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Energy and binding energy of donor impurity in quantum dot with Gaussian confinement

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ABSTRACT

Using the method of the shifted 1/*N* expansion, we investigate the problem of hydrogenic-like donor impurity, located at the center of a spherical semiconductor quantum dot. We have calculated the energy eigenvalues for both ground and first excited sates under the assumption of Gaussian confining potential. The binding energies for three dimensional (3D) and two dimensional (2D) quantum dots are calculated. We show their dependence on dimensionality, dot radius and potential confinement. Our present numerical results show quantitative and qualitative very good agreement with those results obtained by diagonalization, Numerov's integration, and Hartree–Fock methods.

1. Introduction

Advances in modern technology of semiconductor physics has allowed to reduce the effective dimension from three-dimensional bulk materials to quasi-zero dimensional quantum dot structures, where carries confinement can be made by artificial potentials at the nano scale limit in all the three spatial directions (three-dimensional quantum dot) and in two spatial directions (two-dimensional quantum dot). Therefore, energy in such structures is discrete, as in the natural atoms and it depends strongly on its size. Quantum dot structures have attracted considerable attention both experimentally and theoretically [1–12].

Impurities play an essential role in the semiconductor physics, where their presence can dramatically change electronic, optical and transport properties of quantum devices [13]. The Schrödinger equation for the hydrogenic impurity has been solved exactly [14–17]. Zhu et al. [14,15] solved the finite potential well for impurity in the center of spherical quantum dot SQD and obtained the exact solutions by using the method of series expansion. Chuu et al. [16] studied the hydrogenic impurity state energies using exact solution of the Hamiltonian for quantum dots and quantum wires by means of Whittaker function and scattering Coulomb wave function. The fine structure of the energy levels for hydrogenic impurity located in the center of a spherical quantum dot was calculated using exact solution for finite potential well [17]. Gharaati and Khordad used a modified Gaussian potential to calculate energy levels for spherical quantum dot within effective mass approximation [18].

The *variational* approach has been also used to calculate the binding energies of hydrogenic impurity in quantum dot [19–21]. The binding energies were calculated for shallow donors and acceptors in a spherical GaAs-$Ga_{1-x}Al_xAs$ quantum

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dot for both a finite barrier and an infinitely high barrier [19]. The screened donor energies in spherical quantum dot under parabolic potential were studied [20]. Porras-Montenegro and Perez-Merchancano [21] used the variational approach within the effective-mass approximation to calculate the binding energies of hydrogenic impurity in quantum dot. Boda et al. [22] investigated the Gaussian confinement of hydrogenic donor impurity by a very simple variational wave function.

The *perturbative* approach was also used to calculate the binding energies in quantum dot structures. The binding energies of the ground and a few higher exited states for both infinite and finite potential wells as a function of well width and barrier height is calculated using a strong perturbation method within the effective-mass approximation [23]. Bose and Sarkar [24–26] used perturbation method to calculate the energy levels and binding energies of a shallow hydrogenic impurity in SQD with different potential confinement shapes.

In this paper we shall apply the shifted $1/N$ expansion proposed by Sukhatme and Imbo [27,28] to calculate the spectra of an electron and a donor in quantum dots. It is a powerful tool of solving the Schrödinger equation for spherical symmetric potentials [29–32]. Also, it is non-perturbative and can hence be used in problems which do not necessarily involve small coupling constant. It is simple and gives accurate eigenvalues without dealing with wave function of a particle. It was extended successfully to relativistic potentials [33–36]. In this approach, the calculations are carried out for states with arbitrary quantum numbers (the principal and orbital quantum numbers n and ℓ, respectively) using forth-order perturbation theory in the shifted expansion parameter $1/\overline{k}$, where $\overline{k} = N + 2\ell - a$. Here N is the number of spatial dimensions and (a) is a suitable shift parameter which will be discussed later.

The shifted $1/N$ expansion has already been used to study various systems, such as two-dimensional magnetoexcitons [37], shallow donor impurities [38], two-electron spherical quantum dot [39], and two interacting electrons in two-dimensional quantum dots with the presence of magnetic field [40].

This paper is organized as follows. In Section 2, we state the Hamiltonian of donor impurity centered at quantum dot and formulate the shifted $1/N$ expansion method for a symmetric attractive Gaussian potential $V(r)$. In Section 3, we present the numerical energy states and binding energies calculations for hydrogenic donor impurity in both two-dimensional 2D (circular) and three-dimensional 3D (spherical) quantum dots. Finally, the conclusions are provided in Section 4.

2. Theory and method of calculation

Within the framework of an effective-mass approximation, the standard Hamiltonian of an electron in the presence of a hydrogenic donor located at the center of a quantum dot can be written as follows:

$$H_0 = -\nabla^2 - \frac{2w}{r} + V(r) \tag{1}$$

where r represents the position coordinate of the electron, $r = (x,y)$ and $r = (x,y,z)$ for the 2D and 3D systems, respectively. The second term is the coulomb interaction between the donor electron and the hydrogenic nucleus, $w = 0$ or 1 refers the absence or presence of donor atom, respectively. $V(r)$ being the confinement potential.

The confinement potential $V(r)$ is assumed to be in the form of a symmetric attractive Gaussian potential and given by [41]

$$V(r) = -V_0 \exp(-r^2/2R^2) \tag{2}$$

where V_0 the depth of the potential well. R is the range of the confinement potential, which corresponds to the radius of the QD. This model potential is a good qualitative appropriate and realistic one due to its finite depth and continuity at the QD boundaries. Also, it goes smoothly to zero as $r \to \infty$. The Gaussian potential has a parabolic shape near the quantum dot center $(\frac{r}{R} \ll 1)$; $V(r) = -V_0 + V_0 \frac{r^2}{2R^2} = -V_0 + \frac{1}{2} m\omega_0^2 r^2$, ω_0 is the frequency of the harmonic oscillator. By comparison, we get $\omega_0^2 = \frac{V_0}{mR^2} = \frac{2\lambda V_0}{m}$, which gives the Gaussian exponent $\lambda \equiv \frac{1}{2R^2}$ [42].

Following the work of Imbo et al. [28] using $1/N$ expansion method, we begin step by step calculations by formulating the radial Schrödinger equation for an arbitrary spherical potential $V(r)$ as

$$\left(\frac{-\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{(k-1)(k-3)\hbar^2}{8mr^2} + V(r)\right)\psi(r) = E\psi(r) \tag{3}$$

where $k = N + 2\ell$. N being the number of spatial dimensions, $\ell(\ell + N - 2)\hbar^2$ being the eigenvalue of the square of the N-dimensional orbital angular momentum.

In terms of the shifted variable $\overline{k} = k - a$ (a is a shifted parameter), we rewrite Eq. (3) as [28]

$$\left(\frac{-\hbar^2}{2m^*}\frac{d^2}{dr^2} + \overline{k}^2\left(\frac{\hbar^2[1-(1-a)/\overline{k}][1-(3-a)/\overline{k}]}{8m^*r^2} + \frac{V(r)}{Q}\right)\right)\psi(r) = E\psi(r) \tag{4}$$

where Q is a constant which rescales the potential (in large $\overline{k}$ limit) and will be determined below. The energy eigenvalues are given by an expansion in powers of $1/\overline{k}$.