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Observable Ground State Singlet-Triplet Transition in Linear Quantum dots

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Abstract: *The quantum nature of electron spins tells us that they can assume two states- up or down. These spins are the quantum particles that exhibit singlet-triplet transition. In this work, the investigation of a two-electron interaction under the t-U-V-J model on a finite-size lattice in one dimension(1D) was done. The highly simplified correlated variational approach (HSCVA) was the theoretical tool we used to obtain the ground state energies at various variational parameters. The results presented in this work show that when the on-site interaction strength, $U/4t$, nearest neighbor interaction strength, $V/4t$ and nearest* neighbor exchange interaction strength, $J/4t$ are varied at different arbitrary values, phase transition from singlet state to triplet state occurred. The ground state energies this occurred for the singlet state E_s and the triplet state E_t are 18.5859 and 18.5856 respectively for $U/4t = 5$, $V/4t = 5$ and $J/4t = 0.3536$. Also a*t another point of transition, the ground state energies of –20.0994 and -20.0996 for the singlet and triplet states were obtained for $U/4t = 0$, $V/4t = -5$ and $J/4t = 0.0249$ respectively.*

Keywords*: Linear quantum dots, two-electron interaction, singlet-triplet transition,*

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I. Introduction

As attention is turned towards developing or building quantum computers whose capabilities exceed that of classical computers, quantum dots will be one of the research laboratories to focus on in quantum information processing by researchers or scientists. Quantum dots (QDs) are miniature man-made atoms in a solid whose sizes range from nanometer to a few microns with their electronic properties showing several similarities with natural atoms [1]. These quantum dots manufactured artificially in semiconductor quantum material have become candidates for investigating few-body systems with some parameters like the number of electron interactions and their effect when subjected under the influence of magnetic field. Various means and procedures are being used to research on the energy spectrum and the correlation effects of the interacting electrons embedded in a quantum dot under the effect of an applied magnetic field [2]. Some of the effects of electron correlations are the magnetic properties and the spin behaviour of atoms in the ground state of the quantum dot system in the presence of the magnetic field. [3] affirmed this when they carried out a research on the effects of an applied electric field on the magnetic behavior of a triple dots system in a triangular and linear geometry. From their result analysis, an increase of the electric field induces singlet-triplet transitions. The quantum dot has the capacity to be used as a quantum bit of a quantum computer because the magnetic field can be used to tune the transition in the spin of the ground state of the quantum dot from singlet (S=0) to triplet (S=1) state [4]. The main idea of quantum dots is to develop a means to read the state of the quantum particles inside the dot which become a potential and viable quantum bit for information processing. However, for such feat to be achieved smoothly, the coherent nature of the quantum states must be sustained for a long time [5]. A quantum dot of one electron has a quantum bit of a one or a zero state while a two-electron quantum dot has a quantum bit of singlet or triplet state. It is the transition from one state to another that is being seen or regarded as a possible logic state for quantum computers [6]. Beside the quantum computer, quantum dot laser, memory chips, quantum cryptography etc are some of the electronic and optical devices that are the products of quantum dots [7].

This work is aimed at using the highly simplified correlated variational approach (HSCVA) developed by Akpojotor to explore the physics of the t-U-V-J model to investigate the singlet-triplet transition of a two-electron interacting on a finite-sized lattice in one dimension.

In this study, we described briefly the Hubbard model, its Hamiltonian and the extended version of Hubbard model; t-U-V-J model used to study electron correlation and the theoretical calculations in section two. In section three, the numerical results emanating from our calculations and discussions are stated while section four contains our conclusion.

Theoretical Model and Calculations

In solid state physics, there is always a strong correlation when a given lattice site which contains an electron feels the presence of another electron that is located at different lattice site. This interaction (Coulomb interaction) is brought about by the presence of spin and charge between them. In as much as this interaction or relationship exists, the electron are said to be correlated [8].The Hubbard model is given as an approximate means of describing the transition between conducting and insulating systems. The insulating, magnetic and novel superconducting phenomenon in a solid which result from the interactions between electrons is understood with the insight the Hubbard model offers. This model is the simplest model for interacting particles in a lattice. The kinetic term that describes the hopping or itinerant (tunneling) tendency of electrons represented by the letter **t** in the Hamiltonian. This hopping term describes the creation of electrons of spinσon site i and its annihilation on site j (or vice-versa). The symbol $< ij >$point to the fact that hopping is permitted only between two sites which are adjacent. The second term which is the potential, consist of an on-site coulombic interaction represented by the letter **u**. This is the potential energy arising from the charges on the electrons. The final term represents the chemical potential which controls the filling [9]. The Hamiltonian is given by:

$$H_H = -t\left[\sum_{<i,j>\sigma} C_{i\sigma}^{+} C_{j\sigma} + H.C\right] + U\sum_i n_{i\uparrow} n_{i\downarrow} - U\sum_i n_{i\uparrow} n_{i\downarrow} \quad (1)$$

Following the limitation observed in the Hubbard model, it becomes imperative to use the extended version of the Hubbard model, the t-U-V-J which emanated from the t-U-J model by including the nearest neighbour Coulombic interaction V. The t-U-V-J according to Akpojotor [6] is given by:

$$H = -t\left[\sum_{<i,j>} C_{i\sigma}^{+} C_{j\sigma} + H.C.\right] + U\sum_i n_{i\uparrow} n_{i\downarrow} + V\sum_{<i,j>} n_i n_j + J\sum_{<i,j>\sigma,\sigma\sigma^1} C_{i\sigma}^{+} C_{j\sigma\sigma^1}^{+} C_{i\sigma^1} C_{j\sigma} \quad (2)$$

In equation (2), the hopping term in the Hamiltonian is denoted by the letter t the on-site Coulombic interaction is the **U** term , the nearest neighbor (NN) interaction term is **V** and the nearest neighbor exchange term is **J.**

In investigating the singlet-triplet transitions in a two-electron quantum dots, we will obtain the expression for the ground state energy and correlated variational wave function of both the singlet and triplet states.

Following the work of [10], who formulated the correlated variational approach (CVA), the trial wave function according to Chen and Mei is:

$$/\psi> = \sum_i^n X_{jj} /i\uparrow, i\downarrow> + \sum_{<i,j>}^n X_{/i-j/}[\, i\uparrow, j\downarrow> - /\, i\downarrow, j\uparrow>] + \sum_{<i-j>}^n Y_{ij/}[/i\uparrow, j\uparrow>, \quad (3)$$

where$< i, j >$stands for only nearest neighbour interactions equation (3) is the exact ground state wave function. [6] developed a highly simplified formulation of the correlated variational approach (CVA) of equation (3). The equation is:

$$H_{L_{CR}L_R}[R_{L_{CR}}] = \left[E_{\delta L_{CR}L_R} - 4\left(\frac{U}{4t}\right)_{\delta_0 L_{CR}\delta_0 L_R\delta_{RX}} - 4\left\{\left(\frac{V}{4t}\right) + \left(\frac{J}{4t}\right)\right\}_{\delta_1 L_{CR}\delta_1 L_R\delta_{RX}} + 2T_{L_{CR}L_R\delta_{RX}} - 4\left\{\left(\frac{V}{4t}\right) + \left(\frac{J}{4t}\right)\right\}_{\delta_1 L_{CR}\delta_1 L_R\delta_{RY}} + 2T_{L_{CR}L_R\delta_{RY}}\right][R_{L_{CR}}] = [0] \quad (4)$$

Equation (4) is a general matrix equation valid for both singlet and triplet states of two-electron interaction on any lattice size in all the three dimensions. With two-electron interaction on two sites of a linear quantum dot, our analytical calculations with equation (4) yields 3× 3matrix form seen as equation (5)

$$\begin{bmatrix} E-4(U/4t) & 2 & 0 \\ 2 & E-4(V/4t)-4(J/4t) & 0 \\ 0 & 0 & E-4(V/4t)+4(J/4t) \end{bmatrix}\begin{bmatrix} X_0 \\ X_1 \\ Y_1 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad (5)$$

where U/4t is the on-site interaction strength, V/4t is the NN inter-site interaction strength and J/4t is the NN interaction strength

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II. Results and Discussions

The two graphs of figure 1 and 2 plotted from tables 1 and 2 show the behavior of the singlet and triplet states and their point of transitions, $T_p$when the on-site interaction strenght, $U/4t$, nearest neighbour interaction interaction strength, $V/4t$ and nearest neighbour exchange interaction strength, $J/4t$ are varied respectively. From table 1, taking an arbitrary values of J/4t = - 0.5000 to 0.3530 for fixed values of *U/4t* and *V/4t* = 5, the

system assumes a singlet state and its ground state energy is the lowest energy of the singlet state, E_s. That is, at any value of J/4t less than 0.3536,the spins in the quantum dots will anti-align so that the system will read singlet state, ↑↓. This singlet state continues as the values of *J/4t* are increased positively until when J/4t=0.3536. At J/4t=0.3536, there was a transition from singlet state to triplet state. The triplet state which is 18.5856 provides the lowest ground state energy of the system as against 18.5859 of the singlet state as could be seen in table 1.

It is also observed from table 2 that when $U/4t$= 0 and $V/4t$= -5 and varying$J/4t$= - 0.5000 to 0.0240, the singlet state persist until when the value of $J/4t$ =0.0249. It is at this value that the system transit to a triplet state. The ground state energies where this occurred for both the singlet state and the triplet state are – 20.0994 and-20.0996 respectively. We observed on generally note from the graphs, that as the value of *J/4t* is increased, the lowest energy of the singlet state continues to increase while that of the triplet state decreases.

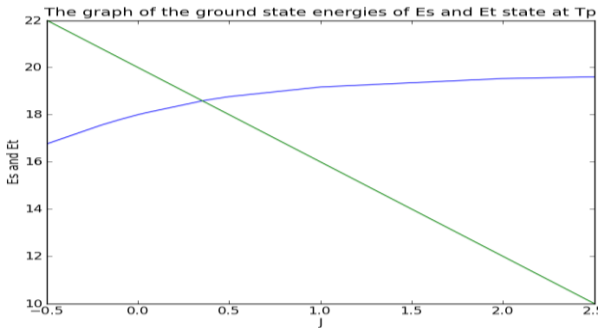

Figure 1: The graph when U/4t= V/4t=5

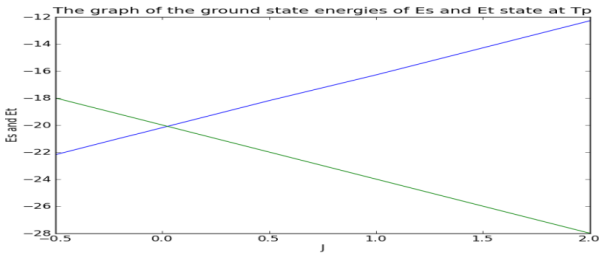

Figure 2: The graph when U/4t = 0 V/4t =5

For the variational parameters, it is observed that for the singlet states (X_o and X_1), they have non-zero values, while that of the triplet state (Y_1) have zeroes.The point of intersection is the transition point. From the graphs, the blue line that rises from left to right represents the ground state energy of the singlet states while the green line that slopes down from left to right represents the ground state energy of the triplet states.

We present the tables showing the ground state energies atvarious transition points, T_p for the singlet and triplet states for two-electron interaction on 2 sites under one dimension.

Table 1: The singlet state

NN Exchange Interaction Strength J/4t	Lowest Energy for Singlet States E_s	Lowest Energy for Triplet States E_t	Variational Parameters		
			X_o	X_1	Y_1
When U/4t = V/4t = 5					
-0.5000	16.7639	22.0000	0.5257	0.8507	0
-0.2000	17.5604	20.8000	0.6340	0.7733	0
-0.1000	17.7900	20.4000	0.6710	0.7415	0
0.000	18.0000	20.000	0.7071	0.7071	0
0.0500	18.0975	19.8000	-0.7246	-0.6892	0
0.3530	18.5850	18.5880	-0.8164	-0.5776	0
0.3536	18.5859	18.5856	0.000	0.0000	1
0.3548	18.5875	18.5808	0.0000	0.0000	1
0.4000	18.6459	18.4000	0.0000	0.0000	1
0.5000	18.7639	18.0000	0.0000	0.0000	1
1.0000	19.1716	16.0000	0.0000	0.0000	1
2.0000	19.5279	12.0000	0.0000	0.0000	1
2.500	19.6148	10.0000	0.0000	0.0000	1
4.0000	19.7538	4.0000	0.0000	0.0000	1

Table 2: The triplet states

When U/4t = 0 and V/4t = -5					
-0.5000	-22.1803	-18.0000	0.0898	0.9960	0
-0.2000	-20.9906	-19.2000	0.0949	0.9955	0
-0.1000	-20.5942	-19.6000	0.0967	0.9953	0
0.0000	-20.1980	-20.0000	0.0985	0.9951	0
0.0200	-20.1188	-20.0800	0.0989	0.9951	0
0.024	-20.1030	-20.1000	0.0990	0.9951	0
0.0249	-20.0994	-20.0996	0.0000	0.0000	1
0.1000	-19.8020	-20.400	0.0000	0.0000	1
0.5000	-18.220	-22.000	0.0000	0.0000	1
1.0000	-16.2462	-24.0000	0.0000	0.0000	1
1.5000	-14.2801	-26.0000	0.0000	0.0000	1
2.0000	-12.3246	-28.0000	0.0000	0.0000	1

III. Conclusion

Phase transitions in quantum dots could be as a result of the effect of magnetic field, electric field, spin behavior in atoms and couloumb interactions. In the quest to understand one of the electronic properties of quantum dots, we have investigated the singlet-tripet transition in linear quantum dots. The results; the ground state energies, the variational parameters with the corresponding graphs in figure 1 and 2 are in good agreement with those of [6].

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