical formulation, section 3 contains the results and discussion, and finally, section 4 present concluding remarks.

2. THEORY

The simplest form of the single – band Hubbard model [5] is given by

$$E = -t \sum_{<ij>\sigma} \left(C^{\dagger}_{i\sigma} C_{j\sigma} + \text{H.C} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \qquad (2.1)$$

where $C^{\dagger}_{i\sigma}$ ($C_{j\sigma}$) and $n_{i\sigma}$ are the creation (annihilation) and number operators, respectively, for an electron of spin σ in the Wannier state on the *i th* lattice site, and $< ij >$ means that only NN site hoppings are allowed in the summation. H.C. denotes Hermitian conjugation and its inclusion in the Hamiltonian guarantees that the expectation values of the dynamical quantities will be real, t is the NN hopping parameter, and each pair (ij) is included only once, and finally U is the on-site or intra-site coulomb interaction parameter.

The hopping of electrons in the single – band Hubbard t – U model of (2.1) is restricted only to nearest – neighbor sites. Since this may be inadequate to provide all the relevant physics of the normal state properties of strongly correlated electron systems, we have extended the t- U Hamiltonian model in this study by including a NNN hopping parameter t'.

Upon the inclusion of the t' the resulting Hamiltonian model [6] is now of the form

$$H = -t \sum_{<ij>\sigma} \left(C^{\dagger}_{i\sigma} C_{j\sigma} + \text{H.C.} \right) - t' \sum_{<<ij>>\sigma} \left(C^{\dagger}_{i\sigma} C_{j\sigma} + \text{H.C.} \right)$$

$$+ U \sum_{i} C^{\dagger}_{i\uparrow} C_{i\uparrow} C^{\dagger}_{i\downarrow} C_{i\downarrow} \qquad (2.2)$$

where $<< ij >>$ means that summation is over NNN.

Chen and Mei [5] have proposed a correlation ground state wave function in the form

$$|\Psi\rangle = \sum_{i} X(i,i) |i\uparrow, i\downarrow\rangle + \sum_{i \neq j} X(i,j) \left\{ |i\uparrow, j\downarrow\rangle - |i\downarrow, j\uparrow\rangle \right\} \qquad (2.3)$$

to be employed for variational studies. Here $|i\uparrow, j\downarrow\rangle$ means that one electron is on lattice i with spin up ($\uparrow$) and the second electron is on lattice site j with spin down ($\downarrow$). The $x_{(ij)}$ are variational parameters.

It is clear that the only correlation covered by (2.3) is the one which requires the two electrons to have antiparallel spins. The physical situation where the two interacting electrons have the same spin is therefore clearly outside the reach of our correlated trial wave function.

Owing to the geometry of the 2D square lattice, it is obvious that the variational parameters $X(i,j)$ should be functions of $|i-j|$ only. In view of this, henceforth we shall adopt the simpler labeling notation

$$X(i,j) \equiv X_{|i-j|} \tag{2.4}$$

For the 4x4 square lattice, six variational parameters arise. These are x_0, x_1, x_2, x_3, x_4 *and* x_5. Substituting (2.2) and (2.3) into (1.1), we get, after some algebra, the analytic expressions

$$\langle \Psi | \Psi \rangle = 16\left(X_0^2 + 4X_1^2 + 4X_2^2 + 2X_3^2 + 4X_4^2 + X_5^2\right) \tag{2.5}$$

$$\langle \Psi | H | \Psi \rangle = 64\left(X_0^2 + 4X_1^2 + 4X_2^2 + 8X_1X_2 + 8X_2X_3 + 4X_3^2 + 8X_1X_4 + 4X_4^2 + 4X_2X_5 + 4X_5^2\right) \tag{2.6}$$

Taking into account (2.5) and (2.6), the variational ground state energy E_g is

$$E_g \langle \Psi | \Psi \rangle = \langle \Psi | H | \Psi \rangle \tag{2.7}$$

By minimizing the expression (2.7) with respect to all the Xi's the ground state energy can be obtained. It is often preferable to convert the problem to an eigenvalue problem. This leads straight forwardly to the matrix equation

$$\begin{pmatrix} E-4(U/4t) & 8 & 8(t'/t) & 0 & 0 & 0 \\ 2 & E+4(t'/t) & 0 & 4(t'/t) & 0 & 0 \\ 2(t'/t) & 4 & E & 4(t'/t) & 4 & 2(t'/t) \\ 0 & 4 & 8(t'/t) & E & 4 & 0 \\ 0 & 0 & 4 & 2 & E+4(t'/t) & 2 \\ 0 & 0 & 8(t'/t) & 8 & 8 & E \end{pmatrix} \begin{pmatrix} X_0 \\ X_1 \\ X_2 \\ X_3 \\ X_4 \\ X_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (2.8)$$

where $E \equiv E_g/t$ is the variational total ground state energy of two electrons interacting under a $t - t' - U$ extended Hubbard model on 4X4 square lattice. Eq. (2.8) has been solved in this study for various sensible values of the parameter $U/4t$ and t'/t.

To have more insight into the dynamics of the two interacting electrons, one usually calculates the pair correlation function (PCF). The PCF can be defined as the probability $P(i,j)$ of finding an electron at site j when there is an electron of opposite spin at site i. It has the representation

$$P_{|i-j|} \equiv P(i,j) = \frac{\left\langle \Psi \middle| C_{i\sigma}^{+} C_{i\sigma} C_{j,-\sigma}^{+} C_{j,-\sigma} \middle| \Psi \right\rangle}{\langle \Psi | \Psi \rangle} \quad (2.9)$$

In a model that goes only up to NNN, the relevant PCFs are P_0, P_1 and P_2, where P_0 is the on – site PCF, P_1 is the NN PCF, and P_2 is the NNN PCF. These have been calculated in this work for various values of U/4t and t'/t.

3. RESULTS AND DISCUSSION

Table 1 shows the calculated values of the variational parameters X_0, X_1, X_2, X_3, X_4, and X_5 for various values of the interaction strength U/4t and t/t (the ratio of the lectronic hopping parameters). In a variational calculation, these variational parameters are the crucial ingredients. They show, comparatively, the weights of the different terms in the trial variational wave function. Table 1 shows clearly two different parameter regimes where the physics of the two interacting electrons is likely to be different.

First as U/4t approaches the value 10 and t'/t takes on a sufficiently positive value, then the variational parameter X_0 becomes significantly smaller than the other variational parameters, showing that the two electrons prefer to remain as far apart as possible. Keeping U/4t at the value 10 and decreasing t'/t from the value 0.25 leads to an enhancement in the magnitude of X_0, X_1, and X_2 and a reduction in the magnitude of X_3, X_4, and X_5.

Second, as U/4t approaches the value – 2, we note that the magnitude of X_0 becomes greater than the magnitude of the other variational parameters, showing that the two electrons prefer to come together on the same site. The role

of t'/t in this parameter regime is similar to the first parameter regime. The values of the total energy and PCFs are exhibited in table 2 for various values of the parameters U/4t and t'/t. Clearly, the trend in the PCFs follows that of the variational parameters, as already noted in the discussion of table 1. The trend for the ground state energy in table 2 shows that a lower ground state energy is achieved as t'/t increases.

Fig. 1 shows the PCFs in the two parameter regimes, characterized by U/4t = 0.25. The two curves in fig. 1 are, essentially, a graphical display of the two conclusions we have already deduced from table 1: As u/4t approaches – 2, the electrons prefer to be at the same site, but as U/4t approaches 0.25 the electrons prefer to stay as further apart as possible. The effect of t' on the two curves in fig. 1 is shown in fig. 2 for U/4t = 0.25, and fig. 3 for U/4t = - 2. The trend is the same for both fig. 2 and fig. 3. As t'/t increases, the PCF is lowered.

Table 1. Calculated values of the variational parameters for various values of the interaction strength U/4t and the parameter t'/t.

Interaction Strength U/4t	t'/t	Variational Parameters					
		X_0	X_1	X_2	X_3	X_4	X_5
10.00	0.25	0.0269	0.2717	0.4279	0.4423	0.5000	0.5447
	0	-0.0608	-0.3620	-0.4400	-0.4400	-0.4772	-0.5004
	-0.25	-0.1027	-0.4741	-0.4754	-0.4327	-0.4323	-0.4056
1.00	0.25	-0.1122	-0.2905	-0.4304	-0.4413	-0.4918	-0.5303
	0	-0.2681	-0.3968	-0.4290	-0.4290	-0.4440	-0.4531
	-0.25	-0.4638	-0.5005	-0.4055	-0.4014	-0.3426	-0.3024
0.25	0.25	0.1510	0.2982	0.4303	0.4396	0.4868	0.5225
	0	0.3629	0.4057	0.4163	0.4163	0.4211	0.4240
	-0.25	-0.6094	-0.4841	-0.3507	-0.3642	-0.2837	-0.2410
-1.00	0.25	-0.3274	-0.3251	-0.4200	-0.4217	-0.4537	-0.4765
	0	-0.6943	0.3901	-0.3208	-0.3208	-0.2911	-0.2742
	-0.25	0.9024	0.3416	0.1418	0.1951	0.0874	0.0566
-2.00	0.25	-0.7649	-0.3168	-0.3001	-0.2814	-0.2739	-0.2651
	0	0.9354	0.2647	0.1410	0.1410	0.0972	0.0758
	-0.25	0.9743	0.2078	0.0297	0.0818	0.0068	-0.0005

Table 2. Values of the total energy and PCFs as functions of the interaction strength U/4t and the parameter t'/t.

Interaction Strength U/4t	t'/t	Total Energy Eg/t	PCFs		
			P_o	P_1	P_2
10.00	0.25	-8.9145	0.0000167	0.0068	0.0169
	0	-7.6292	0.0000810	0.0115	0.0170
	-0.25	-6.1813	0.000213	0.0181	0.0183
1.00	0.25	-9.0425	0.000288	0.0077	0.0170
	0	-7.8389	0.00161	0.0141	0.0164
	-0.25	-6.3820	0.0048	0.0227	0.0149
0.25	0.25	-9.1009	0.000523	0.0082	0.0170
	0	-7.9450	0.00303	0.0151	0.0159
	-0.25	-6.5060	0.00949	0.0240	0.0126
-1.00	0.25	-9.3792	0.00254	0.0100	0.0167
	0	-8.4943	0.0142	0.0179	0.0121
	-0.25	-7.3424	0.0346	0.0198	0.0034
-2.00	0.25	-10.5290	0.0195	0.0134	0.0120
	0	-10.2640	0.0415	0.0133	0.0038
	-0.25	-9.7675	0.0521	0.0095	0.0002

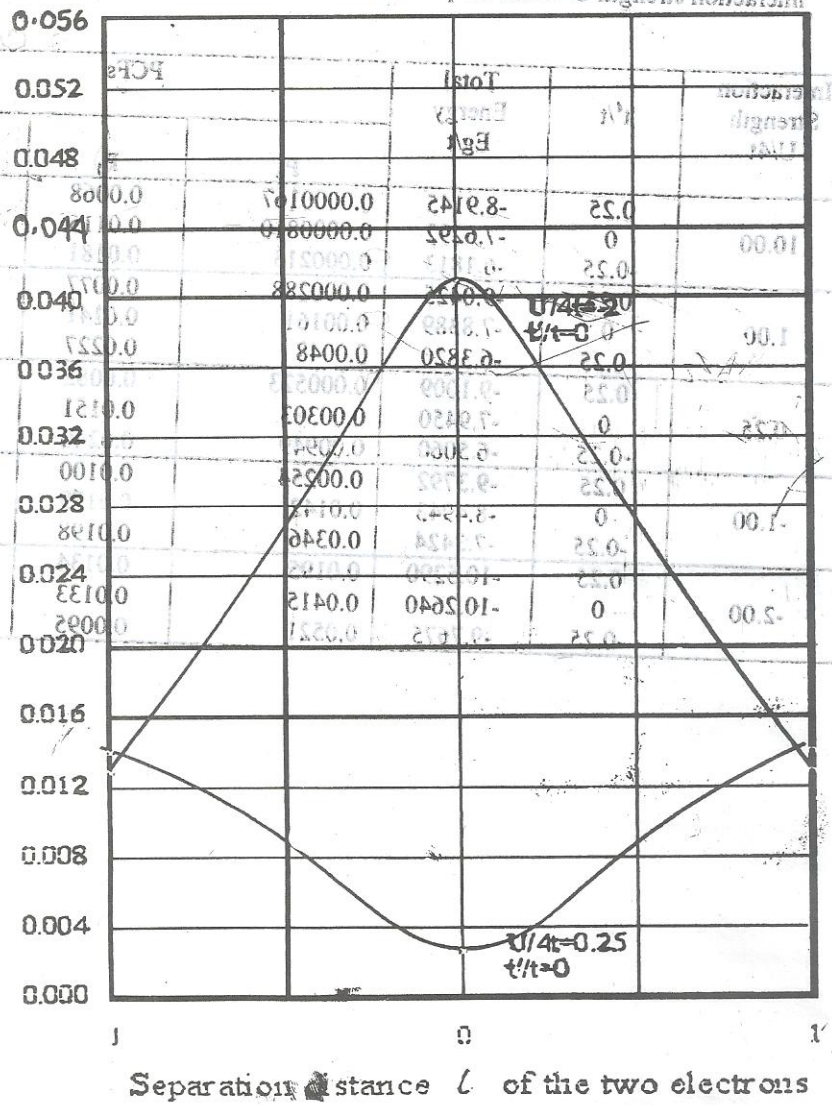
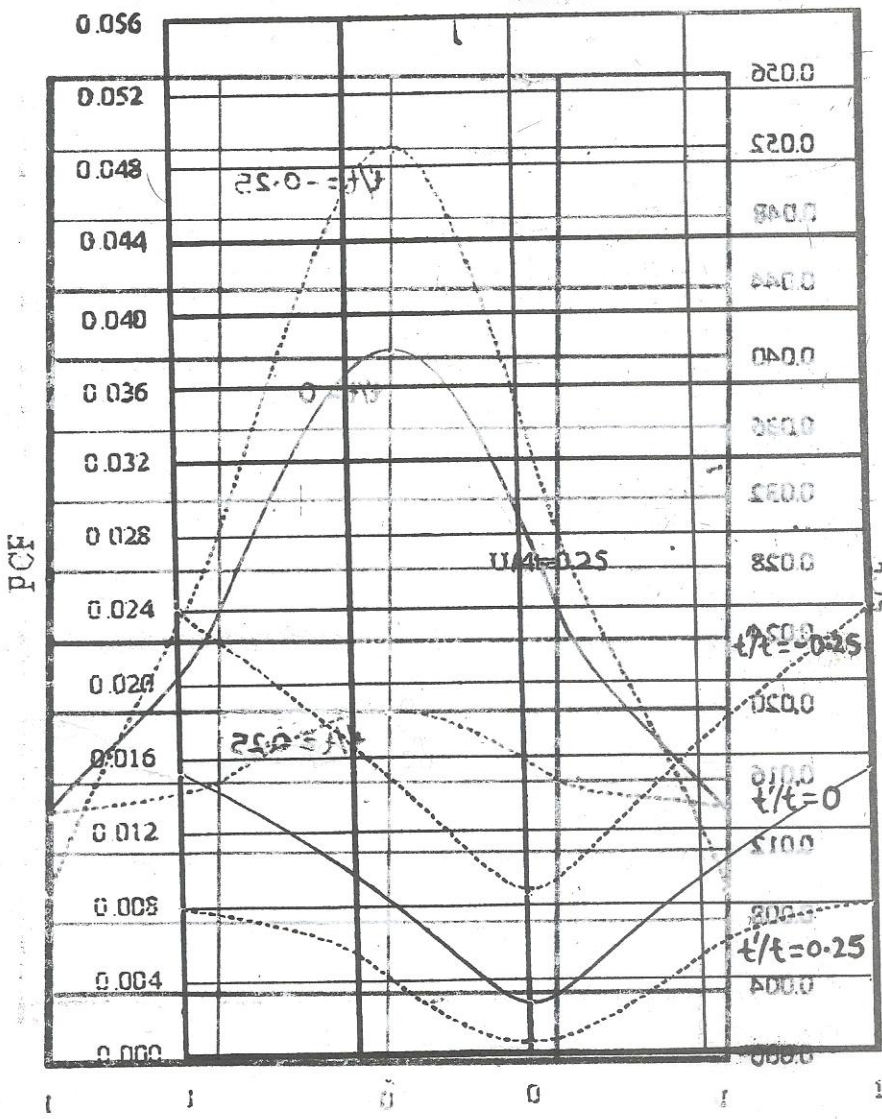


Fig.1 the PCFs for The 2D 4 X 4 square lattice versus the separation distance l of the two electrons. Here an electron is assumed fixed at the lattice position with coordinates (2,2) in the 2D 4X4 square lattice. A separation distance of L = 0 then means that both electrons are at same site (2,2). A separation, of L =1 means that the second electron is at the position (1,2) or (2,3) or (3,2) or (2,1).



Separation distance l of the two electrons

Fig. 2. The PCFs for the 2D 4X4 square lattice versus the separation distance l of the two electrons when U/4t = 0.25

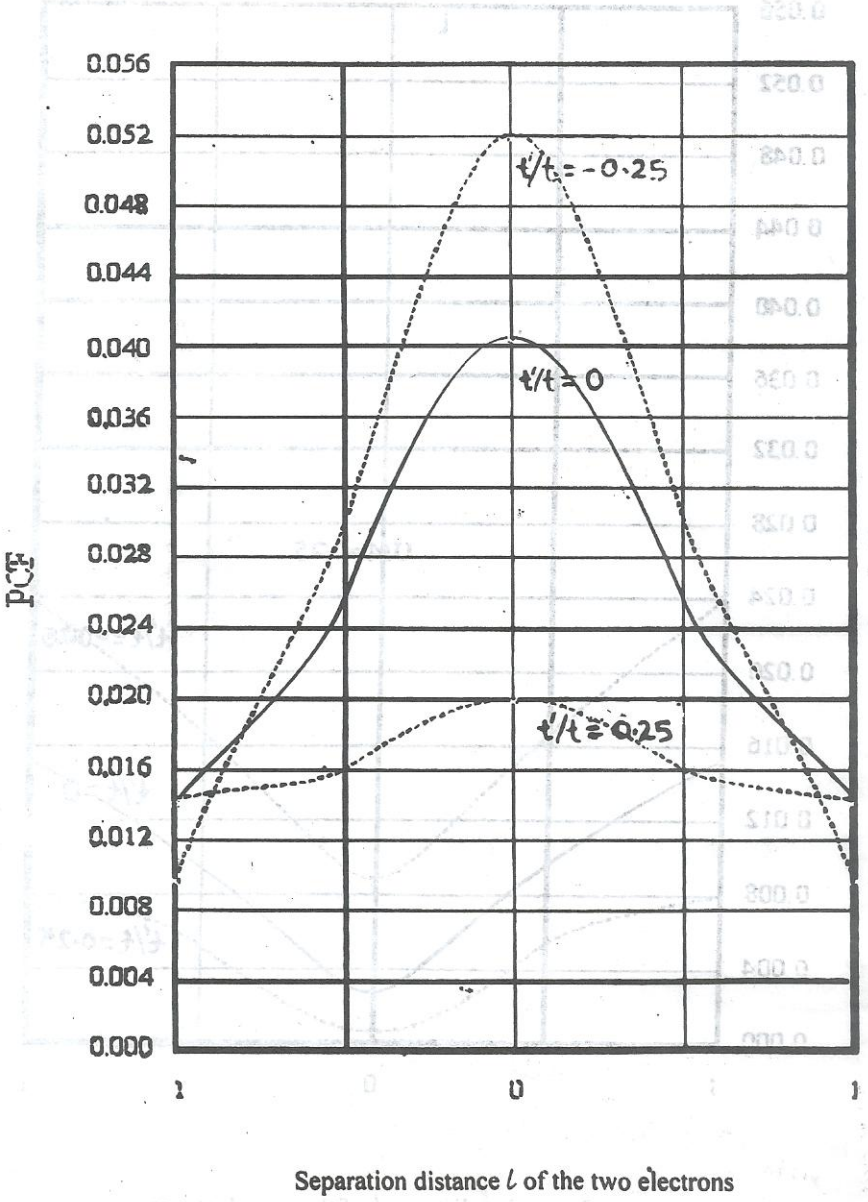


Fig. 3. The PCFs for the 2D 4X4 square lattice versus the separation distance l of the two electrons when U/4t =-2

4. CONCLUSION

In conclusion, we have demonstrated that the $t - t' - U$ model leads to a much richer behavior than the standard $t - U$ model. Depending on the sign of the next – nearest neighbor hopping parameter t', the correlation of the two electrons may be damped or enhanced. Our calculations suggest that the possibility of pair formation is enhanced in the parameter regime where U/4t is sufficiently negative.

The $t - t' - U$ model in this parameter regime may thus be suitable for superconductivity studies. On the other hand when U/4t is sufficiently positive the two electrons prefer to stay as far apart as possible. The $t - t' - U$ model in this parameter regime may thus be suitable for magnetic studies.

It was found in the course of this study that sensible results were obtained when the parameter t'/t lies in the range $-0.5 < t'/t < +0.5$. This result is in accord with the work of Lin and Hirsch [7].

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