Optical and electronic properties of a two-dimensional quantum dot with an impurity

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Abstract

The binding energy and photoionization cross-section (PCS) in a two-dimensional pseudopotential, parabolic potential plus an inverse squared potential, quantum dot (QD) with a donor impurity subjected to a uniform magnetic field directed with respect to the z-axis have been investigated within the compact-density matrix formalism. The dependence of these optical properties on the confinement frequency of the parabolic potential, on the magnetic field and on the external field is studied in detail. Moreover, take into account the position-dependent effective mass and dielectric, the dependence of PCS on the dot radius is investigated. The results reveal that the binding energy and the PCS in a two-dimensional pseudopotential QD have been strongly affected by these factors, and the position effect also plays an important role in the PCS of the pseudopotential QD. In addition, the red-shift (blue-shift) of the PCS is found in this system because of the decreasing (increasing) energy difference between the final and initial states.

1. Introduction

Great success has been achieved in nanofabrication techniques in the past decades [1–3], especially for the low-semiconductor systems, such as superlattices, quantum well, quantum dots and quantum wires. Nowadays, more and more attention has been put on the studies of those systems, and a great deal of experimentations and theoretical works are performed for the purpose of elucidating the physics of these systems [4–10]. The main reasons are as follows: firstly, the low-dimensional quantum systems can cause more obvious nonlinear optical effects than bulk materials; secondly, the nonlinear optical properties have a wide range of potential applications for high-speed electro-optical modulators, far infrared photodetectors, lefthanded materials, semiconductor optical amplifiers and so on [11]. With the advance of the science and technology, much important information has been found with the effect of the external probes [12–15], for instance, the applied electric field, the magnetic field, hydrostatic pressure and temperature and the impurity and so on. Effects of laser radiation on optical properties of disk shaped quantum dot in magnetic field were studied by Prasad and Silotia [16], with the results that the absorption coefficient depends on the optical wave and the strength of the static magnetic field. Philips et al. [17] have reported the photoluminescence study of self-organized InAlAs QDS under pressure.

The effect of pressure and temperature on impurity in a spherical GaAs quantum dots has been studied by Perez-Merchancano et al. [18]. Moreover, not only the pressure and temperature effect, but also the exciton effect has important effect on the optical properties, so amount of the previous works have investigated the excitonic transition and other optical properties in low-dimensional systems [19–21]. On the other hand, the pseudopotential also makes significant contributions to the research of the low dimensional systems [22,23]. For example, optical properties of a donor impurity in a two-dimensional quantum pseudodot have been studied by Wenfang Xie [24], and the result shows that the optical properties of a donor impurity in a two-dimensional pseudoharmonic QD are strongly affected by the zero point of the pseudoharmonic potential, the chemical potential of the electron gas and the Coulomb interaction. In addition, the pseudopotential was applied for interpreting some results from experiments with great success. In the present work, we will focus on studying the binding energy and the photoionization cross-section in a two-dimensional QD with an impurity in the presence of the pseudopotential of a donor impurity in a two-dimensional quantum pseudodot. We present a theoretical investigation of the quantum pseudodot with the effects of the external field, confinement potential and magnetic field.

2. Model and calculations

Let us consider a hydrogenic impurity confined by a QD with a two-dimensional pseudoharmonic potential, subjected to a static...
magnetic field $B$ along the $z$-direction. Within the effective mass approximation, the Hamiltonian of this system can be written as

$$H = \frac{1}{2m^*} \left( \mathbf{p} + e \mathbf{A} \right)^2 + V(r) \frac{e^2}{\epsilon r^2},$$

(1)

where $m^*$ and $e$ are the effective mass and charge, respectively. $\epsilon$ is the dielectric constant, $\mathbf{A} = A_x \mathbf{e}_x + A_y \mathbf{e}_y + A_z \mathbf{e}_z$ is the vector potential of static magnetic field $V(r)$ is pseudopotential which includes parabolic potential and inverse squared potential. It is given as follows [25]:

$$V(r) = \frac{1}{2} m^* \omega_0^2 r^2 + \frac{\hbar^2}{2m^*} \beta^2 r^2 \cdot$$

(2)

where $\omega_0$ denotes the confinement frequency and the dimensionless parameter $\beta$ characterizes the strength of the external field with $\beta \geq 0$ in the present work [11,25].

When without the Coulomb interaction, the Schrödinger equation in plan polar coordinate of this system has the form

$$\left[ -\frac{\hbar^2}{2m^*} \frac{\partial^2}{\partial r^2} + \left( \frac{\hbar^2}{m^*} \omega_0^2 + \frac{\hbar^2}{m^*} \beta^2 \right) r^2 + \frac{1}{2} m^* \omega_0^2 \right] \psi^0 = E^0 \psi^0, \quad$$

(3)

where $\omega_0 = \sqrt{\omega_0^2 + \omega_r^2}/4$ is the total confinement frequency in the magnetic field, $\omega_r = eB/m^*c$ is the cyclotron frequency. $L_z$ is the orbital angular momentum along the $z$ direction, $E^0$ and $\psi^0$ are the energy eigenvalue and eigenstate of the QD with a two-dimensional pseudoharmonic potential without the effect of the impurity, respectively. The two-dimensional eigenfunctions and energy spectrum without the Coulomb interaction can be given by the Refs. [11,25]. Taking into account the Coulomb interaction, the trial function of the electron confined in two-dimensional pseudoharmonic QD with a hydrogenic impurity can be obtained with the help of the variational approach, written as

$$\psi(r, \varphi, z) = N \psi^0(r, \varphi) e^{-\alpha r}$$

$$= Ne^{-\alpha r} N_0 r^{(l+1)/2} \Gamma(l + n + 1) / \Gamma(l + 1) \Gamma(-n, L + 1; r^2) e^{i m \varphi}, \quad$$

(4)

where $N$ is the normalization constant, $N_0 = \sqrt{n! \pi \Gamma(l + n + 1)}$ and $L = \sqrt{m^2 + \beta^2}$, $n$ and $m$ are main quantum number and magnetic number, respectively. $\alpha$ is the variational parameter. The impurity ground state energy is obtained with respect to the minimum of $\alpha$, as given as follows:

$$E_i = \langle \psi(r, \varphi, z, \alpha) | H | \psi(r, \varphi, z, \alpha) \rangle / \langle \psi(r, \varphi, z, \alpha) | \psi(r, \varphi, z, \alpha) \rangle, \quad$$

(5)

where $\alpha_{\text{min}}$ is the value of $\alpha$ corresponding to the minimum of $E_i$. The impurity binding energy is defined as

$$E_B = E^0 - E_i. \quad$$

(6)

In the dipole approximation, the expression of the photoionization cross-section associated with an impurity, starting from Fermi’s golden rule in the well-known dipole approximation, can be obtained by [26,27,29]

$$\sigma(h\omega) = \left( \frac{F_{\text{eff}}}{F_0} \right)^2 \frac{4 \pi^2 \tau_0 \omega_0}{n_i} \left( \frac{m^*}{m_0} \right)^2 \sum_{T} \frac{\langle \psi_{f} | \mathbf{r} - \mathbf{R} | \psi_{i} \rangle^2 \delta(E_f - E_i - h\omega)}{\pi (E_f - E_i - h\omega)^2 + (h\Gamma_f)^2}, \quad$$

(7)

with

$$\delta(E_f - E_i - h\omega) = \frac{1}{\pi} \frac{(h\Gamma_f)^2}{(E_f - E_i - h\omega)^2 + (h\Gamma_f)^2}, \quad$$

(8)

where $n_i$ is the refractive index of the semiconductor, $\alpha_{\text{fs}} = e^2/\hbar c$, the fine structure constant, and $h\omega$ the photon energy, $F_{\text{eff}}/F_0$ is the ratio of the effective electric field $F_{\text{eff}}$ of the incoming photon and the average field $\overline{z}_0$ in the medium [30], $\overline{z}$ is the light wave polarization vectors. The effective field ratio $F_{\text{eff}}/F_0$ may be very large for strongly localized states, but for typical shallow donors with wave functions over many lattice sites, it is quite difficult to calculate $F_0$. Therefore the ratio $F_{\text{eff}}/F_0$ has generally been treated as an adjustable parameter to fix the absolute values of $\sigma$. It is clear that this factor does not affect the shape of the photoionization cross-section. In this work, the ratio is taken to be approximately equal to unity [28]. $\langle \psi_{f} | \mathbf{r} - \mathbf{R} | \psi_{i} \rangle$ is the matrix element between the initial and final states of the dipole moment of the impurity. $\Gamma_f$ is the hydrogenic impurity linewidth and taken as 0.1R$_e$.

### 3. Results and discussions

In this paper, the ground binding energy and PCS in a two-dimensional GaAs QD with an impurity in the presence of the pseudopotential, parabolic potential plus an inverse squared potential, subjected to the uniform magnetic field directed with respect to the $z$-axis have been numerically investigated. The physical parameters for calculations are used as follows [29,31]: $n_i = 3.2$, $\Gamma_f = 0.1R_e$, and $m^* = 0.067m_0$, where $m_0$ is the free electronic mass. The results of our calculations are presented in
In Fig. 1, we present the results for the binding energy of a donor impurity in the GaAs pseudopotential QD as a function of the confinement strength $\omega_0$, for several values of the magnetic field $B$, when $\beta = 0.5$. From this figure, it can be clearly seen that the binding energies are monotonic functions of $\omega_0$, for each $B$, the binding energy is monotonously increased by increasing confinement strength. This physical behavior can be explained as that the increasing $\omega_0$ will lead to an increment of the geometrical confinement in the radial direction. Consequently there is an enhancement of the Coulomb interaction, which results in the enhancement of the binding energy of the two-dimensional GaAs pseudopotential QD. On the other hand, it is noted that the binding energies are increased by the increasing magnetic field $B$ because the carrier is much more confined along the axis of the dot. Moreover, the bending is found in the line for each $B$, and this bending is larger for lower magnetic field values. The physical origin is that the lower one makes more contributions to the radial localization of the impurity. So it is concluded that the magnetic field plays an important role in the studies of the optical properties of the GaAs pseudopotential QD.

In Fig. 2, the binding energies are displayed as a function of the confinement strength $\omega_0$ for the three different values of the applied magnetic field $B$ with $\omega_0 = 1.0 \times 10^{13}$ s$^{-1}$ and $\beta = 0.5$. The binding energies are enhanced by the increasing confinement strength just as shown in Fig. 1. And also, one can observe that the binding energies are increased by the increasing $\beta$. The physical origin for this behavior is that $\beta > 0$ represents repulsive potential, so the increase of $\beta$ strengthens the quantum confinement [11]. As a result, the Coulomb interaction is enhanced. In addition, it should be noted that with the increase in $\omega_0$, the curves corresponding to different values of the external field come close to each other, because the radial quantization becomes significantly stronger than the magnetic one. Obviously, the ground binding energy is greatly affected by the external field. Due to the important role the external field has played in the studies of pseudopotential QD, the effects of $\beta$ on the optical properties should be taken into consideration in optical experiments and application. The PCS is always thought to be another important parameter in optical properties studies of QDs.

In Fig. 3, we present the PCS of a donor impurity in the pseudopotential QD as a function of the incident photon energy $\hbar \omega_0$ in the case of parallel polarization of the incident radiation for different values of the confinement frequency. The magnetic field is set $B = 2$ T, and the external field is set $\beta = 0.5$. From this figure,
it can be easily observed that the PCS is not monotonic functions of $\hbar \omega_0$. For each $\omega_0$, the PCS as a function of $\hbar \omega_0$ has a prominent peak at some position because of the one-photon resonance enhancement. And when the magnitude of $\hbar \omega_0$ is larger than 300 meV, all the PCS will be quite slowly decreased as $\hbar \omega_0$ further increases. Additionally, it is found that the PCS is remarkably decreased by the increasing confinement frequency $\omega_0$. The physical explanation for this physical behavior is that the increase of $\omega_0$ gives rise to an enhancement of the confinement strength, which leads to an enhancement of the binding energy. As a result, PCS is reduced. Moreover, the increase of the $\omega_0$ shifts the peak position of the corresponding PCS to higher frequencies. It indicates a strong confinement-induced blue-shift of a resonance in pseudopotential QDs. This physical behavior originates from an augment of the energy difference between the energy levels with the enhancement of $\omega_0$. So it can be concluded that the PCS of the pseudopotential QD is strongly dependent on the confinement frequency.

Fig. 4 shows the PCS of a donor impurity as a function of the incident photon energy $E_0$ for different values of the magnetic field $B$ with $\omega_0 = 1.0 \times 10^{13}$ s$^{-1}$ and $\beta = 1.0$. The effect of $B$ on the optical properties has been clearly shown in this figure. It can be noted that the PCS is significantly increased with the increase of $B$. This feature can be explained as follows: the resonant peaks of PCS are dependent not only on the dipole transition matrix element but also on the energy internal $E_0$. According to the total confinement frequency $\omega_1 = \omega_0^2 + \omega_c^2/4$, increasing $B$ makes positive contribution to the total confinement frequency $\omega_1$, which arises the enhancement of the PCS in the two-dimensional pseudopotential QD with the effect of the impurity. On the other hand, it is noted that the peak positions move toward the higher energy regions with the enhancement of the strength of magnetic field. The physical reason for this important feature is that as $B$ increases, the quantum confinement of the electron becomes stronger, which results in an increase of the energy interval. Thus, the resonant peaks of the three absorption coefficient above move toward higher energy regions.

Fig. 5 displays the PCS of a donor impurity as a function of the incident photon energy $E_0$ for different values of the external field $\beta$ with $\omega_0 = 1.0 \times 10^{13}$ s$^{-1}$ and $B = 2.0$ T. In this figure, the influence of $\beta$ on the optical properties has been clearly shown. With the increase of $\beta$, the PCS is obviously decreased. The physical origin is that the dipole transition matrix element becomes much larger as $\beta$ increases. Also, one can find that, with the enhancement of $\beta$, the resonant peaks of the PCS exhibit a red-shift. This is due to the fact that, with increasing $\beta$, the energy interval $E_0$ becomes small because of the remarkable influence of the orbital magnetic moment of the electron states. So that, in order to get larger PCS, one should reasonably choose the value of the strength of the external field $\beta$.

It is well known that the effective mass and dielectric are strongly affected by the position of the electron. The relationship between them has been reported by Peter et al. \[32,33\] as follows: for the effective mass $1/m(r) = 1/m^0 + (1 - 1/m^0) \exp(-x/r)$, where $r$ denotes the dot radius, and $\xi$ is a constant which is chosen to be 0.01 a.u.; for the dielectric, $1/e(r) = 1/e_0 + (1 - 1/e_0) \exp(-r/\gamma)$, where $e_0$ is the static dielectric constant of GaAs and $\gamma$ is the screening constant, taken to be 1.1 a.u. By using these expressions, it can be easily explained that there is no appreciable change of the effective mass (dielectric) for a large dot radius, which is to say that the mass (dielectric) variations are unimportant for large dots. Taking into account the position-dependent effective mass and dielectric, the PCS is plotted in Fig. 6 as a function of the incident photon energy $E_0$ for the three different values of dot radius with $\omega_0 = 1.0 \times 10^{13}$ s$^{-1}$, $B = 2.0$ T and $\beta = 1.0$. From Fig. 6, it can be seen that the PCS is clearly decreased with decreasing dot radius $r$.

This physical feature can be explained as that, the smaller the dot radius is, the stronger the confinement strength is, since the size quantization on the radial direction becomes stronger when the QD radius at low values, which more greatly affects the effective mass and the dielectric of the electron. So it is indicated that the PCS is strongly dependent on the position of the electron. So it is concluded that the mass and dielectric variation with position plays an important role in the two-dimensional pseudopotential QD with the effect of the donor impurity.

4. Summary

In this paper, we have presented a detail investigation of the binding energy and PCS in a pseudopotential, parabolic potential plus an inverse squared potential, QD subjected to a uniform magnetic field directed with respect to the $z$-axis within the framework of effective-mass approximation. The dependence of the binding energy and PCS on the confinement frequency of the parabolic potential, on the magnitude of the magnetic field and on the external field has been investigated. Also, it is found that the dot radius has important effects on the PCS in the two-dimensional pseudopotential QD. The results show that the binding energy is an increasing function of the confinement frequency of the pseudopotential. Moreover, the binding energy can also be strengthened with the effects of the applied magnetic field and the external field. On the other hand, the PCS is obviously enhanced by the increasing magnetic field, external field and the dot radius, respectively. Furthermore, the increasing magnetic field can give rise to blue-shift, while the increasing external field can give rise to red-shift due to the effects of them on the energy difference. In general, the binding energy and PCS have strong dependence on these physical parameters. The present results are useful for further understanding the other optical properties of the pseudopotential, parabolic potential plus an inverse squared potential, QD, and we hope that this theoretical study can make a significant contribution to experimental studies and practical applications.

Acknowledgments

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References