The Energy Spectrum of Carriers between Two Concentric Spheres of Kane-Type Semiconductors

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The electronic states of carriers between two concentric spheres of Kane-type semiconductor are theoretically investigated and compared with the results of the parabolic band approximation. Calculations are performed for a hard-wall confinement potential and the eigenstates and the eigenvalues of the Kane Hamiltonian are obtained. Taking into account the real band structure (strong spin-orbital interaction, narrow band gap), the size dependence of the energy of electrons, light holes, and spin-orbital splitting holes in InSb semiconductor concentric spheres are calculated. According to the obtained results both in parabolic and nonparabolic (Kane model) cases, the electron energy levels come close to each other with the increasing of the radius.

1. INTRODUCTION

In recent years, the optical properties of nanosize semiconductor crystals have attracted the attention of many investigators because of their potential applications [1, 2]. The ability to tune their absorption and photoluminescence spectra over a very wide range of energy, as much as, 1.2 eV, by varying the crystal size opens the opportunity of fabricating nanocrystal-based tunable lasers and light-emitting diodes [3]. The progress in submicrometer technology has made possible the fabrication of new type of semiconductor nanostructures whose characteristics change with respect to the geometry of them as quantum dots, quantum wires, and quantum wells. Energy spectrum of carriers in quantum dots, quantum wires, and quantum boxes was investigated theoretically by many groups [3–6]. In [3], the size dependence of the electron and hole quantum size levels in spherical semiconductor nanocrystals were studied. In that work, an analytical theory of the quantum size levels within a spherical eight-band Pidgeon and Brown model, which takes into account both the coupling of conduction band and valence bands and the complex structure of the valence band in nanocrystals with an infinite potential barrier, was developed. The calculated level structures for narrow-gap InSb, moderate-gap CdTe, and wide-gap CdS nanocrystals were presented. It is shown that a new formalism for determining energy eigenstates of spherical quantum dots and cylindrical quantum wires in the multiple-band envelope-function approximation was described in [4]. The bound states were studied for the conduction band and coupled light and heavy holes, as a function of the radius of the GaAs/Al$_x$Ga$_{1-x}$As quantum dot. Implications of the band-coupling effects for optical matrix elements for quantum wires and dots were discussed. The size dependence of the spectra of free carriers in A^3B^5- and A^2B^6-type semiconductor spherical quantum dots is studied [5]. The advantages of a universal method for obtaining equations that are invariant under the transformations of the rotations groups, is that it directly yields a system of equations for the radial functions for any number of bands considered. A nonsymmetrized 8-band effective-mass Hamiltonian for quantum-dot heterostructures (QDHs) in Burt's envelope-function representation was derived [6]. The 8×8 radial Hamiltonian and the boundary conditions for the Schrödinger equation were obtained for spherical QDHs. Electron and hole energy spectra in three spherical QDHs, HgS/CdS; InAs/GaAs; and GaAs/AlAs, were calculated as a function of the quantum-dot radius within the approximate symmetrized and exact nonsymmetrized 8×8 models. In a study of Alonso et al., a relativistic free particle in a one-dimensional box is studied [7].

In the present study, using three-band Kane's model including the conduction band, light, and spin-orbital splitting

hole bands, the energy spectrum of carriers between two concentric spheres is calculated. The system considered here consists of two concentric spheres, and the carriers are assumed to be between the region of two concentric spheres. The potential of the concentric spheres is taken to be infinitive and consequently the wave functions are taken to be zero at the boundary.

In the three-band Kane's Hamiltonian, the valence and conduction bands interaction are taken into account via the only matrix element P (so-called Kane's parameter). The system of Kane equations including the nondispersional heavy hole bands have the following forms [8, 9]:

$$-EC_1 - \frac{Pk_+}{\sqrt{2}}C_3 + \sqrt{\frac{2}{3}}Pk_zC_4 + \frac{Pk_-}{\sqrt{6}}C_5 - \frac{Pk_z}{\sqrt{3}}C_7 - \frac{Pk_-}{\sqrt{3}}C_8 = 0, \tag{1}$$

$$-EC_2 - \frac{Pk_+}{\sqrt{6}}C_4 + \sqrt{\frac{2}{3}}Pk_zC_5 + \frac{Pk_-}{\sqrt{2}}C_6 - \frac{Pk_+}{\sqrt{3}}C_7 + \frac{Pk_z}{\sqrt{3}}C_8 = 0, \tag{2}$$

$$-\frac{Pk_-}{\sqrt{2}}C_1 - (E + E_g)C_3 = 0, \tag{3}$$

$$\sqrt{\frac{2}{3}}Pk_zC_1 - \frac{Pk_-}{\sqrt{6}}C_2 - (E + E_g)C_4 = 0, \tag{4}$$

$$\frac{Pk_+}{\sqrt{6}}C_1 + \sqrt{\frac{2}{3}}Pk_zC_2 - (E + E_g)C_5 = 0, \tag{5}$$

$$\frac{Pk_+}{\sqrt{2}}C_2 - (E + E_g)C_6 = 0, \tag{6}$$

$$\frac{Pk_z}{\sqrt{3}}C_1 - \frac{Pk_-}{\sqrt{3}}C_2 - (\Delta + E + E_g)C_7 = 0, \tag{7}$$

$$-\frac{Pk_+}{\sqrt{3}} \cdot C_1 + \frac{Pk_z}{\sqrt{3}}C_2 - (\Delta + E + E_g)C_8 = 0. \tag{8}$$

Here P is the Kane parameter, E_g is the band gap energy, Δ is the value of spin-orbital splitting, and $k_\pm = k_x + ik_y$, $\vec{k} = i\vec{\nabla}$, and c_i are envelope functions.

2. CALCULATING THE ENERGY SPECTRUM

Substituting the expressions (3)–(8) into formulas (1) and (2), we obtain

$$\left\{ -E - \frac{P^2}{3}\left[\frac{2}{E + E_g} + \frac{1}{E + E_g + \Delta} \right]\Delta_3 \right\}C_{1,2} = 0, \tag{9}$$

where Δ_3 is three-dimensional Laplacian in spherical coordinates,

$$\Delta_3 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r} \right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta} + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}. \tag{10}$$

In spherical coordinates, the eigenfunction is

$$C_{1,2} = R_{1,2}(r)Y_l^m(\theta,\phi), \tag{11}$$

where l is the orbital quantum number and m is the azimuthal quantum number. The radial function $R_{1,2}(r)$ is found to satisfy the following differential equation:

$$\left\{ \frac{P^2}{3}\left(\frac{2}{E + E_g} + \frac{1}{E + E_g + \Delta} \right) \right.$$
$$\left. \cdot \left(\frac{d^2}{dr^2} + \frac{2}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} \right) + E \right\}R_{1,2}(r) = 0. \tag{12}$$

Equation (12) can be rewritten in the form

$$\left(\frac{d^2}{dr^2} + \frac{1}{r}\frac{d}{dr} - \frac{l(l+1)}{r^2} + \mathcal{X}^2 \right)R_{1,2}(r) = 0, \tag{13}$$

where

$$\mathcal{X}^2 = \frac{3}{P^2}\left(\frac{E(E + E_g)(E + E_g + \Delta)}{(3E + 3E_g + 2\Delta)} \right). \tag{14}$$

The solution of (13) is spherical Bessel's equation and it is given by

$$R_{1,2}(r) = AJ_l(\mathcal{X}_{nl}r) + BN_l(\mathcal{X}_{nl}r), \tag{15}$$

where $J_l(\mathcal{X}_{nl}r)$, $N_l(\mathcal{X}_{nl}r)$ are the spherical Bessel functions of the first and second kinds. Two of the first spherical Bessel functions are as follows [10]:

$$J_0(r) = \frac{\sin r}{r}, \qquad N_0(r) = -\frac{\cos r}{r},$$
$$J_1(r) = \frac{\sin r}{r^2} - \frac{\cos r}{r}, \qquad N_1(r) = -\frac{\cos r}{r^2} - \frac{\sin r}{r}. \tag{16}$$

It is required that the wave function satisfy the following boundary condition:

$$R_{1,2}(R_1) = R_{1,2}(R_2) = 0. \tag{17}$$

Equation (17) yields the following result:

$$J_l(\mathcal{X}_{nl}R_1)N_l(\mathcal{X}_{nl}R_2) - J_l(\mathcal{X}_{nl}R_2)N_l(\mathcal{X}_{nl}R_1) = 0. \tag{18}$$

Equations (14) and (17) together show that the radial eigenvalue spectrum is

$$\left(\frac{E(E + E_g)(E + E_g + \Delta)}{(3E + 3E_g + 2\Delta)} \right) = \left(\frac{z_{nl}^2}{R^2} \right)\frac{P^2}{3}, \tag{19}$$

where z_{nl} is the nth root of (18).

Equation (19) determines the energies of electrons, light holes, and spin-orbital splitting holes in Kane-type semiconductor concentric spheres. It is also useful for analyzing the influence of nonparabolicity on the energy spectrum of carriers in concentric spheres.

In Figure 1, the dependence of $E(R)$ on two cases are presented: (a) electrons with parabolic dispersion law and (b) electrons with Kane's dispersion law for InSb concentric spheres. According to this figure, the energy levels in both cases become close to each other with the increasing of the inner radius R_1. At rather small sizes of R_1, the variance in the electron dispersion laws becomes more and more important, and therefore the curves for $E(R)$ keep away from each other.
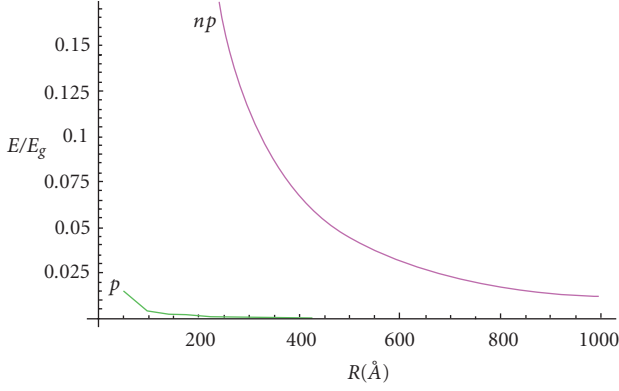
FIGURE 1: Lowest-order energy eigenvalues of electrons as a function of increasing inner radius R_1 for parapolic (p) and nonparapolic (np) dispersion laws.
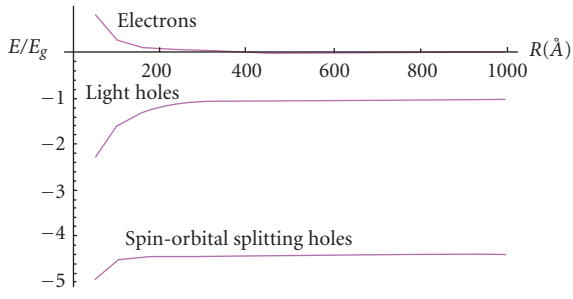

FIGURE 2: The energy spectrum of carriers (electrons, light holes, spin-orbital splitting holes) as a function of the inner radius R_1 in spherical quantum box for InSb.

In Figure 2, the inner radius (R_1) dependence of the energy of carriers is given (electrons, light holes, spin-orbital splitting holes), where $R_2/R_1 = 2$ in nonparabolic dispersion law.

In Figure 3, the dependencies of $E(R)$ of electrons and light holes as a function of inner radius R_1, with R_2 fixed at 400 for nonparabolic dispersion laws, are presented for InSb-type concentric spheres. The energy scale is in units of E_g, E_g is the band gap energy, and the curves are labeled by quantum numbers (ln). According to this figure both in electrons and light holes for a small radius, there is an appreciable separation between states corresponding to different n but equal l quantum numbers.

In the calculations of the carriers energy spectra for narrow gap InSb concentric spheres, we chose the semiconductor band-structure parameters for InSb: energy gap $E_g = 0.2368\,\text{eV}$, spin-orbit splitting is $\Delta = 0.810\,\text{eV}$, the value of the nonparabolicity parameter is $E_P = 23.42\,\text{eV}$ [3].

3. CONCLUSION

The energy spectrum of carriers in InSb concentric spheres is investigated both in parabolic and nonparabolic dispersion laws. It is seen that the energy of electrons in parabolic and
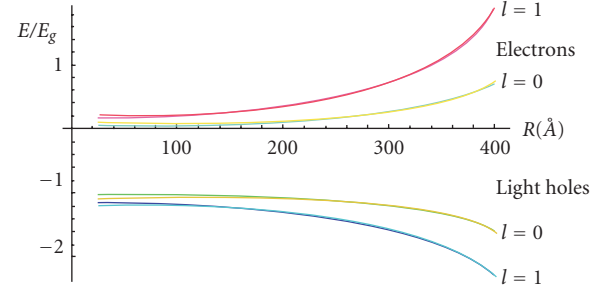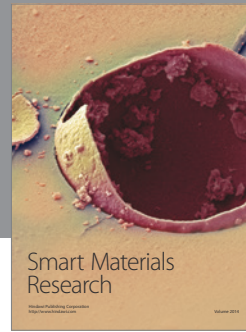

FIGURE 3: Lowest-order energy eigenvalues of electrons and light holes as a function increasing inner radius R_1 and outer radius $R_2 = 500$ for nonparabolic dispersion laws. The (ln) sequence is $\{(01),(0,2),(1,1),(1,2)\}$.

nonparabolic cases becomes close to each other with the increasing of the inner radius R_1. It is shown both in electrons and light holes that for a small radius, there is an appreciable separation between states corresponding to different n but equal l quantum numbers.

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