THE ZEEMAN SPLITTING IN KANE TYPE SEMICONDUCTOR WIRE

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The electronic states of a Kane type semiconductor quantum wire with and without magnetic field are theoretically investigated and compared with those of a quantum wire of the same size. The eigenstates and eigenvalues of the Kane's Hamiltonian are obtained. Numerical calculations are performed for a hard-wall confinement potential and electronic states are obtained as functions of the magnetic field. We calculated the size dependence of the effective *g*-values in bare InSb, GaAs and CdSe nanocrystals. It has been seen that the effective *g*-value of the electrons is decreased with the increasing of quantum wires radius.

1. Introduction

In recent years, there have been many studies about optic properties of quantum nanostructures such as quantum dots, quantum wires, quantum wells and others [1-3]. It is known that the application of a magnetic field could provide additional information about the properties of electrons in solids and in nanostructures. Energy spectrum of carriers in quantum dots and quantum wires, were considered theoretically in [4-8]. In [9] in the absence of magnetic field quantum wire energy spectra and wave functions were obtained for two band Kane model in the case of zero spin orbital interaction and zero magnetic field. The electron energy states were investigated in the uniform magnetic field directed along the quantum wire [4]. In this study the free electron model was used. The energy spectrum was determined as a function of a quantum number m for the finite and infinite potential cases from the boundary conditions. The energy spectrum in the dependent of magnetic field is found to have a minimum for the negative values of quantum number m.

Magneto-optical properties of quantum dots in semiconductors have been considered for the model of hard-wall confinement [6] when the real band structure of InSb-type materials (narrow energy gap and strong spin-orbital interaction) was taken into accaunt. The results of [6] are in a good agreement with the magneto-optical experiments in InSb quantum dots [10]. The effect of quantum confinement and the nanocrystal surface on the *g*-factors are studied in [8] for the ground and excited electron states in bare CdSe and ZnO nanocrystals. The calculation was made by using 8x8 and 14x14 band Kane models second-order $\vec{k}\,.\,\vec{p}$ perturbation theory. The spin-orbital interaction and the contribution of the electrons to the *g* factor were presented in details in [11,12]. For the calculation of the electron *g*-values in [11] the eight-band Kane`s model was used where the nonparabolicity of the electron and light-hole bands and the complex structure of the valence bands had been taken into account simultaneously. This model describes the energy band structure around the Γ point of the Brillouin zone very well. The electron *g*-factor values for quantum wires and quantum dots using the parameters of GaAs/Al_x Ga_{1-x} As hetero-system were calculated by perturbation theory[11]. It was obtained that the *g*-factor is anisotropic ($g_{\parallel} \neq g_{\perp}$) for quantum well and isotropic in cylindrical wire [12].

In this work, using three-band Kane`s model including the conduction band, light and spin-orbital hole bands, the electron spectrum with and without magnetic field and electron effective *g*-factor of quantum wire are calculated. In opposite to [11,1available 2] we take the potential of the quantum wire to be infinitive and consequently the wave functions to be zero at the boundary.

In the eight-band Kane's Hamiltonian the valence and conduction bands interaction is taken into account via the unique matrix element *P* (so called Kane's parameter). The system of Kane equations including the nondispersional heavy hole bands have a from [12, 13]:

$$-EC_1 - \frac{Pk_-}{\sqrt{2}}C_3 + \sqrt{\frac{2}{3}}Pk_z C_4 + \frac{Pk_+}{\sqrt{6}}C_5 + \frac{Pk_z}{\sqrt{3}}C_7 + \frac{Pk_+}{\sqrt{3}}C_8 = 0 \quad (1)$$

$$-EC_2 - \frac{Pk_-}{\sqrt{6}}C_4 + \sqrt{\frac{2}{3}}Pk_z C_5 + \frac{Pk_+}{\sqrt{2}}C_6 + \frac{Pk_-}{\sqrt{3}}C_7 - \frac{Pk_z}{\sqrt{3}}C_8 = 0 \quad (2)$$

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

$$\sqrt{\frac{2}{3}}Pk_z C_1 - \frac{Pk_+}{\sqrt{6}}C_2 - (E+E_g)C_4 = 0 \quad (4)$$

$$\sqrt{\frac{2}{3}}Pk_z C_2 + \frac{Pk_-}{\sqrt{6}}C_1 - (E+E_g)C_5 = 0 \quad (5)$$

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

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

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

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

2. Zero magnetic field

Substituting expressions (3)-(8) into formulas (1) and (2) we obtain:

It needs

$$(-E - \frac{P^2}{3}(\frac{2}{E+E_g} + \frac{1}{E+E_g+\Delta})\Delta_3)C_{1,2} = 0 \quad (9)$$

where Δ_3 three dimensional Laplacian.

In cylindrical coordinates the eigenfunction is

$$C_{1,2} = A_{1,2}\, exp(im\phi + ik_z z)R_{1,2}(\rho) \quad (10)$$

where $A_{1,2}$ is a normalization factor and the radial function $R(\rho)$satisfies

$$\left\{\frac{P^2}{3}(\frac{2}{E+E_g} + \frac{1}{E+E_g+\Delta})\left[\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{m^2}{\rho^2} - k_z^2\right] + E\right\}R_{1,2}(\rho) = 0 \quad (11)$$

The Kane's parameter P is connected with effective mass m_n and can be written in a usual way [15].

$$P^2 = \frac{3\hbar^2}{2m_n}\frac{E_g(E_g+\Delta)}{3E_g+2\Delta} \quad (12)$$

After substitution of the values of P^2 from (12), the equation (11) can be rewritten in the form:

$$\left(\frac{d^2}{d\rho^2} + \frac{1}{\rho}\frac{d}{d\rho} - \frac{m^2}{\rho^2} + \frac{2m_n}{\hbar^2}E'\right)R_{1,2}(\rho) = 0 \quad (13)$$

where

$$E' = \frac{E(E+E_g)(E+E_g+\Delta)(3E_g+2\Delta)}{E_g(E_g+\Delta)(3E+3E_g+2\Delta)} - \frac{\hbar^2 k_z^2}{2m_n} \quad (14)$$

Equation (13) is Bessel's differential equation [16], with the solution bounded at $\rho=0$ being

$$R_{1,2}(\rho) = CJ_m(\chi\rho) \quad (15)$$

where

$$\chi^2 = \frac{2m_n}{\hbar^2}\left(\frac{E(E+E_g)(E+E_g+\Delta)(3E_g+2\Delta)}{E_g(E_g+\Delta)(3E+3E_g+2\Delta)} - \frac{\hbar^2 k_z^2}{2m_n}\right) \quad (16)$$

For an infinite wall at radius R, the boundary condition is $R_{1,2}(R) = 0$, so the eigenvalue equation is

$$J_m(\chi R) = 0 \quad (17)$$

Equations (16) and (17) together show that the radial eigenvalue spectrum is

$$\frac{E(E+E_g)(E+E_g+\Delta)(3E_g+2\Delta)}{E_g(E_g+\Delta)(3E+3E_g+2\Delta)} = \frac{\hbar^2}{2m_n}\frac{z_{mp}^2}{R^2} + \frac{\hbar^2 k_z^2}{2m_n} \quad (18)$$

where z_{mp} is the p-th root of the m-th Bessel function $J(z)$.

Equation (18) determines the energies of electrons, light holes, and the spin-orbit split-off band of holes. This equation can be useful for analyzing the influence of nonparabolicity on the energy spectrum of electrons in a quantum wire.

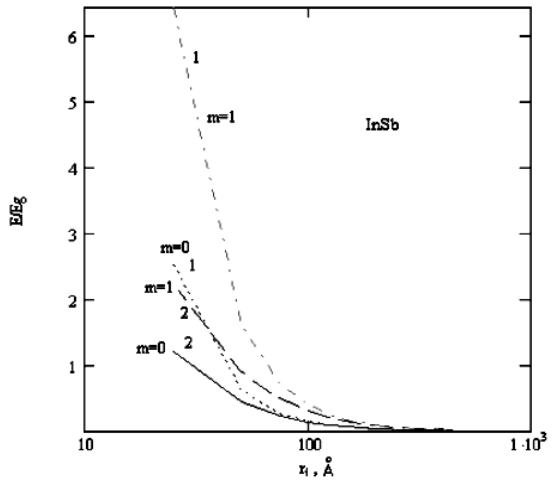

Fig.1. The dependence of the lowest quantum size levels in InSb quantum wire as function of the quantum wire radius. (1) for parabolic dispersion law. (2) for Kane's dispersion law.

In fig.1, the dependencies $E(R)$ for two cases are presented: a) electrons with parabolic dispersion law, b) electrons with Kane's dispersion law for InSb quantum wire. According to this figure, with increase of R, the electron energy levels in both cases are close to each other. At rather small sizes of R, the variance electron dispersion laws become more and more important and therefore, the curves for $E(R)$ keep away from each other.

3. Applied magnetic field, infinite step

The atomic Zeeman splitting is incorporated by adding the terms $\pm\frac{1}{2}g_0\mu_B H$ the diagonal of Kane's Hamiltonian,

μ_B is the Bohr magneton, g_0 is the Lande effective factor. For a uniform magnetic field, H directed along the z axis, the vector potential may be choosen in the form

$$\vec{A} = \frac{1}{2}\left[\vec{H} \times \vec{r}\right] = \left(-\frac{H_y}{2}, \frac{H_x}{2}, 0 \right) \tag{19}$$

and $k_\pm$ have the forms

$$k_\pm \to k_\pm \pm i\frac{1}{2}\lambda_H r_\pm \tag{20}$$

where

$$r_\pm = x \pm iy, \ \lambda_H = \frac{eH}{\hbar c} \tag{21}$$

Substituting expressions (3)-(8) into formulas (1) and (2), and using the (20), (21) relations we obtain:

$$\left(-E_1 + \frac{P^2}{3}\left(\frac{2}{E_1 + E_g} + \frac{1}{E_1 + E_g + \Delta}\right)\left(-\nabla^2 + \lambda_H L_z + \frac{1}{4}\lambda_H^2 \rho^2\right) \pm \frac{P^2 \lambda_H}{3}\left(\frac{1}{E_1 + E_g} - \frac{1}{E_1 + E_g + \Delta}\right) \right) C_{1,2} = 0 \tag{22}$$

where L_z is a z component of in angular momentum operator L, $\rho^2 = x^2 + y^2$ and $E_1 = E \mp \frac{1}{2} g_0 \mu_B H$.

If one seeks the solution of equation (22) in cylindrical coordinates in the form

$$C_{1,2} = A_{1,2}\, exp(im\varphi + ik_z z) exp\left(-\frac{\xi}{2}\right) \xi^{\frac{|m|}{2}} \Phi_{1,2}(\xi) \tag{23}$$

he obtains for the radial function $\Phi(\xi)$ the following equation

$$\xi \frac{d^2\Phi}{d\xi^2} + \left(|m| + 1 - \xi\right)\frac{d\Phi}{d\xi} - \alpha_{1,2}\Phi = 0 \tag{24}$$

Equation (24) is the canonical form of Kummer's equation for the confluent hypergeometric function. In (23) $\xi = \frac{\rho^2}{2l_H^2}$ is the dimensionless variable. The solution of (24) that is bounded at $\rho = 0$ is

$$\Phi(\xi) = M(\alpha_{1,2}, b, \xi) \tag{25}$$

where

$$\alpha_{1,2} = \frac{1}{2} + \frac{m}{2} + \frac{|m|}{2} + \frac{1}{2}k_z^2 l_H^2 - \frac{E_1}{\hbar\omega_c}\frac{(E_1 + E_g)(E_1 + E_g + \Delta)(3E_g + 2\Delta)}{E_g(E_g + \Delta)(3E_1 + 3E_g + 2\Delta)} \pm \frac{\Delta}{2(3E_1 + 3E_g + 2\Delta)} \tag{26}$$

$\omega_c = \frac{eH}{m_n c}$ is the cyclotron frequency, $l_H = \sqrt{\frac{\hbar c}{eH}}$ is the magnetic length and

$$b = |m| + 1 \tag{27}$$

are the parameters of the Kummer function in standard notation. The boundary conditions which correspond to the infinite potential at $\rho = R$ are $C_{1,2} = 0$. These lead to the eigenvalue equations

$$M(\alpha_{1,2}, b, \frac{R^2}{2l_H^2}) = 0 \tag{28}$$

We can find the energy spectrum $E(R, m, l_H, k_z)$ from equation (26). It is necessary for this to find α_1 and α_2 from equation (28) for a given R, azimuthal quantum number m and l_H, and then to substitute them into equation (26). For an infinite medium, $R \to \infty$, equation (28) is replaced by the requirement that M be bounded as $\frac{R^2}{2l_H^2} \to \infty$. This simply means that $\alpha_{1,2}$ is a negative integer [16],

$$\alpha_{1,2} = -l, \ l = 0,1,2,... \tag{29}$$

leading to the result

$$\frac{E_1(E_1 + E_g)(E_1 + E_g + \Delta)(3E_g + 2\Delta)}{E_g(E_g + \Delta)(3E_1 + 3E_g + 2\Delta)} = \left(n + \frac{1}{2}\right)\hbar\omega_c \pm \frac{\Delta}{2(3E_1 + 3E_g + 2\Delta)}\hbar\omega_c + \frac{1}{2}k_z^2 l_H^2 \hbar\omega_c \tag{30}$$

with

$$n = l + m \quad \text{for } m > 0 \tag{31}$$

$$n = l \quad \text{for } m \le 0 . \tag{32}$$

The expression (30) is the same as the expression of the energy spectrums of carriers of bulk Kane type semiconductors in the magnetic field [15].

The magnetic field dependencies of electrons energy spectrum for the lowest sequences of m at the subbands bottom $(k_z=0)$ for InSb quantum wire with R=300Å, in which

the non-parabolicity was taken into account, are shown in Fig.2 (for $g_0=0$).

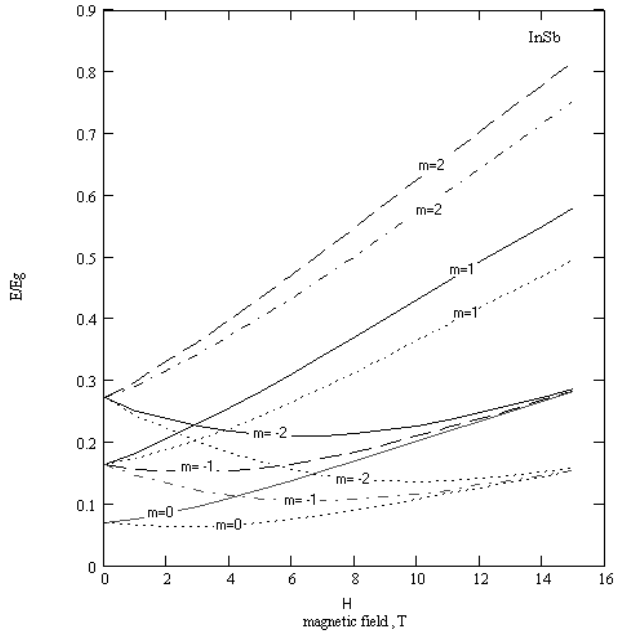

Fig.2. Lowest part of the energy spectrum of electrons as a function of the magnetic field in cylindrical quantum wires for the InSb.

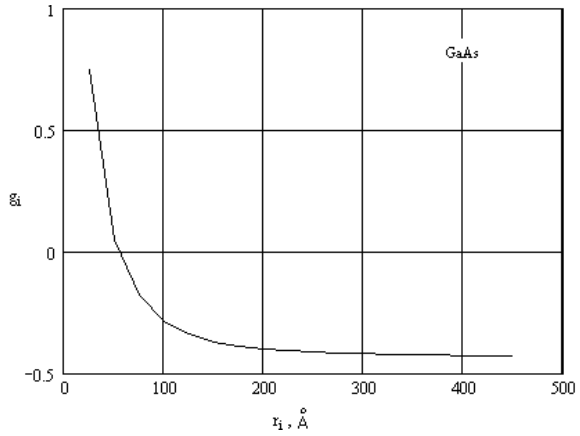

Fig.3. The electron *g* factor calculated as a function of the radius in cylindrical quantum wires for GaAs.

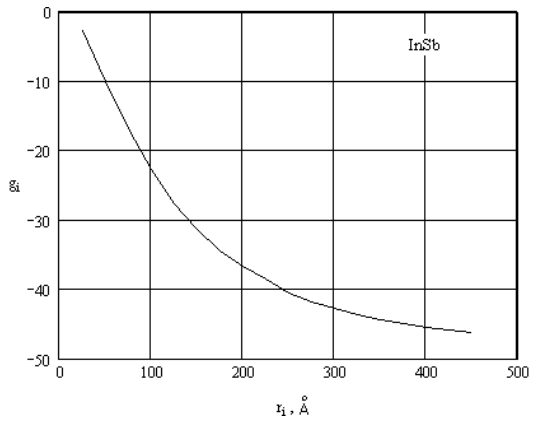

Fig.4. The electron g factor calculated as a function of the radius in cylindrical quantum wires for InSb.

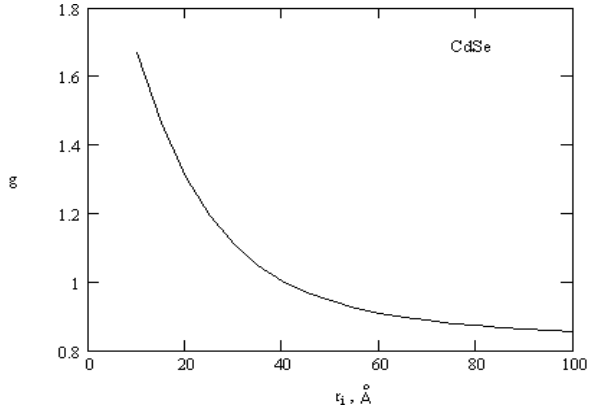

Fig.5. The electron *g* factor calculated as a function of the radius in cylindrical quantum wires for CdSe.

The light hole and spin-orbital splitting subbands can be obtained by the same way for two other roots of equation (26). As it is seen from fig.1 the magnetic field dependence of energy has a minimum only for subbands with the negative *m*. These results are in good agreement with those given in [4].

Note that for the quantum wire with the finite length *d*

$$k_z = \frac{\pi}{d} l \ , l=1,2,3,... \qquad (33)$$

and the minimal value for k_z must be taken as $\frac{\pi}{d}$.

The expression for the *g*-factor obtained in the second order of $\vec{k}.\vec{p}$ perturbation theory has the form [15]

$$g(E) = 2\left[1 + (1 - \frac{m_0}{m_n})\frac{\Delta}{3E + 3E_g + 2\Delta}\right] \qquad (34)$$

But in magneto-optical experiments, transitions from the bottom of the subbands take place and the effective *g*-factor can be determined from the Zeeman splitting of subbands

$$g(E) = \frac{E_\uparrow - E_\downarrow}{\mu_B H} \qquad (35)$$

Here $E_\uparrow$ and $E_\downarrow$ are the electron energy for spin $+z$ and $-z$ directions, respectively. Note that the *g*-factor determined by the equations (34) and (35) are the same if one considers the bottom of the lowest subband.

Figures 3, 4 and 5 show the electron g-factor dependence on *R* calculated by the equation (35) for GaAs, InSb and CdSe quantum wires for the fixed magnetic field value *H=0.5T*, respectively. As seen from fig.3 in GaAs quantum wire, the electron *g* factor value changes its sign with a radius. The following band parameters have been used for GaAs $E_g = 1.52$ *eV*, $\Delta = 0.34$ *eV*, $2p_{cv}^2/m_0 = 28.9$ *eV* (here $p_{cv}=m_0P/\hbar$, m_0 is the free-electron mass) [11]. The contribution of remote bands is taken into account by adding the constant $\Delta g = -0.12$ to the Kane's model values of *g* [12]. This result is also found in [11] for $GaAs/Al_{0.35}Ga_{0.65}$ as structures in the finite barrier case. It is obvious that the same will occur in the case of fixed R with increasing of magnetic field. The figure which shows the *g*-factor dependence on *R*

for CdSe (figure 5) is in good agreement with the reference [8].

It should be noted that the obtained results can be applied to quantum wires of InAs and zero-gap semiconductor HgTe and narrow-gap semiconductor Cd_{1-x} Hg_xTe also.

4. Conclusion

In this work using the eight band Kane's model the electron spectrum with and without magnetic field and electron effective *g*-factor for quantum wire is calculated. It was shown that the effective *g*-factor of electrons decreases with increasing of quantum wires radius and changes its sign for GaAs quantum wires.

The size dependence of the spectra of electrons in A^3B^5 and A^2B^6-type semiconductor cylindrical quantum wires was studied. It was taken into account the nonparabolicity of the spectrum of light holes, electrons and spin-orbit splitting valence band.

[1] *J.I.Alferov*.FTP N1,32, 1, p.3-18, (1998).
[2] *J.I.Alferov*. FTP N4, 32, 1, p.385-410, (1998).
[3] *M.Masale*. Physica E 5 98-107, (1999).
[4] *N.C.Constantinou, M.Masale and D.R.Tiley*. J. Phys:Condens.Matter 4 , 4499-4508, (1992).
[5] *N.C.Constantinou and M.Masale.* Phys. Rev. B 48, 11, 128, (1993).
[6] *W.Zawadski and M.Kubisa*. Semicond.Sci. Technol. 8 , S240-S242, (1993).
[7] *A.Garcia-Cristobal, V.M. Fomin and J.T.Devreese*. Physica B 256-258 190-193, (1998).
[8] *A.V. Rodina, Ai.L. Efros, M. Rosen, B.K. Meyer.* Material Science and Engineering C 19 435-438 (2002).
[9] *Chhi-Chong Wu and Chau-Ju Lin*. J.Appl.Phys 83 (3), 1390-1395, (1998).
[10] *Ch. Sikorski and V. Merkt*. Phys.Rev.Lett 62 ,2164, (1989).
[11] *A.A.Kiselev, E.L. Ivchenko*. Pismo v JETF 67, 1,41-45, (1996).
[12] *A.A.Kiselev, E.L. Ivchenko U.Rössler*. Phys. Rev. B58, 24, 16353-15359, (1998).
[13] *B.M. Askerov*. Kinetic Effects in Semiconductors (Nauka, Leningrad, 1970).
[14] *A.I. Anselm*. Introduction to Semiconductor Theory (Nauka, Moscow, 1978; Prentice-Hall, Englewood.
[15] *B.M. Askerov.* Electron Transport Phenomena in Semiconductors (World Scientific, 1994, Singapur).
[16] *V.M. Galitskii, B.M. Karnakov, V.I. Kogan.* A collection of problems Quantum mechanics Science, Moscow, 1981 (in Russian).
[17] *L.D.Landau and E.M.Lifshitz.* Quantum Mechanics, 1977 Pergamon press Cliffs.

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KEYN TİPLİ YARIMKEÇİRİCİ KVANT MƏFTİLLƏRDƏ ZEYMAN PARÇALANMASI

Keyn tipli yarımkeçrici kvant məftillərdə maqnit sahəsində və sahənin sıfır qiymətində elektron halları tapılmış və eyni ölçülü yarımkeçrici kvant məftillin elektron halları ilə müqayisə edilmişdir. Keyn hamiltonianı üçün məxsusi qiymətlər və dalğa funksiyaları tapılmışdır. Ədədi hesablamalarla sonsuz məhdudlaşdırıcı potensial üçün elektronun enerjisinin maqnit sahəsindən asılılığı tapılmışdır. İnSb, GaAs və CdSe nanokristalları üçün elektronların effektiv *g*-faktorunun sistemin ölçüsündən asılılığı hesablanmışdır. Göstərilmişdir ki, ölçü kiçildikcə *g*-faktorun qiyməti artır.

А. М. Бабаев

ЗЕЕМАНОВСКОЕ РАСЩЕПЛЕНИЕ В КЕЙНОВСКИХ ПОЛУПРОВОДНИКОВЫХ КВАНТОВЫХ ПРОВОЛОКАХ

Найдены электронные состояния в кейновских полупроводниковых квантовых проволоках в магнитном поле и в отсутствии поля. Проведены сравнения с обычной полупроводниковой квантовой проволокой того же размера. Получены собственные значения и собственные функции кейновского гамильтониана. Проведены численные расчеты для бесконечного ограничивающего потенциала и найдены электронные состояния в зависимости от магнитного поля. Рассчитаны величины электронного эффективного *g*-фактора в зависимости от размера в наноструктурах полупроводников InSb, GaAs, и CdSe. Показано, что значение эффективного *g*-фактора растет с уменьшением размера квантовой проволоки.

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