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Corresponding author
Raymond C. Abenga
raymondabenga@ymail.com

Pair Correlation Function for Two Interacting Electrons in a Square Lattice System

Raymond Chiviter Abenga[1] and Sunda Onyefie Agada[2]

[1&2]Department of Pure and Applied Physics, Veritas University, Abuja, Nigeria

ABSTRACT

The study of electron-electron interaction has stimulated significant interest in mean field theory calculations and physical properties of condensed matter physics. In this study, we have computed the pair correlation functions in the two dimensional Hubbard model using the correlated variational approach in a finite sized lattice system. The result of the computed pair correlation functions for both on-site and off-site interaction for two interacting electrons is presented. The result shows that, as the interaction strength $(\frac{U}{4t})$ decreases the pair correlation function values for on-site interaction increases. This indicates that, the two electrons will prefer to stay at the same site and align themselves together due to the less forces of repulsion while for the off-site interaction, as the interaction strength $\frac{U}{4t}$ decreases, the pair correlation function $\mathrm{P}_1, \mathrm{P}_2, \mathrm{P}_3, \mathrm{P}_4$ and P_5 also decrease indicating that, the two electrons will prefer to stay at different site due to the large repulsive force.

Keywords Hubbard model, Pair correlation function, Unit step Hamiltonian

INTRODUCTION

The Hubbard model has received increasing attention for its relevance for high-T_c superconductivity, anti-ferromagnetism and ferromagnetism, thus playing a central role in the theoretical investigation of strongly correlated systems [1]. The Hubbard model offers one of the simplest ways to get insight on how the interactions between electrons can give

rise to insulating, magnetic and even Nobel superconducting effects in solids. This model has been applied to the understanding of many systems from heavy fermions systems to high temperature superconductivity [2]. Indeed it is an amazing feature of the model that, despite its simplicity it exhibits behaviours relevant to many of the most subtle and beautiful properties of solid state systems.

The Hubbard model has been studied by the full range of analytic techniques developed by condensed matter theorists, from simple mean field approaches to field theoretic methods employing Feynman diagrams, expansions in the degeneracy of the number of flavours (spin, orbital angular momentum) etc. It has also been extensively studied with numerical methods like diagonalization method, Quantum Monte Carlo method and the variational Monte Carlo method [3] and [4]. In either of the above theories electron interaction plays an important role. An electron located at a given lattice site would always feel the presence of another electron which is located at a different lattice site. This interaction is due to the presence of spin and charge between them. So long as this relationship exists the electrons are said to be correlated [5]. In a lattice system, the interacting electrons are located at lattice sites. In a system of two interacting electrons with one at site i and the other at site j, if an electron is located at site i how do we know the position of the second electron. This paper provides a good justification for this work in which the sole aim is to determine the probability of finding an electron at site j when an electron is at site i.

This paper is organized as follow, in Section 2 we give a brief summary of the Hubbard model and the method used for the calculations. In Section 3 we present a brief description of pair correlation function for a non-symmetric argument and in Section 4 we discuss the results. The final Section is devoted to the conclusion of the paper.

THEORETICAL BACKGROUND

The Hubbard Model for Two Dimensional Systems

The Hubbard model was originally proposed as a simple model to describe the physics of metallic ferromagnetism. Apart from the fact that it exhibits anti-ferromagnetism, it also gives rise to ferromagnetism for large values of the on-site Coulomb repulsion within mean field theory as well as within other approximations [6]. However, subsequent work has shown that an on-site Coulomb repulsion by itself will not give rise to metallic

ferromagnetism except in special situations, such as a single hole in a half-filled band or special lattice geometries [7]. It appears in general, that electrons of anti-parallel spin can more easily avoid paying the price of on-site Coulomb repulsion by developing spatial correlations rather than by spin polarization, contrary to the predictions of mean field theory [8] and [9].

The reduction of the full many-body Hamiltonian to a simple effective model is in itself a complicated problem and in general the resulting models cannot be solved exactly. A variety of approximate and numerically exact methods have been developed, but there are a number of shortcomings to each of these approaches. In its simplest form, the single-band Hubbard model reads [10] and [11].

$$\mathrm{H} = -t\sum_{\langle i,j\rangle\sigma}(C_{i\sigma}^{+}C_{j\sigma} + H.C) + U\sum_{i} n_{i\sigma}n_{i\sigma}, \qquad (1)$$

where $C_{i\sigma}^{+}C_{j\sigma}$ and $n_{i\sigma}$ are the creation (annihilation) and number operators respectively, for an electron of spin σ in the Wannier state on the ith lattice site, $\langle i,j\rangle$ means that only nearest-neighbor site hopping is allowed, $H.C$ is the Hermitian conjugate and its presence ensures that the dynamical quantities are real, t and U are respectively the hopping and on-site interaction weighting factor. The term U in the Hamiltonian accounts for the dominant part of the Coulomb repulsion.

To solve the problem of a variational calculation, we employ a two-site Hubbard model. In this case the Hamiltonian *H* in the form of the Hubbard model is written explicitly by [12] as

$$H = -t\left(C_{0\uparrow}^{\dagger}C_{1\uparrow} + C_{1\uparrow}^{\dagger}C_{0\uparrow} + C_{0\downarrow}^{\dagger}C_{1\downarrow} + C_{1\downarrow}^{\dagger}C_{0\downarrow}\right) + U(n_{0\uparrow}n_{0\downarrow} + n_{1\uparrow}n_{1\downarrow}) \qquad (2)$$

The Hubbard Hamiltonian becomes very cumbersome to handle when the size of the Hilbert space of a given dimensional lattice increases [13], hence the need for the application of approximation technique.

Electronic States of the Interacting Electrons

The problem of pair correlation function for two interacting electrons under the Hubbard model can at best be studied by first determining the electronic states of the interacting electrons in a finite-sized lattice system. In [14] the wave function of the two interacting electrons was defined as

$$|\Psi\rangle = \sum_{i=1,j=1}^{N} R_{ij}|\ i\sigma, j\sigma^{1}\rangle \qquad (3)$$

where $|\ i\sigma, j\sigma^{1}\rangle$ is the electronic state when there is an electron at site i with spin σ and the second electron at site j with spin σ ^{1}and R_{ij} are the expansion coefficients.

To write out equation (3) correctly to determine the electronic states in a wave function, the lattice system is drawn in full with appropriate periodic boundary conditions as shown in Figure 1.

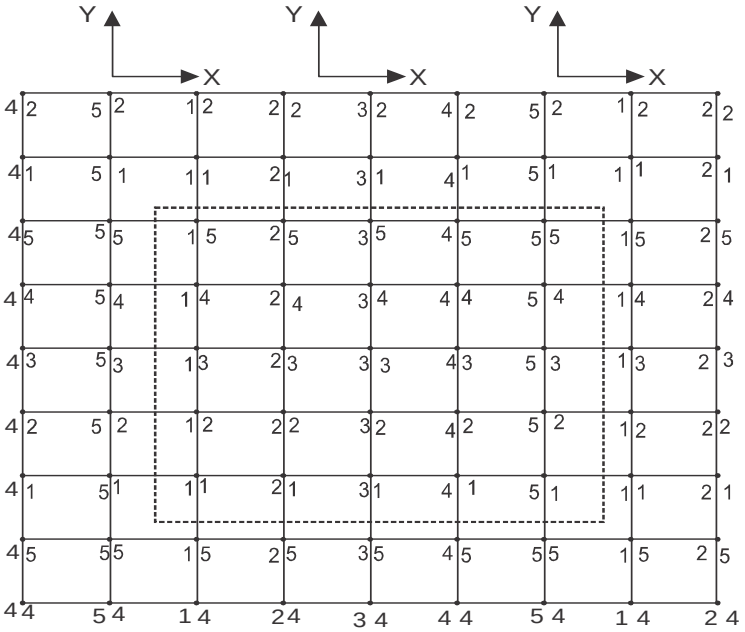

Figure 1: Two dimensional 5 x 5 lattice with periodic boundary conditions.

The trial wave function for the correlated variational approach is given in the form [13].

$$|\Psi\rangle = \sum_{i=j} x_{ij} |i\uparrow i\downarrow\rangle + \sum_{i\neq j} x_{Li-jL}(|i\uparrow j\downarrow\rangle - |i\downarrow j\uparrow\rangle) \qquad (4)$$

With a careful application of equations (3) and (4) we can conveniently determine the electronic states and hence the ground-state energy of the two interacting electrons in finite-size lattice provided the two basic conditions stated below are duly followed.

i. The field strength tensor

$$\langle i|i\rangle = \delta_{ij} \begin{cases} 1 & \text{if and only if } \ i = j \\ 0 & \text{if and only if } \ i \neq j \end{cases}$$

ii. The Marshal rule for non-convergence of parity

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

However, to overcome the finite-size lattice defects, we developed the unit step model as an approximate solution to the Hubbard Hamiltonian in other to solve effectively any higher and larger dimensional lattices. Considering the case of two electrons interacting in

a two dimensional N x N lattice, if one electron is at site (x, y) and the second one is at site (x_1, y_1) then the state will be $|xy\sigma, x_1\ y_1\bar{\sigma}\rangle$ where the relative spins of the two electrons are $(\bar{\sigma}) = \uparrow (\downarrow)$. The details of the electronic states of the two electrons interaction in a cluster of a square lattice is summarized as in Table 1.

Table 1: The summary of the relevant information derived from the analytical geometry of the 2D 5 x 5 cluster on a square lattice

Lattice separation l between the two electrons and the actual separation distance d		Pair wave function $\|\Psi_l\rangle$	Number of pair electronic states at lattice separation l $\langle\Psi_l\|\Psi_l\rangle$	Pair electronic states $\|i\uparrow, j\downarrow\rangle$
l	d			
0	0	$\|\Psi_0\rangle$	25	$\|11\uparrow,11\downarrow\rangle, \ldots, \|55\uparrow,55\downarrow\rangle$
1	a	$\|\Psi_1\rangle$	100	$\|11\uparrow,12\downarrow\rangle, \ldots, \|54\uparrow,55\downarrow\rangle$
2	$\sqrt{2}a$	$\|\Psi_2\rangle$	100	$\|11\uparrow,22\downarrow\rangle, \ldots, \|45\uparrow,51\downarrow\rangle$
3	2a	$\|\Psi_3\rangle$	100	$\|11\uparrow,13\downarrow\rangle, \ldots, \|53\uparrow,55\downarrow\rangle$
4	$\sqrt{5}a$	$\|\Psi_4\rangle$	200	$\|11\uparrow,23\downarrow\rangle, \ldots, \|43\uparrow,55\downarrow\rangle$ Or $\|11\uparrow,32\downarrow\rangle, \ldots, \|34\uparrow,55\downarrow\rangle$
5	$\sqrt{8}a$	$\|\Psi_5\rangle$	100	$\|11\uparrow,33\downarrow\rangle, \ldots, \|35\uparrow,53\downarrow\rangle$
Total number of electronic states			625	625

The Unit Step Hamiltonian

The approximation to the Hubbard Hamiltonian study is actually necessary because of the strong limitation and difficulty pose by the Hubbard Hamiltonian as we move away from finite-size lattices to larger N–dimensional lattices. The unit step model takes advantage of the symmetry of the Hubbard model given by (1). The kinetic hopping term (t) can only distribute the electrons within only nearest-neighbor (NN) sites in a given lattice according to +1 or -1. The *U* part can only act on the on-site electrons (double occupancy) while it is zero otherwise. Also from the geometry of the 2D 5 x 5 square lattice we recast (3) in the form

$$|\Psi\rangle = \sum_{l=0}^{l} X_l |\Psi_l\rangle \qquad (5)$$

In an explicit form the operation of the unit step Hamiltonian in two dimensional square lattices is defined as [13].

$$\begin{aligned} H|(ij)\uparrow,(kl)\downarrow\rangle = -t(&|(i+1)j\uparrow,(kl)\downarrow\rangle + |(i-1)j\uparrow,(kl)\downarrow\rangle + |i(j+1)\uparrow,(kl)\downarrow\rangle \\ &+|i(j-1)\uparrow,(kl)\downarrow\rangle + |(ij)\uparrow,(k+1)l\downarrow\rangle + |(ij)\uparrow,(k-1)l\downarrow\rangle \\ &+|(ij)\uparrow,k(l+1)\downarrow\rangle + |(ij)\uparrow,k(l-1)\downarrow\rangle) + U|(ii)\uparrow,(ii)\downarrow\rangle \end{aligned} \qquad (6)$$

Thus as the unit step Hamiltonian model acts on (5) we obtained the result

$$H|\Psi\rangle = H\sum_l X_l|\Psi_l\rangle = -t\sum_{(ij)}\left\{\frac{nX_l\langle\Psi_l|\Psi_l\rangle|\Psi_j\rangle}{\langle\Psi_j|\Psi_j\rangle}\right\} + U\sum_l X_l|\Psi_l\rangle \quad (7)$$

here n is the total number of states generated within a given lattice separation, $\langle\Psi_l|\Psi_l\rangle$ is the inner product of the state acted on by the unit step Hamiltonian, $\langle\Psi_j|\Psi_j\rangle$ is the total number or the inner product of the new state generated after operating on the eigen state, l is the particular lattice separation, $|\Psi_j\rangle$ is the new state generated.

On the basis of the information provided in Table 1 and the trial wave function given by equation (5), the action of the Hubbard Hamiltonian on the surviving anti-parallel spins state yields;

$$H|\Psi_0\rangle = -tx_0(2|\Psi_1\rangle) + Ux_0|\Psi_0\rangle$$
$$H|\Psi_1\rangle = -tx_1\{8|\Psi_0\rangle + 4|\Psi_2\rangle + 3|\Psi_3\rangle\}$$
$$H|\Psi_2\rangle = -tx_2\{4|\Psi_1\rangle + 2|\Psi_4\rangle\}$$
$$H|\Psi_3\rangle = -tx_3\{2|\Psi_1\rangle + 2|\Psi_4\rangle\}$$
$$H|\Psi_4\rangle = -tx_4\{4|\Psi_2\rangle + 4|\Psi_3\rangle + 4|\Psi_5\rangle\}$$
$$H|\Psi_5\rangle = -tx_5\{2|\Psi_4\rangle\}$$

Thus we have that;

$$H|\Psi\rangle = -t\{2x_0|\Psi_1\rangle + 8x_1|\Psi_0\rangle + 4x_1|\Psi_2\rangle + 2x_1|\Psi_3\rangle + 4x_2|\Psi_1\rangle + 2x_2|\Psi_4\rangle + 2x_3|\Psi_1\rangle +$$
$$2x3\Psi4+4x4\Psi2+4x4\Psi3+4x4\Psi5+2x5\Psi4+Ux0\Psi0 \quad (8)$$

Thus with the use of the field strength tensor condition as stated in Section 2, it is established after multiplying through (5) and (8) by the BRA of (5) and this yields

$$\langle\Psi|\Psi\rangle = 25(x_0^2 + 4x_1^2 + 4x_2^2 + 4x_3^2 + 8x_4^2 + 4x_5^2) \quad (9)$$

$$\langle\Psi|H|\Psi\rangle = -25t\{4x_0x_1 + 8x_1x_2 + 4x_1x_3 + 8x_2x_4 + 8x_3x_4 + 8x_4x_5 + 2x_3^2 + 4x_4^2 +$$
$$4x52-U4tx02$$

(10)

RESULTS AND DISCUSSION

The Variational Ground State Energy

The variational ground state energy is defined as [13]

$$E_g = \frac{\langle \Psi|H|\Psi\rangle}{\langle \Psi|\Psi\rangle} \tag{11}$$

where E_g, is the correlated ground state energy and Ψ is the guessed trial wave function.

Substituting (9) and (10) into (11) yields

$$E_g = \frac{-25t\left\{4x_0x_1+8x_1x_2+4x_1x_3+8x_2x_4+8x_3x_4+8x_4x_5+2x_3^2+4x_4^2+4x_5^2-\frac{U}{4t}x_0^2\right\}}{25(x_0^2+4x_1^2+4x_2^2+4x_3^2+8x_4^2+4x_5^2)} \tag{12}$$

where $\frac{E_g}{t} = E$, is the energy possess by the two electrons in the ground state and $\frac{U}{4t}$ is dimensionless and it is called the interaction strength.

Equation (12) is differentially minimized in the form

$$\langle \Psi|\Psi\rangle \frac{\partial E_g}{\partial x_i} + E_g \frac{\partial \langle \Psi|\Psi\rangle}{\partial x_i} = \frac{\partial \langle \Psi|H|\Psi\rangle}{\partial x_i} \tag{13}$$

Subject to the condition that the correlated ground state energy of the two interacting electrons is a constant of the motion

$$\frac{\partial E_g}{\partial x_i} = 0, \forall\, i = 0,1,2,3 \tag{14}$$

Minimization of equation (12) with respect to $x_i; i = 0,1,2,3,4,5$, and the turning point constraint yield the following results;

$$\left.\begin{array}{c} \left(E - 4\frac{U}{4t}\right)x_0 + 8x_1 = 0 \\ 2x_0 + Ex_1 + 4x_2 + 2x_3 = 0 \\ 4x_1 + Ex_2 + 4x_4 = 0 \\ 2x_1 + (E+2)x_3 + 4x_4 = 0 \\ 2x_2 + 2x_3 + (E+2)x_4 + 2x_5 = 0 \\ 4x_4 + (E+4)x_5 = 0 \end{array}\right\} \tag{15}$$

To obtain the variational ground state energy, of equation (15) is transformed into a matrix to give a homogeneous eigen value problem of the form

$$[A - \lambda_l I]\vec{X}_i = 0, \tag{16}$$

where A is an N×N matrix which takes the dimension of the number of separations, λ_i is the eigen value to be determined, I is the identity matrix which is also of the same order as A and $\vec{X}_i$ are the various eigen vector. After some algebraic transformation we obtain the matrix

$$\begin{pmatrix} E-4\frac{U}{4t} & 8 & 0 & 0 & 0 & 0 \\ 2 & E & 4 & 2 & 0 & 0 \\ 0 & 4 & E & 0 & 4 & 0 \\ 0 & 2 & 0 & E+2 & 4 & 0 \\ 0 & 0 & 2 & 2 & E+2 & 2 \\ 0 & 0 & 0 & 0 & 4 & E+4 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad (17)$$

Equation (17) is the matrix from which the ground state energy and corresponding variational parameters for the various arbitrary values of the interaction strength are determined and the result presented in Table 2 at different values of $\frac{U}{4t}$.

Table 2: Variational energy and the variational parameters

Interaction strength $\frac{U}{4t}$	Total energy E (eV)	Variational Parameters x_i					
		x_0	x_1	x_2	x_3	x_4	x_5
50.00	-7.7585	0.0131	0.3390	0.4242	0.4538	0.4837	0.5148
40.00	-7.7602	0.0162	0.3399	0.4244	0.4537	0.4835	0.5143
30.00	-7.7630	0.0214	0.3412	0.4247	0.4537	0.4830	0.5134
20.00	-7.7684	0.0313	0.3438	0.4253	0.4535	0.4821	0.5117
10.00	-7.7834	0.0587	0.3506	0.4266	0.4528	0.4794	0.5068
5.00	-7.8084	0.1039	0.3613	0.4279	0.4508	0.4739	0.4978
1.00	-7.9013	0.2631	0.3914	0.4240	0.4351	0.4462	0.4575
0.00	-8.0000	0.4082	0.4082	0.4082	0.4082	0.4082	0.4082
-1.00	-8.3668	0.7235	0.3945	0.3176	0.2934	0.2695	0.2468
-5.00	-20.8086	0.9947	0.1005	0.0200	0.0114	0.0034	0.0008
-10.00	-40.4010	0.9987	0.0501	0.0050	0.0026	0.0004	0.0000
-20.00	-80.2001	0.9997	0.0250	0.0012	0.0006	0.0000	0.0000

Table 2, shows that;

i. The total energy possesses by the two electrons decreases as the interaction strength is decreased.

ii. x_0 increases as the interaction strength is decreased.

iii. x_1 increases until the interaction strength $\frac{U}{4t} = 0$ and then it starts to decrease as $\frac{U}{4t}$ is decreased.

iv. x_2 increases until the interaction strength $\frac{U}{4t} = 5$ and then it starts to decrease as $\frac{U}{4t}$ decreases.

v. $x_3, x_4,$ and x_5 decreases consistently as $\frac{U}{4t}$ decreases.

The negative values of the total energy also confirms to the fact that, there is attraction between the interacting electrons. Table 2 also shows clearly that the variational parameters for any given system are of equal weights when $\frac{U}{4t} = 0$. This implies that the probability of double occupancy is the same as single occupancy. When the interaction strength is zero, we observe a free electron system. This implies that, the two electrons are not under the influence of any given potential, they are free to hop to any preferable lattice site. It is therefore clear that for positive values of the interaction strength x_i increases and decreases for negative values of the interaction strength which implies that the two interacting electrons will prefer to remain close together and this is what is responsible for some of the physical properties of condensed matter physics such as superconductivity and magnetism. However for the negative values of the interaction strength the two electrons prefers to stay far apart as possible and as the potential energy U decreases this gives room for dominance in the hopping term of the Hubbard model and consequently leads to the exchange of electrons. This exchange is responsible for ferromagnetism.

Pair Correlation Function (PCF)

The pair correlation function is defined as the probability of finding an electron at site j when there is an electron at site i. In terms of density correlation it is defined by[15] as

$$\mathrm{P_{(ij)}} = \frac{\langle\Psi|\mathrm{n_i n_j}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \tag{18}$$

For on-site interaction (18) becomes

$$\mathrm{P(ij)} \rightarrow \mathrm{P_0} = \frac{\langle\Psi|\mathrm{n_i{\uparrow}n_i{\downarrow}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{\mathrm{x_0^2}}{\langle\Psi|\Psi\rangle} \tag{19}$$

Similarly, for off-site interaction (18) turns

$$\mathrm{P(ij)} \rightarrow \mathrm{P_1} = \frac{\langle\Psi|\mathrm{n_i{\uparrow}n_j{\downarrow}+n_i{\downarrow}n_j{\uparrow}}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = \frac{4\mathrm{x_1^2}}{\langle\Psi|\Psi\rangle} \tag{20}$$

Equations (19) and (20) are the PCF calculated for a non-symmetric argument i.e. $P_l(l > 0)$ is essentially made up of two probabilities. The pair correlation function values are calculated using equations (19) and (20) and the result presented in Table 3.

Table 3: Pair Correlation Function

Interaction Strength $\frac{U}{4t}$	Pair correlation function					
	P_0	P_1	P_2	P_3	P_4	P_5
50.00	1.391×10^{-6}	3.725×10^{-3}	5.833×10^{-3}	6.675×10^{-3}	0.03136	8.591×10^{-3}
40.00	2.127×10^{-6}	3.745×10^{-3}	5.838×10^{-3}	6.672×10^{-3}	0.01515	8.574×10^{-3}
30.00	3.711×10^{-6}	3.773×10^{-3}	5.847×10^{-3}	6.672×10^{-3}	0.01512	8.544×10^{-3}
20.00	7.939×10^{-6}	3.841×10^{-3}	5.863×10^{-3}	6.667×10^{-3}	0.01507	8.487×10^{-3}
10.00	2.792×10^{-5}	3.985×10^{-3}	5.899×10^{-3}	6.645×10^{-3}	0.01480	8.326×10^{-3}
5.00	8.748×10^{-5}	4.231×10^{-3}	5.935×10^{-3}	6.587×10^{-3}	0.01456	8.033×10^{-3}
1.00	5.611×10^{-4}	4.966×10^{-3}	5.827×10^{-3}	6.137×10^{-3}	0.01291	6.785×10^{-3}
0.00	1.350×10^{-3}	5.401×10^{-3}	5.401×10^{-3}	5.401×10^{-3}	0.01082	5.401×10^{-3}
-1.00	4.242×10^{-3}	5.045×10^{-3}	3.270×10^{-3}	2.790×10^{-3}	4.709×10^{-3}	1.974×10^{-3}
-5.00	8.018×10^{-3}	3.274×10^{-4}	1.297×10^{-5}	4.213×10^{-6}	7.494×10^{-7}	2.075×10^{-8}
-10.00	8.083×10^{-3}	8.136×10^{-5}	8.104×10^{-7}	2.191×10^{-7}	1.037×10^{-8}	0.0000
-20.00	8.099×10^{-3}	2.026×10^{-5}	4.668×10^{-8}	1.167×10^{-8}	0.00000	0.000

Table 3 show that, as $\frac{U}{4t}$ decreases the pair correlation function values for on-site interaction increases for P_0. This indicates that, the two electrons will prefer to stay at the same site and align themselves together due to the less forces of repulsion while for the off-site interaction, as the interaction strength $\frac{U}{4t}$ decreases, the pair correlation function P_1, P_2, P_3, P_4 and P_5 also decrease indicating that, the two electrons will prefer to stay at different site due to the large repulsive force. It is inferred from the results that when the interaction strength is more negatively large, then the electrons tend to remain close together (Cooper pairing). However as the interaction strength turns positive, the two electrons prefer to stay far apart as possible and this is synonymous with ferromagnetism. This result shows that, the interacting electrons at large positive interaction strength tend to gain the lowest ground state energy and hence the highest potential.

CONCLUSION

The effect of the interaction strength $\frac{U}{4t}$ to pair correlation function in a single band Hubbard model in 2-D lattice system has been investigated. The variational method is applied in the determination of the pair correlation function. The pair correlation function of two interacting electrons under the Hubbard model has been discussed in a two-dimensional lattice with appropriate periodic boundary conditions. The pair correlation function is calculated to explain some physical properties of condensed matter physics such as superconductivity, magnetism, ferromagnetism etc.

Table 2 show that, the energy (E) decreases as the interaction strength decreases and the variational parameters $x_{0,1,2,3}$ increases as $\frac{U}{4t}$ decreases. It can also be seen from Table 2 that the variational parameters follow the ordering $x_0 < x_1 < x_2 < x_3 < x_4 < x_5$ which implies that for large $\frac{U}{4t}$ the electrons prefer to stay far apart as possible. Table 3 has it that, as $\frac{U}{4t}$ decreases the pair correlation function values for on-site interaction increases indicating that the two electrons will prefer to stay at the same site and align themselves together due to the less forces of repulsion while for the off-site interaction, as the interaction strength $\frac{U}{4t}$ decreases, the pair correlation function $\mathrm{P}_3, \mathrm{P}_4$ and P_5 also decrease indicating that, the two electrons will prefer to stay at different site due to the large repulsive force.

Conclusively this research work has shown that, physical properties of condensed matter physics such as superconductivity, magnetism, ferromagnetism etc can be explained by the correlated variational approach. Particular attention has been paid to the variational parameters as it shows that for large *U* the electrons will prefer to stay far apart as possible. In general, it is found that as *U* decreases, the pair correlation function for on-site interaction increases indicating that the two electrons will prefer to occupy the same site while that of the off-site interaction decreases indicating that the two electrons will prefer to occupy different site.

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