Quasi-bound states in Kane type semiconductor quantum dots

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In the present study, it is considered that a A^3B^5 type spherical semiconductor quantum dot surrounded by a very thin insulating spherical layer is placed in an another A^3B^5 type semiconductor region. It is assumed that the δ -type potential barrier for the very thin insulating spherical layer has a radius of a. By using Kane Hamiltonian, it is investigated the scattering resonances of electrons which are scattered from the boundary of the semiconductor dot. By using the continuity conditions for the wave functions and flux discontinuous at the boundary of the semiconductor quantum dot, we have analytically calculated the phase shift and the partial cross section for the scattering of electrons. It has been shown that the quasi-bound states appear as peaks in the cross section.

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1. Introduction

In recent years, there have been intensive studies in connection with features of quantum nanostructures such as quantum wells, wires and dots [1]. Electrons traversing through ultra-small semiconductor microstructures give rise to a fascinating regime of quantum transport [2]. When the system size is reduced to near or below the mean free path of charge carriers, a variety of phenomena associated with quantum interference can be easily observed. These include the study of the universal conductance fluctuations in the mesoscopic regime [3], the Aharonov-Bohm effects [4], the quenching of the quantum Hall effects [5], and the junction resonances [6]. Interference of the ballistic charge carriers in one-dimensional (1D) rings formed by two quantum wires in the self-ordered silicon quantum wells was investigated [7].

Recent progress on the synthetic chemistry of semiconductor nanocrystals has made it possible to access high quality semiconductor nanocrystals with controlled size, shape and optical properties. Current technologies can be used to fabricate quantum dots of various types, including both core–shell ones [8] and those embedded in a matrix made of a different semiconductor material. It has been shown experimentally that core–shell quantum dots can be effectively used in biology and medicine [9–11]. Core–shell quantum dots are primarily used for in vivo imaging and identifying living cells. Core–shell quantum dots have a nanometer sized semiconductor core coated with a thin layer of a shell material. The carrier spectrum in such a dot strongly depends on the core radius and the thickness of the coating shell. The scattering of two dimensional massless Dirac electrons was investigated in presence of a random array of circular mass barriers. The differential and total cross section, the inverse momentum relaxation time and the perpendicular component of resistivity were also calculated [12].

By using the one-band effective mass approximation model, the optical properties of the spherical shaped CdSe/ZnS and CdSe/ZnSe core–shell quantum dots were computed. A theoretical analysis of the radiative recombination lifetime of core-shell quantum dots has been presented and discussed [13]. The interband optical absorption and Stark shift in the ensemble of InSb spherical quantum layers were investigated. Calculations were carried out for both, the cases of parabolic and Kane's dispersion laws [14]. Barrier penetration through a square potential barrier and a step potential barrier was studied in the framework of the eight-band Kane Hamiltonians [15]. It is well known that during the scattering on a spherical cavity of radius R, the resonant states occur for the electrons with narrow energy bands around the zeros of the denominator of phase shift [16]. The exact solution of the Schrödinger equation was made for 1D well formed by a repulsive delta barrier in front of an impenetrable well, and the relation between scattering resonances and exponential decay from the well was also obtained [17]. An attractive delta potential has been used as a barrier to study resonance phenomena in scattering theory [18]. Hernandes et al. [19] investigated a one channel model with a double pole δ-barrier potential and showed that a double pole of the S-matrix can be induced by tuning the parameters of the model.

The energy spectrum is parabolic only in the A^3B^5 type semiconductors near the bottom of their conduction band. In the majority of other substances, non-parabolicity of the energy spectrum plays an important role. The

experimental advantages of using narrow-gap semiconductors for the reduced dimensionality make it necessary to take into account the real band structure of materials. While considering the non-parabolicity of the electron dispersion in narrow and medium gap semiconductors the coupling of conduction and valance bands should be taken into account. This is the purpose of our work.

In this paper, the electron scattering problem was investigated for a δ-type potential barrier in A^3B^5 type semiconductors using three-band Kane model, and calculated the cross section to demonstrate how possible the quasi-bound states reveal themselves in the scattering cross section. By using the method in refs. [16]-[18], positions of resonant states were obtained and energies of quasi-bound states were calculated for the InAs/Insulator/InSb nanosystem.

2. Theory

The model which is considered in the present study consist of an open spherical quantum dot which is a semiconductor sphere (i.e., InAs type semiconductor as labelled B) and has a radius a. It is surrounded by a very thin insulating spherical layer and placed in an another semiconductor region (i.e., InSb type semiconductor as labelled A).

In the first step, it is assumed that an electron with an energy *E* travels from outer of the quantum dot through the inner part of the quantum dot. We treat the thin insulating spherical layer as a δ-type potential at $r=a$, $U(r)=U\,a\,\delta(r-a)$, where $\delta(r-a)$ is the Dirac delta function .

The theory of quantum structures has been built within the single-band effective mass approximation. However, this is invalid for narrow-gap semiconductors, where the electron effective mass is small. We use the Kane zone structure model (which takes into account the interaction of the conduction band and three hole bands) in the spherical approximation. For the 3-D electron, the Kane Hamiltonian [20] in spherical coordinates is

$$\left\{-\frac{\hbar^2}{2m(\varepsilon)}\Delta_3-\varepsilon+Ua\delta(r-a)\right\}\Psi(r,\theta,\phi)=0\,, \quad (1)$$

where Δ_3 is three-dimensional Laplacien and $m(\varepsilon)$ represents the electronic effective mass in nonparabolic approximation and given by

$$\frac{\hbar^2}{2m(\varepsilon)}=\frac{P^2}{3}\frac{3\varepsilon+3E_g+2\Delta}{\left(\varepsilon+E_g\right)\left(\varepsilon+E_g+\Delta\right)}, \quad (2)$$

where P is the matrix element accounting for the interaction between the conduction band and the valence band. The matrix element P is expressed in terms of the effective mass at conduction band bottom and other parameters (E_g is the band gap and Δ is the spin-orbit splitting energy of the valence bands) and given by

$$\frac{P^2}{3}=\frac{\hbar^2}{2m_n}\frac{E_g(E_g+\Delta)}{(3E_g+2\Delta)}\,, \quad (3)$$

[21]. The Schrödinger equation may be factorized so that its solutions becomes

$$\Psi(r,\theta,\phi)=\frac{\chi_l(r)}{r}Y_{lm}(\theta,\varphi) \quad (4)$$

where $Y_{lm}(\theta,\varphi)$ are spherical harmonic functions [16]. The radial equation found to satisfy the following differential equation:

$$\left\{\frac{d^2}{dr^2}-\frac{l(l+1)}{r^2}+\frac{2m(\varepsilon)}{\hbar^2}\left(\varepsilon-Ua\delta(r-a)\right)\right\}\chi_l(r)=0 \quad (5)$$

For $l=0$, at the origin fixes the interior solution to

$$\chi_0(\rho)=\sin(k_Br)\,. \quad (6)$$

The solution for the outer part is

$$\chi_0(\rho)=A\sin\left(k_Ar+\delta_0\right) \quad (7)$$

where δ_0 is phase shift and

$$k_i=\sqrt{\frac{3}{P^2}\frac{\varepsilon(\varepsilon+E_{g_i})(\varepsilon+E_{gi}+\Delta_i)}{(3\varepsilon+3E_{gi}+2\Delta_i)}}\,, \quad (8)$$

We have imposed the wave function is continuous at $r=a$ and first derivative is discontinuous at $r=a$. Thus, we have

$$\chi_{a+}(a)=\chi_{a-}(a) \quad (9)$$

$$\frac{1}{m_A(\varepsilon)}\frac{d\chi_{a+}}{dr}-\frac{1}{m_B(\varepsilon)}\frac{d\chi_{a-}}{dr}=\frac{2}{\hbar^2}Ua\chi(a) \quad (10)$$

where indices ± indicate limit from right and left. For the determine the phase shift and amplitude, we use the boundary conditions (9)-(10), and we get

$$Cot\delta_0=\frac{1+Cot\left(z_A\right)\cdot\left(\frac{\Omega}{z_A}d+Cot\left(z_B\right)\cdot\frac{z_B}{z_A}\cdot\frac{m_A(\varepsilon)}{m_B(\varepsilon)}\right)}{Cot\left(z_A\right)-\frac{\Omega}{z_A}d-Cot\left(z_B\right)\cdot\frac{z_B}{z_A}\cdot\frac{m_A(\varepsilon)}{m_B(\varepsilon)}}\,, \quad (11)$$

$$A=\frac{\sin\left(z_B\right)}{\sin\left(z_A+\delta_0\right)}\,, \quad (12)$$

where we defined dimensionless parameters:

$$d=\frac{\left(\varepsilon+E_{gA}\right)\left(\varepsilon+E_{gA}+\Delta_A\right)}{3\varepsilon+3E_g+2\Delta_A}\frac{3E_{gA}+2\Delta_A}{E_{gA}(E_{gA}+\Delta_A)} \quad (13)$$

$$\Omega=\frac{2m_{nA}Ua^2}{\hbar^2},\ z_A=k_Aa,\ z_B=k_Ba. \quad (14)$$

Ω characterizes the penetrability of the barrier. The value $\Omega\to\infty$ corresponds to a completely impenetrable barrier, while the value $\Omega=0$ corresponds to the case of complete penetration, or the absence of any scatter.

The scattering matrix S_0, written as a function of the phase shift δ_0, is

$$S_0=Exp[2i\delta_0]=\frac{1+i\tan\left(\delta_0(\varepsilon)\right)}{1-i\tan\left(\delta_0(\varepsilon)\right)}, \quad (15)$$

[18]. Resonant states are represented by the poles of scattering matrix:

$$1-i\tan\left(\delta_0(\varepsilon)\right)=0. \quad (16)$$

With this exact expression of the phase shift $\delta_0(E)$ we can locate the position of its complex poles

$$\varepsilon=\varepsilon_r-i(\Gamma/2), \quad (17)$$

where Γ is the width of the quasi-bound states.

The analytical expression for the amplitude is obtained by using Eqs. (9)-(10)

$$A=\left[\left\{\frac{\Omega}{z_A}d\sin\left(z_B\right)+\frac{z_B}{z_A}\cdot\frac{m_A(\varepsilon)}{m_B(\varepsilon)}\cdot\cos\left(z_B\right)\right\}^2+\sin^2\left(z_B\right)\right]^{1/2}. \quad (18)$$

Now we shall study the evolution of a wave coming out from the quantum dot, with solution given by

$$\chi_0(\rho)=A_1\sin(k_Br). \quad (19)$$

The solution for the outer part is

$$\chi_0(\rho)=\sin\left(k_Ar+\delta_0\right), \quad (20)$$

Then, when $A_1=1/A$, the phase shift will the same as before.

For $l=0$, the partial cross section σ_0 becomes

$$\sigma_0=\frac{4\pi}{k_A^{\,2}}\sin^2\delta_0. \quad (21)$$

E may be performed from the δ_0 curve as a function of the energy of the incident particle.

3. Results and discussion

It is presented a numerical example for the InAs/insulator/InSb nanosystem. It is used the values of the effective mass of electrons $m_B=0.025m_0$ and $m_A=0.016m_0$ for InAs and InSb, respectively, where m_0 is the mass of free electron. The values of the band gaps ε_g and spin-splitting Δ for InAs and InSb are selected $E_{gB}=0.42eV$, $\Delta_B=0.34eV$, $E_{gA}=0.23eV$, $\Delta_A=0.9eV$, respectively [22]. The inner radius was taken as $r=100A^\circ$.

In Fig. 1, the dependence of the amplitude on the electron energy is shown for the value of the dimensionless parameter, $\Omega=30$. The curves for the amplitudes of electrons through the outer part (from the semiconductor B to the semiconductor A) and coming from the outer part (from the semiconductor A to the semiconductor B) are labeled as "1" and "2", respectively. As it is seen from Fig. 1 the amplitude of the electron coming from the inner part is zero for particular values of energy. The amplitudes of the electrons coming from the outer part are maximum at those particular values of energy. These energy values are the energies of quasi-bound states. The incident wave from semiconductor A may undergo multiple collisions before leaving the well. When this happens the duration time of the electron in the well increases and quasi bound sates occurs [23, 24]. If the energy of the electron coming from the outer part is close to the energy of quasi-bound states in the inner part the amplitude of the incident electron will be maximum.

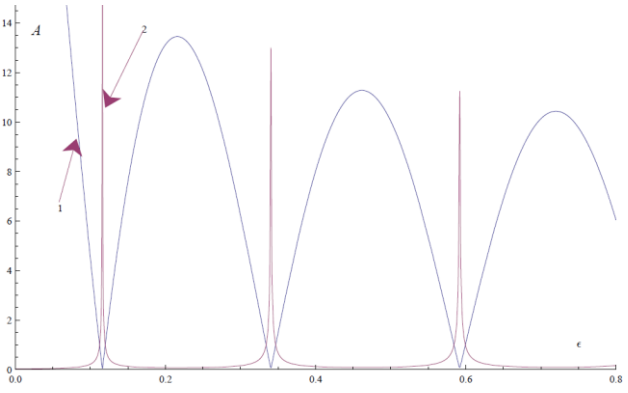

Fig. 1. The amplitude of the wave function for the InAs/insulator/InSb type nanosystem plotted as a functions of the energy for $\Omega=30$.

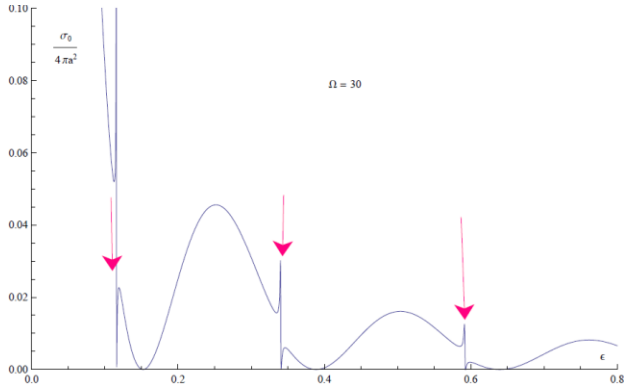

Fig. 2. The scattering cross section $\sigma_0(\varepsilon)$ *for* $\Omega = 30$.

The energy of quasi-bound states with δ-type potential barrier is found by solving Eq.(16). The account for quasi-bound states one normally solves the time-dependent Schrödinger equation which is very complicated problem when compared to the standard eigenvalue problem. Here, we follow the method presented in detail in [18, 20] and calculate the poles scattering matrix. For the InAs/insulator/InSb nanosystem, values of energies of quasi-bounds states and with half width $\Gamma/2$ were calculated as $(\varepsilon, \Gamma/2)$: (0.1159, 0.00012), (0.3403, 0.0005), (0.5918, 0.00066). The positions of the poles in the complex plain are functions of two independent parameters as the radius of quantum dot and the potential barrier strength U.

If the energy of the incident electrons is close to the energy of quasi bound states of electrons in the inner parts, its wave function inside will be strongly coupled with its wave function outside, and the wave function in the inner part will have a large amplitude, resulting in resonance scattering (as seen in Fig. 3).

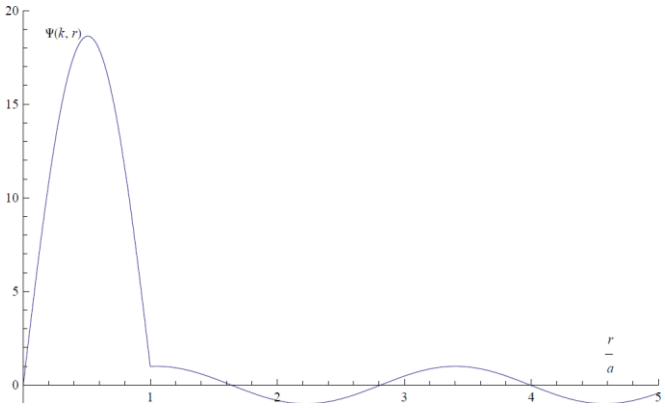

Fig. 3. The scattering wave function as a function of r, evaluated at ε *=0.1159eV. In the inner region, the amplitude of the scattering wave function increases.*

For $\Omega \to \infty$, the resonance levels lie close to the energy eigenvalues of the quantum dot [16]. They therefore are called quasi-bound states of the system. The peaks of amplitude indicate the quasi-bound states. The energy of the quasi-bound states is complex, where the negative imaginary part of the energy becomes small. The positions of poles depend on the potential strength Ω. If Ω is very large but still finite, the dot is penetrable and it has no bound states corresponding to quasi-bound states.

The energies and widths of quasi-bound states cannot be directly measured experimentally, whereas such characteristic as the scattering cross section σ is measurable. Therefore, it makes sense to analyze and clarify the dependence of σ_0 on ε and its features can be used to determine the spectral parameters of quasi-stationary electron states with reasonable accuracy. In order to do this, we must study the properties of the partial cross section σ_0.

The numerical results for the lowest contribution (l=0) to the total cross section as a function of energy are shown in Fig. 2. The vertical arrows indicate the ε values corresponding quasi-bound states. Narrow peaks appear close to the positions of the bound states of the dot that are defined by the equation $sin(z_B) = 0$. A series of narrow resonances is apparent. From the Fig. 1 and Fig. 2, it can be seen that the resonance energies exactly coincide, correspondingly, with the peak positions of the function A(ε) on the energy scale. Off resonance, the wide bumps in the cross section are typical of hard sphere scattering.

4. Conclusion

By using the Kane Hamiltonian, the electron scattering from spherical quantum dot surrounded by the δ-type potential barrier is studied. It was demonstrated that the resonance energies and resonance width of quasi-bound states of electrons in the open quantum dot can be calculated by the complex poles scattering matrix. For the InAs/ınsulator/InSb nanosystem, the energy and the width of the quasi-bound states are calculated by using the scattering matrix.

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