

Quantum Dots in Ferromagnetic Heisenberg Model

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Quantum Dots (QDs) are semiconductor-nanostructure materials which are also called artificial atoms. QDs are classified as ferromagnetic material. Theoretically, Heisenberg model is regarded as a good model in describing these QDs. We applied Spin Wave Theory (SWT) on the above mentioned model to explore the physical properties of these materials, such as ground state energy, excitation energy and magnetization. We found that the ground state energy ε_g increased with the applied external magnetic field B as $B^{0.3}$. A phase transition was also observed around $B \sim 1T$, which indicate a transition from singlet to a triplet state. Staggered magnetization reaches saturation around this point of transition.

Keywords: Quantum Dots, Ferromagnetism, Heisenberg Hamiltonian, Spin Wave Theory

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I. Introduction:

Extensive attention was paid in the past decade toward Nano technology in both theoretical as well as experimental branches.¹⁻¹² This technology deals with tiny material of size ranging between 1 to 10nm. At this level these materials show different behavior from that of bulk ones.⁸

This different behavior gave these materials wonderful characteristics, amazing and vast applications in several fields.¹⁻⁴ The reason behind this behavior is due to two factors: the surface to volume ratio and secondly due to Heisenberg uncertainty principle.⁹

Quantum dots (QDs) also referred to as artificial atoms are classified as nano materials. They are made from several semiconductor materials such as: Cadmium Selenide (CdSe) Cadmium Sulfide (CdS) and Cadmium Telluride (CdTe) . Also QDs were made from Zinc Sulfide (ZnS) and Zinc Selenide (ZnSe).^{4,10,11}

As mentioned above QDs are of size ranges from 1 – 10nm. Each QD may contain in it from a single electron to several thousand up. They do consist of two parts: the core which is made of a semiconductor material such as CdSe, and a shell which is also a semiconductor like ZnS.⁴ For some applications a coating for QDs is made from polymers to prevent leakage of toxic materials into them and to help them dissolving in water. The coating also makes them very useful in several biological applications.^{4,10,11}

As semiconductors, quantum dots have a band gap between the covalent band and the conducting band. Excitons (which are electron-hole pairs) are confined in three dimensions.^{2,3,5}

Scientists succeeded in confining electrons in a quantum dot similar to the well-known example of a particle in a box. The electrons are allowed to remain within these boundaries which are of the size atoms called nano space. The limitation of space appears as an increase in electron energy and makes it quantized which gives unique electrical as well as optical properties to the quantum dot.^{2,3} These properties make QDs applicable in several technical applications. Beside their quantum confinements, quantum dots have another advantage regarding their size. The flexibility of QD size allows researchers to grow and manufacture it in several ways. This gives QD extra wide range of life applications.

The properties and wide applications of quantum dots attracted attention of many researchers (both experimentalists as well as theorists). Experimentally several compounds of QDs were under study and investigation such as Gallium arsenide (GaAs) which is used in making logic gates for supercomputers.¹²

Theorists subjected QDs to a keen investigation to be able to understand them and use them in large number of applications. During these studies researchers applied several theoretical models to investigate quantum dots in order to understand and explore their characteristics.

II. Spin wave theory and Heisenberg model

It is well-known by theorists that these ferromagnetic quantum dots can be described by Heisenberg model. In our research, we used Heisenberg model in quantum dots containing unlimited number of electrons subjected to an external magnetic field B in z -direction.

$$\hat{H} = \sum_{i,j} J_{ij} S_i \cdot S_j + \mu_B g_l B \sum_{i,j} (S_i^z - S_j^z) \quad (1)$$

Where J_{ij} is the exchange constant between the site i and j , μ_B Bohr magneton, g_l gyromagnetic ratio and B external magnetic field.

Using the lowering and raising spin operators:

$$S^\pm = S^x \pm iS^y \quad (2)$$

The above Hamiltonian becomes:

$$\hat{H} = \sum_{i,j} J_{ij} \left[\frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) \right] + \mu_B g_l B \sum_{i,j} (S_i^z - S_j^z), \quad (3)$$

In spin-wave theory, the quantum spin operators in the Hamiltonian are transformed to bosonic operators using a well-defined transformation such as Holstein-Primakoff (HP) transformations or the Dyson-Maleev (DM) transformations. We will use HP¹⁴ transformations since the DM transformations make the above Hamiltonian non-Hermitian. For the two sublattices the HP transformations are:

$$S_i^+ = a_i^+ (2s - a_i^+ a_i)^{\frac{1}{2}} \quad (4)$$

$$S_i^- = (2s - a_i^+ a_i)^{\frac{1}{2}} a_i \quad (5)$$

$$S_i^z = s - a_i^+ a_i \quad (6)$$

$$S_j^+ = (2s - b_j^+ b_j)^{\frac{1}{2}} b_j \quad (7)$$

$$S_j^- = b_j^+ (2s - b_j^+ b_j)^{\frac{1}{2}} \quad (8)$$

$$S_j^z = b_j^+ b_j - s \quad (9)$$

A linearized Hamiltonian is obtained by substituting HP transformations into Eq.(3) and keeping terms up to quadratic order in the spin-deviation operators a and b . The linearized Hamiltonian in Fourier transformed variables is

$$\tilde{H} = \sum_k [A(k)(a_k^\dagger a_k + b_k^\dagger b_k) + B(k)(a_k^\dagger b_k^\dagger + a_k b_k) + c] \quad (10)$$

with

$$A(k) = Js + B_z \tag{11}$$

$$B(k) = 2Js\cos(kx) \tag{12}$$

$$C = 2sB_z - Js^2 \tag{13}$$

and

$$B_z = \mu_B g_l B \tag{14}$$

The linearized Hamiltonian in Eq.(10), can be diagonalized using Bogoliubov transformations defined as

$$a_k = u_k \alpha_k + v_k \beta_k^\dagger \tag{15}$$

$$b_k = u_k \beta_k + v_k \alpha_k^\dagger \tag{16}$$

and their conjugates to

$$\tilde{H} = \varepsilon_g + \sum_k [E(k)(\alpha_k^\dagger \alpha_k + \beta_k^\dagger \beta_k)] \tag{17}$$

where α_k and β_k are the normal mode boson operators, and the transformation coefficients u_k, v_k are constrained by the condition $u^2 - v^2 = 1$.

The ground state energy per ε_g site is given by

$$\varepsilon_g = C + 2A + \sum_k \zeta_k \tag{18}$$

The excited energy $E(k)$ is

$$E_k = \zeta_k \tag{19}$$

The staggered magnetization M is

$$M = s - \langle D \rangle \tag{20}$$

such that

$$\zeta_k = \sqrt{(2A)^2 - 4B^2(k)} \tag{21}$$

$$u_k = \sqrt{\frac{2A(k) + \zeta_k}{\zeta_k}} \tag{22}$$

$$v_k = \sqrt{\frac{2A(k) - \zeta_k}{\zeta_k}} \tag{23}$$

$$\langle D \rangle = \langle a_k^\dagger a_k \rangle = \langle b_k^\dagger b_k \rangle \quad (24)$$

$$= \frac{1}{N} \sum_k v_k^2 \quad (25)$$

with $\langle D \rangle$ is the average taken in the ground state, which is the Neel state, at zero temperature.

The physical quantities defined above are calculated as a function of external magnetic field B for spin $s = 1/2$ system.

III. Results and discussion

Linear spin wave theory shows that the ground state energy defined in Eq.(18.) increases with increasing the external magnetic field B as shown in Fig(1). This increase took the form as $\sim B^{1/2}$. A point of transition from a singlet to a triplet state at $B \sim 1T$ was observed in agreement with previous studies.⁸

Excitation spectrum of the QD was computed using Eq.(19.). A gapless mode at momentum $K = 0$ in the absence of external magnetic field $B = 0$ T is observed in agreement with other ferromagnet materials Fig. (2). But a gap appears in the spectrum and increases linearly with B as soon as the magnetic field is switched on. This linear behavior differs before and after the transition point $B \sim 1T$ as illustrated in Fig. (3).

Finally magnetization curve shows an increase to a saturated value with B - as expected - , Fig.(4), since the external magnetic field forces the spins to align in its direction. This increase goes as $M \sim B^{0.3}$. We also observe a transition point around $B \sim 1T$.

In conclusion, LSWT shows a transition point from singlet to a triplet state in QDs at $B = 1T$. The external magnetic field disturbed the system by increasing the ground state energy. All the physical quantities increased by increasing the external magnetic field B .

Still many efforts have to be done in studying QDs to clarify and understand all of their characteristics to make them more applicable in many medical applications, security, industry, computer logic gates and other applications. We hope that we contributed to these investigations in making QDs a little bit more clear.

IV. Research Bibliography

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Figure captions

FIGURE 1. Ground state energy under the influence of a magnetic field.

FIGURE 2. The energies of excitement for several values of the magnetic field.

FIGURE 3. The excitation mode at $K = 0$ as a function of external magnetic field. The change of linear behavior is clear at $B = 1$ T indication a phase transition from singlet to a triplet state.

FIGURE 4. Magnetization M Vs. B . The system reaches saturation at the transition point.





