The Analytical Effects of a Hydrostatic Pressure on the Ground State Energy of GaAs Quantum Dot at Low-Temperature: Algebraic Method

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Received March 29, 2022
Revised August 29, 2022
Accepted for publication August 29, 2022

This analytical study focused on discussing the collective effects of hydrostatic pressure and temperature on the ground state energy for two electrons trapped in GaAs parabolic quantum dot in the presence of a magnetic field using the effective mass approximation. The electronic interaction was approximated by the Johnson–Payne potential model, where its parameters were carefully chosen to match the Coulomb interaction. It is noted that the ground state energy decreases with an increment in pressure while it increases linearly slightly with increasing temperature. As is customary, it was found that ground state energy decreases with increasing dot size and reach its bulk value as the dot becomes wider. Among the most prominent notes related to this study were as follows: (i) The largest contribution to the total ground state energy is caused by the relative motion since the effect of pressure on this part is more pronounced than the part of the center of mass that often does not feel the presence of pressure. (ii) Ground state energy shows temperature insensitivity while pressure exerts a tangible effect on the ground state energy in the strong magnetic field confinement. (iii) The effect of temperature on the ground state energy is always the opposite of the pressure effect. (iv) With regard to the increase in pressure, it was found that it reduces the electron separation (r), therefore the ground state energy decreases in the presence of the harmonic interaction that is directly proportional to the square of r, but compared to previous works mentioned in the literature, energy showed increased behavior because Coulomb's interaction is inversely proportional to the electron separation. (v) In the region of weak confinement $(R > a_B^*)$, the effect of pressure on ground state energy becomes neglected, while this effect becomes noticeable in the region of strong confinement $(R < a_B^*)$.

Keywords: Quantum Dots, Hydrostatic Pressure, Harmonic e-e Interaction.

DOI: 10.21883/SC.2022.10.54905.9847

1. Introduction

Quantum dots (QDs) are tiny particles of nanometer size trapped in three dimensions, which are composed of hundreds to thousands of atoms. These semiconducting materials can be made from an element, such as silicon or germanium, or from compounds such as GaAs, InAs, CdS or CdSe. A quantum dot exists as a box that limits the motion of the particles, where the number of particles can be adjusted through a voltage difference applied to the system, this result in quantization of energy levels, which leads to noticeable changes in the electrical and optical properties of these structures, enabling us to design artificial atoms with targeted tasks, which involve potential applications in many technology fields [1–11].

Numerous previous studies have used approximate methods to study the electronic, thermal and optical properties of a quantum dot in the presence of a uniform magnetic field, an electric field or an impurity under the influence of hydrostatic pressure based on the effective mass approximation [12–20]. The energy levels of a single GaAs QD with an infinite confinement potential well were studied using the second quantization method [21]. The authors noticed that the energy is modified noticeably with the application of hydrostatic pressure moreover; the energy levels exhibit a linear behavior with Hydrostatic pressure when the magnetic field remains unchanged. Sr.G. Jayam et al. [22] used the perturbation method to investigate the combined effects of pressure and electric field on the donor ionization energy of a spherical GaAs QD soaked in $Ga_{1-x}Al_xAs$. They found that, the ionization energy enhances with both hydrostatic pressure and electric field and this enhancement becomes pronounced for a wider dot. The Hass variational method has been used to study the variation of the susceptibility of a donor in cylindrical GaAs QD under the influence of hydrostatic pressure [23]. They stated that for wider dots, the magnitude of susceptibility decreases significantly with increasing pressure, whereas narrower dots almost do not feel the effect of hydrostatic pressure. Using exact diagonalization method, the ground state energy of shallow impurity in heterostructure of GaAs/AlGaAs has been investigated under the influence of temperature and pressure [24]. They reported that the increase in pressure enhances the donor binding energy, while it diminishes as the temperature increases and these changes are noticeable when the confinement frequency is large enough.

The aim of this study is to give an accurate and profound effect of hydrostatic pressure on the ground state energy of GaAs QD. The importance of pressure emerges because it works as a unit for operating system in the optoelectronic devices. To achieve a precise effect of hydrostatic pressure on the energy spectrum, it was necessary to search for a model of e-e interaction potential to obtain an analytical solution; since the e-e interaction controls the energy spectrum of the QDs. Among these models is the Johnson–Payne model [25]. The reason is as follows: As is known, due to the effects of the image charges in the nearby layers, Coulomb's interaction weakens if the electron separation is large, while at small separation distances, it is cut off due to the limitation of the electron wave function in the direction of growth [26]. Consequently, the Coulomb interaction can be modeled by the Johnson–Payne interaction. It is noteworthy that the harmonic interaction is valid only for a certain range of distances between electrons. Therefore, to make it represent a real interaction, the parameters of the model must be carefully tuned to give the most suitable results as we will demonstrate this later.

This study is arranged as follows: Section 2 displays the effective Hamiltonian of the system and the pressure effect is introduced through the effective mass approximation. The analytical results and discussions are presented in Section 3. In the last section, we conclude this study with the most important and prominent conclusions.

2. Theory and model

We utilize the effective mass approximation to scrutinize the effect of hydrostatic pressure on the ground state energy of a two-dimensional parabolic GaAs QD in the presence of a perpendicular magnetic field $B = B\hat{k}$ at low-temperature. Therefore, the effective Hamiltonian of the spinless system can be written as

$$\hat{\mathscr{H}} = \sum_{i=1}^{2}\left(\frac{1}{2m^*(P,T)}\left(\mathbf{p}_i + e\mathbf{A}(\mathbf{r}_i)\right)^2 + \frac{1}{2}m^*(P,T)\omega_0^2 r_i^2\right) + 2V_0 - \frac{1}{2}m^*(P,T)\Omega^2|\mathbf{r}_1 - \mathbf{r}_2|^2, \tag{1}$$

where $\mathbf{p}_i$ and $\mathbf{r}_i$ are the linear momentum and the position vector associated with the ith electron respectively, $\mathbf{A}$ is the vector potential which has been chosen as $\mathbf{A} = \frac{1}{2}\mathbf{B}\times\mathbf{r}$, Ω — represents the interaction strength. V_0 and Ω are the characteristic parameters of the harmonic interaction and we will discuss them later, ω_0 denotes the frequency strength of the confining potential and $m^*(P,T)$ is the pressure-temperature dependent effective mass of the electron that can be represented by [27]

$$m^*(P,T) = \frac{m_0}{1 + E_P^\Gamma\left(\frac{2}{E_g^\Gamma(P,T)} + \frac{1}{E_g^\Gamma(P,T)+\Delta_0}\right)}, \tag{2}$$

where $E_P^\Gamma = 7.51\,\text{eV}$, denotes the energy associated with the matrix element of the momentum, $\Delta_0 = 0.341\,\text{meV}$, indicates the splitting in energy due to spin-orbit interaction and $E_g^\Gamma(P,T)$ is the energy gap under the application of hydrostatic pressure which is given at the Γ point by [28,29]

$$E_g^\Gamma(P,T) = E_g^\Gamma(0,T) + bP + cP^2, \tag{3}$$

where P in kbar, $b = 10.7\,\text{meV}\cdot\text{kbar}^{-1}$, $c = -3.77\cdot10^{-5}\,\text{eV}\cdot\text{kbar}^{-2}$ and

$$E_g^\Gamma(0,T) = 1.519 - 5.405\cdot10^{-5}\frac{T^2}{T+204}. \tag{4}$$

In our calculations, a small field like $B = 3\,\text{T}$ is adequate to guarantee a spin-polarized state of the system; consequently the Zeeman term can be disregarded. Therefore, in the symmetric gauge one can rewrite Eq. (1) as

$$\hat{\mathscr{H}} = \sum_{i=1}^{2}\left(\frac{p_i^2}{2m^*(P,T)} + \frac{1}{2}m^*(P,T)\omega^2 r_i^2 + -\frac{1}{2}\omega_c\hat{L}_{i,z}\right) + 2V_0 - \frac{1}{2}m^*(P,T)\Omega^2|\mathbf{r}_1 - \mathbf{r}_2|^2, \tag{5}$$

where

$$\omega = \sqrt{\omega_0^2 + \omega_c^2/4}, \quad \omega_c = \frac{eB}{m^*(P,T)}$$

is the cyclotron frequency of the electron and $\hat{L}_{i,z} = x_i p_{iy} - y_i p_{ix}$, is the angular momentum operator of i-th electron. The Hamiltonian can be solved analytically by presenting the new coordinates for the center of mass and relative motion using the following transformation [30,31]

$$\mathbf{R} = (X,Y) = (\mathbf{r}_1 + \mathbf{r}_2)/2, \quad \mathbf{P} = (P_X, P_Y) = \mathbf{p}_1 + \mathbf{p}_2,$$
$$\mathbf{r}_{12} = (x_{12}, y_{12}) = \mathbf{r}_1 - \mathbf{r}_2,$$
$$p_{12} = (p_{12,x}, p_{12,y}) = (\mathbf{p}_1 - \mathbf{p}_2)/2. \tag{6}$$

Now the Hamiltonian of Eq. (5) can be decomposed into two familiar parts through the use of the raising and lowering operators for both the center of mass motion $(A^\pm, B^\pm)$ and the relative motion $(a_{12}^\pm, b_{12}^\pm)$ and they were chosen in a way that suits the problem as follows [31]:

$$A^\pm = \frac{2\omega m^*(P,T)(X \mp iY) \mp i(P_X \mp P_Y)}{\sqrt{8\hbar\omega m^*(P,T)}},$$
$$B^\pm = \frac{2\omega m^*(P,T)(X \pm iY) \pm i(P_X \pm P_Y)}{\sqrt{8\hbar\omega m^*(P,T)}}, \tag{7}$$
$$a_{12}^\pm = \frac{\omega m^*(P,T)(x_{12} \mp iy_{12}) \mp i(p_{12,x} \mp p_{12,y})}{\sqrt{4\hbar\Omega_0 m^*(P,T)}},$$
$$b_{12}^\pm = \frac{\omega m^*(P,T)(x_{12} \pm iy_{12}) \mp i(p_{12,x} \pm p_{12,y})}{\sqrt{4\hbar\Omega_0 m^*(P,T)}},$$

where $\Omega_0^2 = \omega^2 - 2\Omega^2$. We assume that $\omega_0 = \frac{\Omega}{\sqrt{2}_0}$, to ensure that the electrons are trapped within the quantum dot no matter how the strength of the magnetic field is, in other words $\Omega_0 > 0$. These ladder operators fulfill many commutation relations, for example $[A^-, A^+] = 1 = [B^-, B^+]$,

$[A^{\pm}, B^{\pm}] = 0 = [A^{\pm}, a_{12}^{\pm}]$ and $[a_{12}^{-}, a_{kl}^{+}] = [b_{12}^{-}, b_{kl}^{+}] = c_{12kl}$, where c_{12kl} is given by

$$c_{12kl} = \begin{cases} -2, & l = 1 \text{ and } k = 2, \\ -1 & l = 1 \text{ and } k \neq 2, \\ 0, & k, l \neq 1 \text{ and } k, l \neq 2, \\ 1, & l \neq 2 \text{ and } k = 1, \\ 2, & l = 2 \text{ and } k = 1. \end{cases} \quad (8)$$

Therefore, the Hamiltonians of the center of mass and relative motion respectively are as follows

$$\mathscr{H}_{cm} = \left(\hbar\omega - \frac{1}{2}\hbar\omega_c\right)A^+A^- + \left(\hbar\omega + \frac{1}{2}\hbar\omega_c\right)B^+B^- + \hbar\omega, \quad (9)$$

$$\mathscr{H}_{\text{rel}} = \frac{1}{4}\left[2V_0 + (2\hbar\Omega_0 - \hbar\omega_c)a_{12}^+a_{12}^- + (2\hbar\Omega_0 + \hbar\omega_c)b_{12}^+b_{12}^- + \hbar\Omega_0\right]. \quad (10)$$

Therefore, one can calculate the total ground state energy at a strong magnetic field as follows [30]

$$E = 2V_0 + \hbar\omega + 2\hbar\Omega_0 - \frac{1}{2}\hbar\omega_c. \quad (11)$$

Also in the case of independent electrons, the total ground state energy becomes [32,33]

$$E = 3\hbar\omega - \frac{1}{2}\hbar\omega_c. \quad (12)$$

In the next section, the dependence of the ground state energy on the pressure and temperature will be discussed in the presence of harmonic e-e interaction incorporating the effects of the magnetic field and dot size. Moreover, the parameters of harmonic interaction were also justified.

3. Results

Our analytical calculations were performed for GaAs quantum dot using its characteristic parameters: electron effective mass $m^* = 0.067m_0$ calculated at $T = 0$ K and $P = 0$ kbar where m_0 is the bare mass of an electron, effective Bohr radius $a_B^* = 9.8$ nm and effective Rydberg constant $R_y = 5.85$ meV. It is worth noting that the electron-electron interaction has been modeled by the harmonic interaction potential that depends on two characteristic parameters V_0 and Ω, whose values were chosen by matching our results for the ground state energy dependence on the magnetic field with the exact diagonalization results of M.K. Elsaid et al. [14]. By choosing $V_0 = 5.1$ meV, $\Omega = 6.5$ meV and $R = 1.25a_B^*$, we find that there is a fairly accurate agreement obtained between our results and the exact diagonalization results in Fig. 3 and Fig. 4 of Ref. [14].

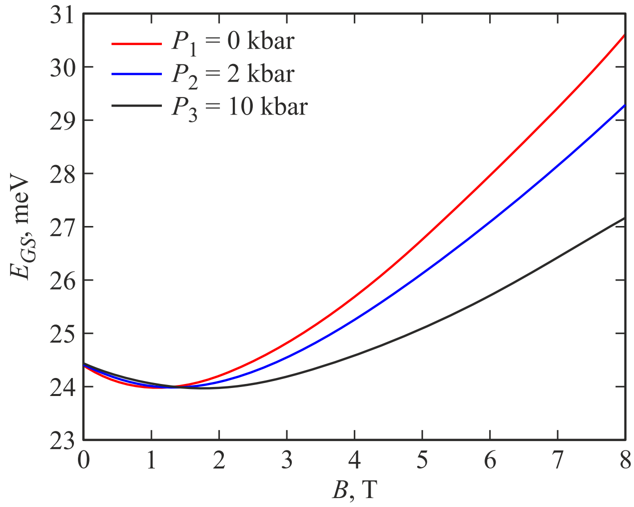

Figure 1. The ground state energy vs the magnetic field for GaAs QD at $T = 0$ K with dot size $R = 1.25a_B^*$, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV for different values of hydrostatic pressure ($P = 0$, 2 and 10 kbar).

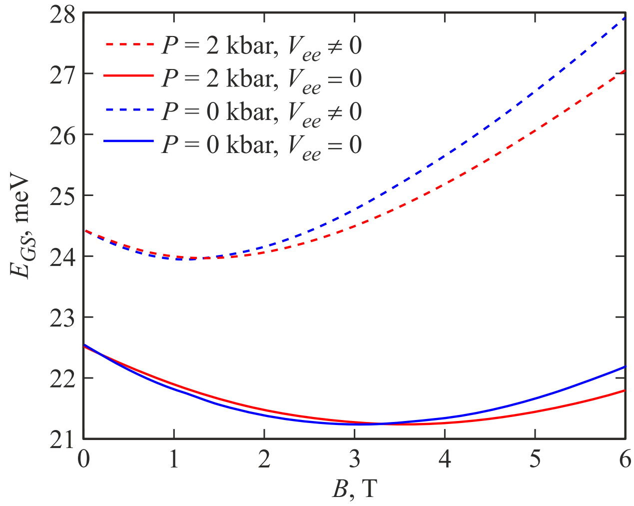

Figure 2. The ground state energy vs the magnetic field for GaAs QD with dot size $R = 1.25a_B^*$C, $T = 0$ K, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV.

Fig. 1 presents the variation of the ground state energy (E_{GS}) of GaAs QD with the magnetic field for dot size $R = 1.25a_B^*$ and temperature $T = 1$ K for three values of static pressure: $P = 0$, 2 and 10 kbar. It is noted that for $B < 2T$, the ground state energy becomes insensitive to the pressure while for $B > 2T$, the effects of pressure becomes tangible and the ground state energy of a QD increases noticeably. This is due to the decrement of the effective separation of two electrons as the magnetic field increases (effect of magnetic confinement), and this increases the interaction energy $(V_{ee} \approx -m^*(P, T)\Omega^2 r^2)$, which leads to an increase in the total ground state energy of the system. Moreover for a fixed magnetic field value the (E_{GS}) shows a significant decrease as the hydrostatic pressure increases. This signalizes that the wave function of the electron is highly localized within the quantum dot due to an increment in the pressure. It is also evident that the slope of the curves depends on the hydrostatic pressure, i. e., the smaller the hydrostatic pressure is, the larger the slope of the curves will be, and in the weak magnetic field region, the ground state energy becomes insensitive to the change in the hydrostatic pressure. These results show that the ground state energy depends strongly on the magnetic field as well as the pressure.

In Fig. 2 the effect of the harmonic e-e interaction on the ground state energy of the GaAs QD is investigated as a function of a magnetic field incorporating the effects of hydrostatic pressure. We present the results for two different cases–one with $V_{ee} = 0$, another with $V_{ee} \neq 0$. As expected, in the presence of e-e interaction, the ground state energy of the QD is significantly greater than the case in its absence as the magnetic field increases. This is a consequence of the increase in the magnetic confinement on the electrons. Also, in the case of interacting electrons, the application of hydrostatic pressure i. e. $P = 2$ kbar decreases the ground state energy in the high magnetic field region, while for independent electrons, the pressure effect on the ground state energy is almost ignorable regardless the magnetic field value. The decrease in the ground state energy with the application of pressure can be attributed to the change in the parameters of the quantum dot as follows: when the pressure increases for a fixed magnetic field value, the mass of the electron $m^*(P, T)$ increases, resulting in a decrease in the kinetic energy of the electrons, also the harmonic e-e interaction V_{ee} decreases (due to the reduction in the e-e separation) resulting in a decrease in the ground state energy. On the other hand, for $B < 2T$, for interacting electrons, the ground state energy shows insensitivity to pressure. Generally, the ground state energy will be strengthened with the enhancement of the magnetic field and this enhancement is more significant in the case of interacting electrons. Indeed, the presence of e-e interaction with magnetic and geometrical confinements under the application of pressure modifies the energy spectrum of the free electrons. This is to say, the electrons will have a high probability of excitation for higher states when the interaction is present, as a result the ground state energy increases. This behavior is qualitatively consistent with the results in the Ref. [24].

In Fig. 3 we have plotted the ground-state energies for the center of mass and relative motion as a function of the magnetic field for two different cases–one with $P = 0$, another with $P = 2$ kbar. We can notice that the ground state energy of the relative motion enhances noticeably with magnetic field, while it increases slowly for the center of mass motion. Also, the energy of the relative motion is always greater than the energy of the center of mass motion. This is because the interaction effect — as is known — is only visible in the relative motion of the electrons ($\mathscr{H}_{\mathrm{rel}}$), as it was found that the ground state energy decreases with the application of pressure, which means that the application of hydrostatic pressure enhances the interactions between electrons, whereas, the center of mass part $\mathscr{H}_{cm}$ is governed by the magnetic confinement and the parabolic confinement potential, hence there is a competition between them. One can realize that for weak confinement ($R = 1.25a_B$), the magnetic confinement effect on the ground state energy wins over as the magnetic field increases result in a decrease of the ground-state energy for the center of mass motion. We also find that, the pressure exerts a tangible effect on the ground state energy of a relative motion and the relative motion brought the largest contribution to the total ground state energy. On the other hand, the ground state energy of the center of mass motion shows pressure insensitivity. Thereby, as a first approximation, the ground-state properties of our system can be scrutinized using the Hamiltonian of the relative motion. Moreover, the ground state energy increases approximately as a quadratic function of the magnetic field; this is due to the presence of the B^2 term in the relative Hamiltonian.

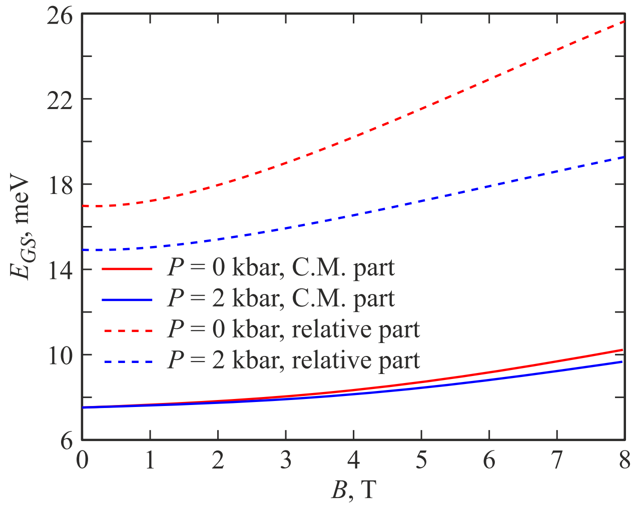

Figure 3. The ground state energy for the center of mass (c.m) and relative part of the Hamiltonian *vs* the magnetic field for GaAs QD with dot size $R = 1.25a_B^*$, $T = 0$ K, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV.

The variation of the total ground state energy with temperature for different values of pressure is shown in Fig. 4. It is evident that the energy enhances slightly linearly with temperature when the applied pressure is very low ($P = 0$ kbar) while at high-pressure value ($P = 10$ kbar) the effect of the temperature on the ground state energy becomes intangible. This behavior is qualitatively consistent with the results in the Ref. [34]. Furthermore, for a fixed value of temperature, it can be seen that the energy increases as the pressure decreases. The linear behavior of the energy is attributed to the changes in the kinetic energy and the harmonic interaction energy that result from the

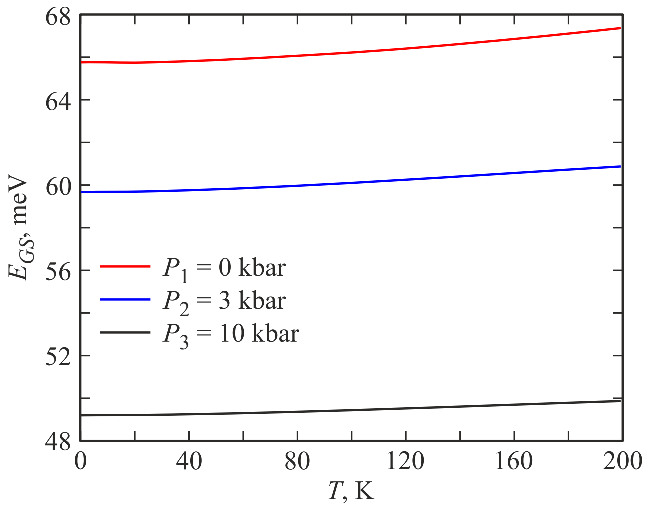

Figure 4. The ground state energy *vs* the temperature for GaAs QD with dot size $R = 1.25a_B^*$, $B = 2T$, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV.

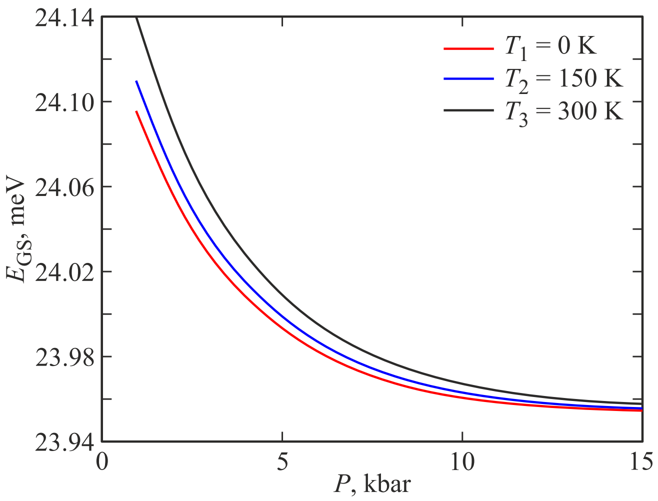

Figure 5. The ground state energy *vs* the temperature for GaAs QD with dot size $R = 1.25a_B^*$, $B = 2T$, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV.

increase in the effective mass of the electron due to the increase in the pressure. This linear relationship indicates that the system is operating under hydrostatic pressure and temperature can be used to adjust the output of the optoelectronic devices without adjusting the geometrical size of the QD. Also, it can be seen that when the temperature is applied, its effect is mostly seen on the ground state energy in the absence of the external hydrostatic pressure. This is to say, the effect of temperature remains less important compared to the effects of magnetic field and hydrostatic pressure.

Fig. 5 displays the dependence of the total ground state energy on the pressure for three values of temperature ($T = 0$, 150 and 300 K) with magnetic field strength $B = 2T$ and dot radius $R = 1.25a_B$. It is clear that the variation of the ground state energy with temperature being less prominent. For fixed value of pressure, the ground state energy decreases smoothly as the temperature decreases. Moreover, it decreases as the pressure increases. The physical interpretation of this behavior is related to the effect of the harmonic repulsion interaction in the system since the effective mass increases as the pressure increases results in a reduction in both the kinetic energy $(-\frac{\hbar^2}{2\mu^*}\nabla^2)$ and harmonic interaction energy $(-\frac{1}{2}\mu^*(P,T)\Omega^2r^2)$ of the system. Moreover, we have noticed that the effect of pressure on energy is more pronounced than the temperature, also due to the enhancement of the harmonic repulsion interaction; this is explained by the effect created by the hydrostatic pressure added to the geometrical confinement. From Figs 4 and 5, the effects of pressure and temperature on the energy have reverse effects.

The variation of the ground state energy with the dot radius for three different values of pressure ($P = 0$, 2 and 10 kbar) is presented in Fig. 6. The energy was computed in unit of effective Rydberg energy, $R_y = 5.85$ meV at $T = 0$ K. The figure shows two important features: The first is that in the case of strong confinement ($R < 10\,\text{nm} \cong a_B^*$), the energy shows a strong dependence on the pressure. The largest contribution to the ground state energy comes from the geometrical confinement and that the parabolic potential overcomes the magnetic confinement. Secondly is that in the case of weak confinement ($R > 10$ nm), the pressure effect on the energy becomes weaker as the radius of the QD increases. With an insight into the energy curves, we notice that it converges to the bulk value of the semiconductor material, i.e., $E_{GS} = 1R_y$ for the large QDs. Moreover, for a fixed value of the dot radius, a decrement in pressure results in an increment in the ground state energy. This can be explained as follows: an increment in pressure causes the wave function

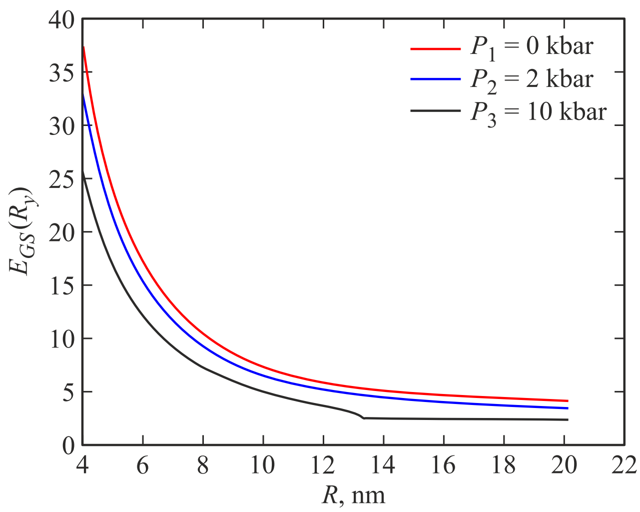

Figure 6. The ground state energy *vs* the dot radius for GaAs QD at $T = 0$ K, $B = 2T$, $\Omega = 5.1$ meV and $V_0 = 6.4$ meV.

of the electrons to shrink, thereby reducing the interaction between them, so the ground state energy decreases. This result indicates that, there is a competition between the geometrical confinement and the one created by the application of the magnetic field or the pressure. The variation of energy with dot radius is a well-known feature in literature [35].

On the other hand, there is a competition between the geometrical confinement and the one created by the application of the magnetic field or the pressure.

4. Conclusion

In this study we have investigated analytically the influence of the hydrostatic pressure and temperature simultaneously on the ground-state energy for two-electron parabolic GaAs QD in the presence of a magnetic field by means of effective mass approximation. We have presented the calculations using Johnson−Payne potential as a model for the e-e interaction. We have analyzed the dependence of the ground state energy on the confinement frequency and magnetic field. It was found that the ground state energy enhances with magnetic field and the pressure effects become pronounced as the magnetic field increases. Also, a decrement in pressure leads to an increment in ground state energy. This is because applying pressure causes a modification in the effective-mass of the electron. Moreover, the well-known enhancement behavior of the ground state energy with the magnetic field was achieved in the presence of e-e interaction. The results showed that the ground state energy of the interacting electrons decreases with increasing pressure and the pressure effect disappears for a weak magnetic field, while the effect of the pressure increment on the energy becomes less pronounced in the case of independent electrons. Also we have found a distinctive feature of this work which is that, the largest contribution to the ground state energy of the system is caused by the relative motion of electrons, and the increase in pressure significantly reduces it with the increase in the magnetic field, while the effect of pressure was almost not appreciable on the motion of the center of the mass. Furthermore, we studied how the ground state energy depends on the radius of the QD under pressure, and the results are as follows: (i) for a strong confinement, the ground state energy depends on pressure noticeably. (ii) for a weak confinement, the effect of pressure on the ground state energy is intangible. However, the ground state energy approaches the bulk value of the semiconductor material as the dot radius continues to increase. Finally, our results also showed that the ground state energy is insensitive to temperature change, as it increases very slightly linearly with the increase in temperature.

In general, this work may have merits in developing semiconductor devices. A key property of QDs is the emission of photons under excitation. The photon emission wavelength depends not only on the material but on the QD size. The ability to precisely control the size of a QD thus enables a manufacturer to tune the wavelength of emission over a wide range of wavelengths. This feature plays an important role in the manufacture of optoelectronic devices under the simultaneous effect of both pressure and temperature so that the operating output can be controlled without the need to adjust the geometrical size of the QD.

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