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EXCITON BINDING ENERGY IN SYMMETRICAL STEP QUANTUM WELLS

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ABSTRACT

We consider a double-step potential model that consist of a narrow well imbedded inside of a large well, which is produced by a symmetrical structure of $GaAs/Ga_{1-x}Al_xAs/Ga_{1-y}Al_yAs$. The exciton trial function is taken as a product of the ground state wave functions of both the unbound electron and hole in the heterostructure, with an arbitrary correlation function that depends only on electron-hole separation. A renormalized Schrödinger equation for the correlation function, which coincides with one for a hydrogen atom in an effective isotropic and non-homogeneous space, is deduced. Ground state binding energies as a function of the external well width are calculated for an exciton in this heterostructure by using the trigonometric sweep method. Two peaks in the binding energy curves associated with the wave function leakage into the inner and outer barrier region are obtained. In the particular case of the single well, our results are in a good agreement with previous variational calculations and available experimental data.

INTRODUCTION

In the past decade, the effect of the dimensionality reducing on the neutral and charged excitons ground state binding energy in quantum wells (QWs) has attracted considerable attention. Many variational calculations of the ground and first excited states energies for exciton in QWs with rectangular and parabolic confining potential have been performed by using a trial functions with one, two or more variational parameters [1-7]. To obtain the exciton binding energy with reasonable accuracy this method generally implies tedious calculations. In the paper [8] it has been proposed as alternative a simple fractional-dimension approach, in which the problem for exciton confined in QW is reduced to the hydrogen problem in effective isotropic homogeneous space with non-integer dimension. Later it has been proposed [9] the numerical procedure that permits to find the dimension of this effective space.

These approaches can be improved by considering an effective space in which the dimension depends on the electron-hole separation, varying from three-dimensional for very small electron-hole distance to two-dimensional as it becomes very large. In this work by using the method of functional derivation we deduce a wave equation for the electron-hole correlation function of an exciton confined in a QW which describes the hydrogen problem in an isotropic effective space with variable dimension. We found an explicit expression for the volume measure function of this space that provides a simple algorithm for calculating the exciton ground state binding energy in a QW with arbitrary shape of confining potential. In this way, we analyze an exciton in a symmetrical heterostructure which consists of a narrow well imbedded inside of a large well.

THEORY

Within the isotropic effective mass approximation the dimensionless Hamiltonian for a correlated electron-hole pair in a QW can be written as [2]

$$H = \eta_e \nabla_e^2 + V_e(z_e) + \eta_h \nabla_h^2 + V_h(z_h) - 2/r \ , \ r = |\mathbf{r}_e - \mathbf{r}_h| \qquad [1]$$

where m_e^*, m_h^* and $V_e(z_e), V_h(z_h)$ are the effective masses and potential profiles for the electrons and holes, respectively, $\eta_e = \mu/m_e^*$, $\eta_h = \mu/m_h^*$ and μ is the reduced mass of the exciton. All lengths in the Hamiltonian (1) have been scaled in terms of the exciton Bohr radius $a_0^* = \varepsilon \hbar^2/\mu e^2$ and the energies in the exciton Rydberg $Ry^* = e^2/2\varepsilon a_0^*$.

To calculate the exciton ground state energy, we choose a trial wave function as

$$\Psi(\mathbf{r}) = f_e(\mathbf{r}_e) f_h(\mathbf{r}_h) \Phi(r_{eh}) \qquad [2]$$

where r_{eh} is the distance between the electron and hole, $f_e(\mathbf{r}_e)$ and $f_h(\mathbf{r}_h)$ are the ground state wave function of the unbound electron and hole confined in the QW, respectively, which are solution of the eigenvalue problem

$$\left[\eta_i \nabla_i^2 + V_i(z_i)\right] f_i(\mathbf{r}_i) = E_i f_i(\mathbf{r}_i); \quad (i = e, h) \qquad [3]$$

with E_e (E_h) being the unbound electron (hole) lowest energy in the QW. Φ is an unknown function to describe the electron-hole correlation, which is assumed to depend only on the electron-hole separation. The exciton ground state energy, E can be found by minimizing the functional: $F[\Phi] = \langle f_e f_h \Phi | H - E | f_e f_h \Phi \rangle$ taking the functional derivative with respect to Φ one can obtain the Euler-Lagrange equation:

$$-\frac{1}{S_0(r)} \frac{d}{dr}\left[S_0(r) \frac{d\Phi(r)}{dr} \right] - \frac{2}{r}\Phi(r) = -E_b \Phi(r), \ E_b = E_e + E_h - E \qquad [4]$$

where E_b is the ground state binding energy of the exciton in the QW, and S_0 is a volume measure function in an isotropic and non-homogeneous given space. So is interpreted as a relative radial probability distribution (unnormalized) for the uncorrelated electron-hole pair in the QW,

$$S_0(r) = \overline{|f_e(\mathbf{r}_e)|^2 |f_h(\mathbf{r}_h)|^2} = \iint_{|\mathbf{r}|=r} |f_e(\mathbf{r}_e)|^2 |f_h(\mathbf{r}_h)|^2 \, d\mathbf{r}_e d\mathbf{r}_h \qquad [5]$$

Equations (4) and (5) describe the problem of a hydrogen atom in a space with variable dimension D^*. The relation between the volume measure function (5) and the fractal dimension [10] is given by the formula $S_0(r) \approx r^{D^*(r)-1}$. As the electron-hole distance is

very small the integral (5) is proportional to r^2 and the effective space is three-dimensional. As the electron-hole distance increases its wave functions in the well interfaces vanishes and the wave function flux remains only through the spherical band within the well. $S_0(r)$ increases in this case with the sphere radius growth linearly, that corresponds to two-dimensional effective space. In our problem is necessary interchange $\mathbf{r}_i$ for the z variable in Eq. (5),

$$S_0(r) = r \int_{-\infty}^{+\infty} f_e^2(z_e)\, dz_e \int_{z_e - r}^{z_e + r} f_h^2(z_h)\, dz_h \qquad [6]$$

In our numerical procedure we first solve Eq. (3) separately for an electron and hole by using the trigonometric sweep method [7]. We calculate $S_0(r)$ from Eq. (6) and afterward we solve Eq. (4) by means of the trigonometric sweep method.

RESULTS AND DISCUSSION

To check the accuracy of our method, first we calculate the binding energies for the ground state of an exciton in a square-well GaAs/$Ga_{0.7}Al_{0.3}As$ QW, as a function of the well width. Our results in Fig. 1 (lower curve) are in agreement with those obtained in Ref. [5] (solid circles).

The insignificant discrepancy between our results and the previous variational calculations can be ascribed to the fact that in Ref. [5] it was taken into account the anisotropy of the hole mass, whereas we have assumed for simplicity an isotropic model.

Also, in Fig. 1 shows the results of the calculation of the exciton ground state binding energy in a $Ga_{0.55}Al_{0.45}As/Ga_{0.8}Al_{0.2}As/GaAs/Ga_{0.8}Al_{0.2}As/Ga_{0.55}Al_{0.45}As$ heterostructure with a double-step confining potential which consists of a small rectangular well (of length L_1) inside a large one (of length L). Following Greene and Bajaj [1, 2], we use the empirical formula $\Delta E_g = 1.155x + 0.37x^2$ [eV] to determine the energy-band-gap, with 60% and 40% of ΔE_g the contribution corresponding to the conduction and valence bands discontinuity, respectively. The confinement potential is defined as, $V(z) = 0$ for $|z| < L_1/2$; $V(z) = V_1$ for $L_1/2 < |z| < L/2$; and $V(z) = V_2$ for $|z| > L/2$, where V_1 and V_2 are the values of the potential barriers determined by the *Al* concentrations 0.8 and 0.45, respectively.

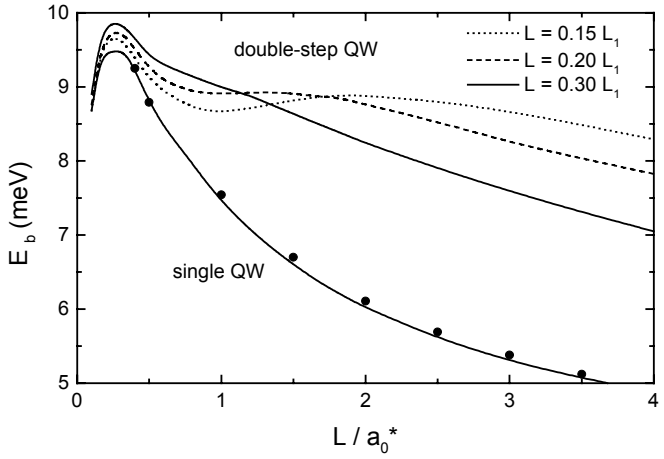

Figure 1. Exciton ground state binding energies as a function of the well width in the following semiconductor heterostructures: (i) a $GaAs/Ga_{0.8}Al_{0.2}As/Ga_{0.55}Al_{0.45}As$ double-step QW (upper curves) and for several values of the internal well width L_1; (ii) a square-well $GaAs/Ga_{0.7}Al_{0.3}As$ QW (lower curve).

The existence of two peaks in the curves of the binding energy for $L = 0.15L_1$ and $L = 0.20L_1$ can be attributed to the leakage the compressed exciton wave function into exterior region that in this structure is realized in two stages: for large well from the internal well to external one and afterwards for small well width from the external well into barrier region. The leakage of the exciton wave function into exterior regions provides a sharp increasing of the electron-hole separation and a noticeable diminishing of the binding energy. As the well width becomes very small the exciton energy level is pushed up into the exterior barrier region and 3D character of the exciton wave function is restored, meanwhile E_b begins to fall up to the correspondent bulk value.

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