Correlation Energy of Low-Lying States in Spherical Quantum Dot

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Abstract- **Correlation energy in $1s-1s$ and $1s-2s$ states of a two-electron spherical quantum dot with finite confining potential is calculated using the effective mass approximation, variational method and mean value theorem. The results show that the correlation energy is more significant for dots of smaller radii and larger barrier heights. The correlation energy decreases as the radius increases. The results are compared to other investigations.**

Keywords*- *Quantum Dot; Correlation Energy; Mean Value Theorem

I. INTRODUCTION

The study of confined quantum systems has been the interesting subject of investigation since the beginning of quantum theory. The interest in the study of the physical properties of confined quantum systems such as quantum wells, wires, and dots, has increased, with the recent progress in semiconductor nanotechnology [1-5]. Quantum size effects in these structures, lead to formation of atomic-like discrete energy levels (subbands), as opposed to the energy bands in bulk crystals. The effects of these energy levels on the physical properties of these quantum structures have been widely investigated [6-8]. These studies demonstrate that quantum confinement of carriers in quantum dots (QDs) has improved physical properties, as compared to semiconductor quantum wells and wires, for high-performance optoelectronic devices [9]. In these nanostructures in which the carrier motion is restricted to a narrow region of a few nanometers in dimension, the correlation among the electrons is shown to be appreciable [10].

The binding energies of two electrons in a spherical QD with square well potential confinement have been considered in [11]. The energy levels of two electrons in a square quantum well box have been studied by Bryant [12]. Brus [13] considered the effect of dielectric mismatch between the dot material and the surrounding. Zhu et al., [14] have pointed out the significance of size and shape effects on electron-electron interactions in a parabolic confinement. The energy spectra of two electrons in low-lying excited states in a spherical QD with different barrier heights are studied by John Peter and Saravan Kumar [10]. Correlation energies in a triplet state of a two electron spherical QD with square well potential confinement are estimated in Ref. [15]. In this paper the variational method is used for calculating the correlation energy of low-lying states in a spherical quantum dot. In this regard, a trial wave function based on the carrier wave function in spherical quantum dot is introduced and some integrals are calculated using mean value theorem.

In Section 2, the Hamiltonian and the calculation method are given. The numerical calculations and discussion on typical GaAs material are presented in Section 3.

II. THEORY

A. Single Electron In Spherical Quantum Dot

Within the framework of effective mass approximation, the Hamiltonian for carriers in spherical quantum dot in the absence of impurity is written as

$$H_i = \sum_i -\frac{\hbar^2}{2m^*_i}\nabla^2 + V_i(r) \tag{1}$$

Where m^*_i and $V_i(r)$ are the effective mass of the electrons and barrier height. The confining potential $V_i(r)$ is given by

$$V_i = \begin{cases} 0 & r < R \\ V_0 & r \geq R \end{cases} \tag{2}$$

Where $V_0 = Q_c \Delta E_g(x)$. Q_c is the conduction band offset parameter, which is taken as 0.658 [10]. The band gap difference between GaAs and $Ga_{l-x}Al_xAs$ is given by

$$\Delta E_g(x) = 1.115x + 0.37x^2(\mathrm{eV}) \tag{3}$$

The eigen function for *ns* states within the dot is

$$\Psi_i(r) = \begin{cases} N_n \dfrac{\sin(\alpha_n r)}{\alpha_n r} & r \leq R \\ N_n \dfrac{\sin(\alpha_n R)\, e^{-\beta_n r}}{\alpha_n r} & r > R \end{cases} \tag{4}$$

Where N_n is normalization constant and α_n and β_n are given by

$$\alpha_n = \sqrt{2m^* E_n} \quad , \quad \beta_n = \sqrt{2m^*(V_0 - E_n)} \tag{5}$$

Matching the wave function and their derivatives at the boundary $r = R$, the normalization constant and energy eigenvalues are determined by solving the transcendental equation

$$\boldsymbol{\alpha_n R \cot(\alpha_n R) + \beta_n R = 0} \tag{6}$$

B. Two Interacting Electrons in Spherical Quantum Dot

The Hamiltonian for this system is

$$H = H_1 + H_2 + H_{12} \tag{7}$$

Where H_{12} is the perturbation term,

$$H_{12} = \frac{e^2}{4\pi\varepsilon_0 |\vec{r_1} - \vec{r_2}|} \tag{8}$$

The Coulomb interaction energy is calculated using the variational method. In this regard the wave functions of system for 1s and 2s states are written as

$$\Psi_{1s-1s} = \Psi_{1s}(r_1)\Psi_{1s}(r_2)e^{-\lambda}|\vec{r_1} - \vec{r_2}| \quad (9)$$

and

$$\Psi_{1s-2s} = \Psi_{1s}(r_1)\Psi_{2s}(r_2)e^{-\lambda}|\vec{r_1} - \vec{r_2}| \quad (10)$$

Where λ is variational parameter . The correlation energies are obtained as

$$\begin{aligned} E_{1s-1s} &= min_\lambda \frac{e^2}{4\pi\varepsilon_0} < \Psi_{1s-1s} \left|\frac{1}{\vec{r_1} - \vec{r_2}}\right| \Psi_{1s-1s} > \\ &= (\frac{4\pi N_1^2 e^2}{\alpha_1^2 \varepsilon_0}) \min_\lambda \{ \left(\frac{R}{4} - \frac{\sin(\alpha_1 R)}{4\alpha_1}\right)(Z_1 + z_2) \\ &+ \left(\frac{N_1^2}{\alpha_1^2}\right)\left[\frac{e^{-2\lambda R}}{R}\left(\frac{R}{4} - \frac{\sin(\alpha_1 R)}{4\alpha_1}\right)\right. \\ &+ \frac{e^{-4\lambda R}}{2R}\left(\frac{R}{4} - \frac{\sin(2\alpha_1 R)}{4\alpha_1} + \frac{\sin(\alpha_1 R)}{4\alpha_1}\right) \\ &\left. + e^{-4\lambda R}\frac{\sin^2(\alpha_1 R)}{4\beta_1 R}\right] \\ &\times \left[\frac{R}{4} - \frac{\sin(2\alpha_1 R)}{4\alpha_1} + \frac{\sin(\alpha_1 R)}{4\alpha_1}\right. \\ &\left. + \frac{\sin^2(\alpha_1 R)}{2\beta_1}\right]\} \end{aligned} \quad (11)$$

and

$$\begin{aligned} \Delta E_{1s-2s} &= min_\lambda \frac{e^2}{4\pi\varepsilon_0} < \Psi_{1s-2s} \left|\frac{1}{\vec{r_1} - \vec{r_2}}\right| \Psi_{1s-2s} > \\ &= (\frac{4\pi N_1^2 e^2}{\alpha_1^2 \varepsilon_0}) \min_\lambda \{ \left(\frac{R}{4} - \frac{\sin(\alpha_1 R)}{4\alpha_1}\right)(J_1 + J_2) \\ &+ \left(\frac{N_2^2}{\alpha_2^2}\right)\left[\frac{e^{-2\lambda R}}{R}\left(\frac{R}{4} - \frac{\sin(\alpha_2 R)}{4\alpha_2}\right)\right. \\ &+ \frac{e^{-4\lambda R}}{2R}\left(\frac{R}{4} - \frac{\sin(2\alpha_2 R)}{4\alpha_2} + \frac{\sin(\alpha_2 R)}{4\alpha_2}\right) \\ &\left. + e^{-4\lambda R}\frac{\sin^2(\alpha_2 R)}{4\beta_2 R}\right] \\ &\times \left[\frac{R}{4} - \frac{\sin(2\alpha_1 R)}{4\alpha_1} + \frac{\sin(\alpha_1 R)}{4\alpha_1}\right. \\ &\left. + \frac{\sin^2(\alpha_1 R)}{2\beta_1}\right] \end{aligned} \quad (12)$$

Where

$$Z_1 = N_1^2 \int_0^R \sin^2(\alpha_1 r) \frac{e^{-2\lambda r}}{\alpha_1^2 r} dr \quad (13)$$

$$Z_2 = N_1^2 \sin^2(\alpha_1 R) \frac{e^{2\beta_1 R}}{\alpha_1^2} \int_R^\infty e^{-2\beta_1 r} \frac{e^{-2\lambda r}}{r} dr \quad (14)$$

$$J_1 = N_2^2 \int_0^R \sin^2(\alpha_2 r) \frac{e^{-2\lambda r}}{\alpha_2^2 r} dr \quad (15)$$

$$J_2 = N_1^2 \sin^2(\alpha_2 R) \frac{e^{2\beta_2 R}}{\alpha_2^2} \int_R^\infty e^{-2\beta_2 r} \frac{e^{-2\lambda r}}{r} dr \quad (16)$$

Some of the integrals are calculated using the mean value theorem [16].

III. RESULTS AND DISCUSSION

In this study, the numerical calculations are carried out on a typical $GaAs/Ga_{l-x}Al_xAs$ QD. We have used the following parameters in the calculations: $m^* = 0.067m_0$, x = 0.2.

Figure 1 shows the variations of the total energies with (dash curve) and without (solid curve) Coulomb term as a function of dot radius for 1s−1s states. As it is seen, the confined energy decreases as the dot size increases, a feature that is well known in Literature [17]. The correlation energy is positive and increases with decreasing in dot size. For comparison, the calculations are carried out with wave function $\phi_{1s-1s} = \Psi_{1s}(r_1)\Psi_{1s}(r_2)$, and the results are presented in Fig. 2. The total energy with and without correlation energy decreases as dot radius increases. The energies have greater value than Figure 1 for a given value of dot radius. This is because the wave function (Eq. 9) includes an interaction term which is not considered in the wave function ϕ_{1s-1s}. The results of Fig. 2 are similar to work done by Sivakami and Navaneethakrishnan [11].

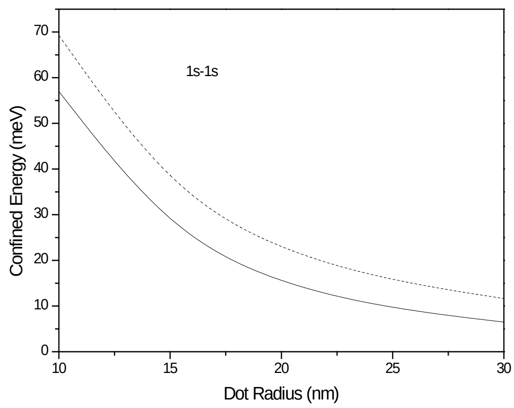

Fig. 1 The variations of confined energies of 1s-1s states versus the dot radius in the finite barrier model

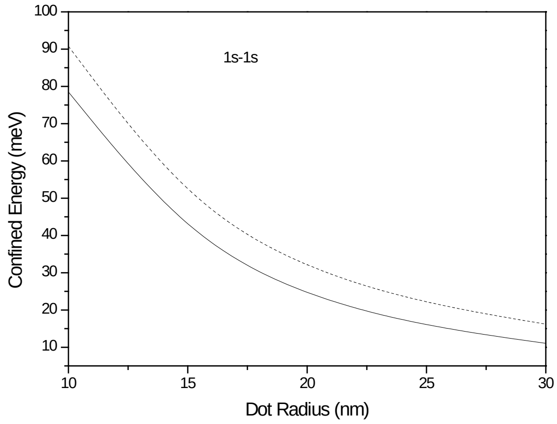

Fig. 2 The variations of confined energies in terms of the dot radius in the finite barrier model for $\phi_{1s-1s} = \Psi_{1s}(r_1)\Psi_{1s}(r_2)$

The total energies for 1s − 2s states in terms of radius of quantum dot are calculated using variational method and wave function Ψ_{1s-2s}, and are shown in Fig. 3. As it can be seen, the total energies with (dash curve) and without (solid curve) correlation energy decrease as the radius of dot increases. For comparison the total energy for $1s-2s$ states with wave function without interaction term, $\phi_{1s-2s}=\Psi_{1s}(r_1)\Psi_{2s}(r_2)$, is calculated and shown in Fig. 4. The correlation energy decreases as the dot size increases. The confined energy with wave function ϕ_{1s-2s}has greater value than Figure 3 for a given value of dot radius. This is also because the wave function Ψ_{1s-2s} includes interaction terms.

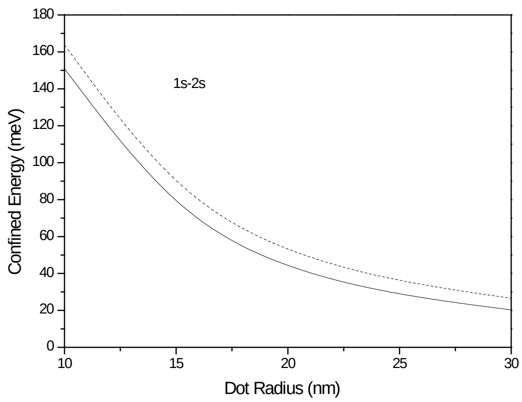

Fig. 3 The variations of confined energies of 1s-2s states versus the dot radius in the finite barrier model

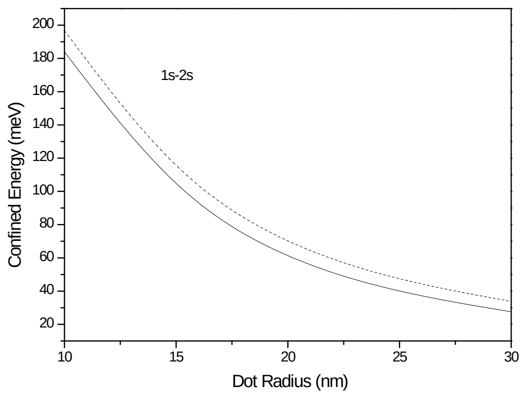

Fig. 4 The variations of confined energies in terms of the dot radius in the finite barrier model for $\phi_{1s-2s}=\Psi_{1s}(r_1)\Psi_{2s}(r_2)$

IV. CONCLUSION

The total energies including Coulomb interaction in a spherical quantum dot using variational method and appropriate wave function are calculated for $GaAs/Ga_{l-x}Al_xAs$ structures. The results clearly indicate that the total energy decreases as the dot size increases and correlation energy increases as the radius of dot decreases. The results are similar the Sivakami's report for $1s-1s$ states. The significant conclusion that emerges from the figures is that the correlation effects are important for smaller dots and should be considered in the studies of all low dimensional systems.

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