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RENORMALIZED SCHRODINGER EQUATION FOR EXCITON GROUND STATE IN A SPHERICAL QUANTUM DOT

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ABSTRACT

We calculate the exciton ground state energy in a spherical quantum dot using a trial function taken as the product the exact ground state wave function of the uncoupled electron and hole with an unknown function that describes the confinement of the relative electron-hole separation. The one-dimensional Schrödinger-type equation is deduced by using variational principle. The results of calculation of the exciton ground state energy in a spherical quantum dot as functions of the dot radius for rectangular and parabolic confinement potential shapes are presented.

INTRODUCTION

Recent progress [1] in nanometer technology has made possible the fabrication of new types semiconductor structures, such as quantum wells (QW), well wires (QWW) and dots (QD), whose characteristic dimensions become comparable to the de Broglie wavelengths of free carriers. The theoretical analysis of the electronic properties these systems in the past decade have attracted a great deal of attention [2-4]. It has been found that the electron and hole mobility in these structures can be restricted in varies directions and the space dimensionality can be reduced from three up to zero in QD. A strong quantum-confinement effect produced in these structures increases highly electron-hole Coulomb interaction, the excitons, confined in QD becomes more stable and can be present at room temperature in both absorption and emission spectra. There fore, many novel devices using excitonic transitions in QD can be proposed. Although many theoretical studies have been devoted to excitonic states in QW [2], QWW [3] and quantum disk [4], up to we know only one paper [5,6] in spherical QD, considering the infinite barrier model. In this paper, we present the general method to calculate the ground state energy of an exciton in QD, suitable for models both with infinite and finite electron and hole barriers.

THEORETICAL MODEL

Within the framework of the effective-mass approximation the dimensionless Hamiltonian of exciton in a spherical GaAs-(Ga, Al)As QD can be written as [2]:

$$H = H_e(r_e) + H_h(r_h) - 2/r_{eh};$$
$$H_e(r_e) = -\eta_e \Delta_e + V_e(r_e); \quad H_h(r_h) = -\eta_h \Delta_h + V_h(r_h) \qquad [1]$$

where $H_e(r_e), V_e(r_e)$ and $H_h(r_h), V_h(r_h)$ are one-particle Hamiltonians and confining potentials for uncoupled electron and hole respectively. In this work we

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consider two different models of the isotropic confinement: 1) rectangular: $V_i(r_i)=0$ for $r_i < R_0$ and $V_i(r_i)=V_0^{(i)}$ for $r_i > R_0$, and 2) $V_i(r_i)=0.5\,r_i^2/R_0^2$, where $i=e,h$. The dimensionless parameters η_e and η_h are related in (1) with the electron m_e, hole m_h and reduced μ masses by means of relations: $\eta_e=\mu/m_e\,;\eta_h=\mu/m_h\,;\quad \mu=m_e m_h/(m_e+m_h)$. The effective Bohr radius $a_0^*=\varepsilon\hbar^2/\mu e^2$ as the unit of length and the effective Rydberg $Ry^*=e^2/2a_0^*\varepsilon$ as the energy unit are used in (1). The Schrödinger equation for coupled electron-hole pair with the Hamiltonian (1) cannot be solved exactly and therefore we propose for a ground exciton state a trial function as a product of the one-particle electron and hole ground state wave functions with unknown function $\Phi(r_{eh})$, that depends only on the hole-electron separation r_{eh}:

$$\psi\,(r_e\,,r_h\,,r_{eh}\,)=\,f_e\,(r_e\,)f_h\,(r_h\,)\Phi\,(r_{eh}\,) \qquad [2]$$

where $f_e(r_e)$ and $f_h(r_h)$ are well-known solutions of the Schrödinger equation for spherical QW with rectangular or parabolic potentials:

$$[-\eta_i\Delta_i+V_i(r_i)]f_i(r_i)=\varepsilon_i\,f_i(r_i);\quad i=e,h \qquad [3]$$

In the trial function (2) the confinement of the electron and hole are described by two firsts factors meanwhile the last one takes into account the electron-hole interaction. The wave function (2) have a structure similar to one proposed by Bastard [7], with the difference that we do not restrict the unknown function $\Phi(r)$ by one particular function class (exponential, gaussian, etc.) but assume that it can be any function from a total L_2 metric space. One can deduce a differential equation for the best function $\Phi(r)$ in this space that minimize the total energy

$$E[\Phi]=\frac{\langle f_e(r_e)f_h(r_h)\Phi(_{eh}\,r)|H\,|\,f_e(r_e)f_h(r_h)\,\Phi(_{eh}\,r)\rangle}{\langle f_e(r_e)f_h(r_h)\Phi(r_{eh})|\,f_e(r_e)f_h(r_h)\Phi(r_{eh})\rangle} \qquad [4]$$

considering $E[\Phi]$ as a functional whose value depends on the function $\Phi(r)$. Substituting (6) in (7) and taking into account the relations (4) and (5) one can obtain the explicit expression for $E[\Phi]$,

$$E[\Phi]=\varepsilon_e+\varepsilon_h+\int_0^\infty S(r_{eh})\left[\left(\frac{\partial\Phi}{\partial r_{eh}}\right)^2-\frac{2}{r_{eh}}\Phi^2\right]dr_{eh}\Bigg/\int_0^\infty S(r_{eh})\Phi^2 dr_{eh} \qquad [5]$$

Where

$$S(r) = 8\pi^2 r \int_0^\infty r_e f_e^2(r_e) dr_e \int_{|r_e - r|}^{r_e + r} r_h f_h^2(r_h) dr_h \qquad [6]$$

The last summand in Eq. (5) describes the lowering of the uncoupled electron energy in cylindrical QWW due to bounding with ion. This lowering depends on choice of de function $\Phi(r)$ and attains a minimum value for a function $\Phi(r)$ for which the variational derivative $\delta E[\Phi]/\delta\Phi$ is equal a zero. Following the standard procedure of the calculus of variations one can demonstrate that $E[\Phi]$ defined by (5) has a minimum value for a function $\Phi(r)$, which is the solution of the Schrödinger-type equation for central-force problem corresponding to the lowest eigenvalue E_h,, Φ is the solution of the following Schrödinger-type equation corresponding to the lowest eigenvalue E_b:

$$-\frac{1}{S(r_{eh})}\frac{d}{dr_{eh}}\left[S(r_{eh})\frac{d\Phi}{dr_{eh}}\right] + -\frac{2}{r_{eh}}\Phi = E_b\Phi; \quad E = \varepsilon_e + \varepsilon_h + E_b \qquad [7]$$

where E and E_b are the exciton total and binding energies respectively.

RESULTS AND DISCUSSION

In order to evaluate the function $S(r)$ defined by the relation (6) we need an effective numerical method with high accuracy. For a given set of the material parameters the values of this function have been evaluated numerically, stored in the computer and approximated by B-spline functions. Furthermore, by using this approximation for $S(r)$ we solve numerically the equation (7) by means of the trigonometric sweep procedure [8]. The results of calculation of the binding energy vs. QD radius for the model of the $GaAs/Ga_{0.7}Al_{0.3}As$ and $GaAs/Ga_{0.45}Al_{0.3}As$ with rectangular confining potential and for parabolic QDs are presented in Fig. 1.

From the Figure it is seen the difference between curves for the rectangular and parabolic confining potential. In first case the binding energy attains a maximum value with decreasing QD radius. This result can be ascribed to the effect of the wave function leakage into barrier region when the QD's size becomes less than a critical value. In contrast for parabolic QD this effect does not appear due to infinite barrier height.

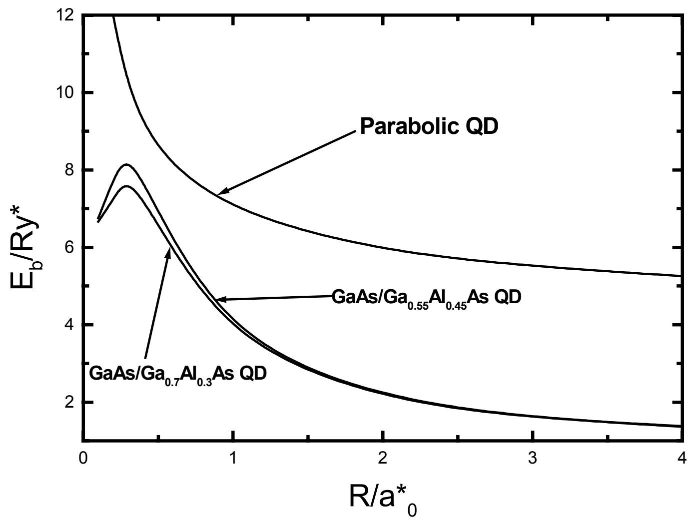

Fig.1. The exciton binding energy as function of the QD radius for the models with rectangular and parabolic confining potentials

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