Section 3. Physics

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DIMENSIONALLY QUANTIZATION OF THE ENERGY SPECTRUM OF HOLES IN A P-Te QUANTUM WELL

Absract. The dimensionally quantization in a potential well grown on the basis of a gyrotropic crystal (for example, p-Se or p-Te) is theoretically investigated.

Expressions are obtained for the wave functions of holes depending on the dimensionally quantization number.

It was shown that the dimensionally-quantized spectrum of holes in gyrotropic crystals depends on the ratio of the hole energy to the height of the potential barrier. In particular, the energy spectrum of holes in the well consists of a set of dimensionally-quantized levels that do not intersect with each other due to the presence of an energy gap between subbands of the valence band.

Keywords: dimensionally quantization, wave function, holes, energy spectrum.

I. Introduction

Recently, considerable attention has been drawn to dimensionally quantization (DQ), which has applications in optoelectronics [1]. For semiconductors with a simple band structure, the study of interlevel optical transitions in structures for an arbitrary potential was carried out in [2; 3]. At the same time, interlevel optical transitions in semiconductor structures with hole conductivity are of interest because of the nonzero absorption for light of arbitrary polarization, which have practical applications [4]. A theoretical study of this kind of problem is hampered by the complexity of the band structure of the crystal.

In particular, in [5–7], such a problem in the case of a rectangular dimensionally quantized well (DQW) with a fixed thickness was solved numerically. However, even a small variation in the thickness or depth of the RQW can greatly change the final result, which makes it difficult to analyze intermediate calculations. In [8], on the basis of perturbation theory, analytical expressions [9] were obtained; the energy spectrum, the wave function of holes, and the intersubband absorption of polarized radiation

in an infinitely deep quantum well of a semiconductor were studied. The calculations were carried out in the Luttinger-Kohn approximation [10; 11] for semiconductors with a zinc blende lattice.

However, the theoretical study of dimensional quantization in a potential well (DQW) grown on the basis of a gyrotropic crystal (for example, *p-Se* or *p-Te*) remains open, which is the subject of this communication.

Note that the study of a number of phenomena, in particular, optical or photovoltaic effects in dimensionally-quantized structures (QW) requires knowledge of the energy spectrum and wave functions of electron current carriers.

II. Basic ratios

For a quantum well with a potential $U(z)$, the effective Hamiltonian for a quantum well with a potential $U(z)$ is the effective Hamiltonian of electrons in *p-Te* in the form

$$\widehat{H} = \widehat{H}_0 + \sum_{\alpha=x,z} A_\alpha \sigma_\alpha , \qquad (1)$$

where $\widehat{H}_0 = Ak_\perp^2 + Bk_z^2$, $A_x = \Delta$, $A_z = \beta k_z$ and it is assumed that the phases of t $M_{1,2}^{'}$ he function are chosen so that the coefficient at k_z is real, 2Δ – spin-orbit splitting of the valence band at the M(P) point of the Brillouin zone), $k_\perp^2 = k_x^2 + k_y^2$, A, B, β_V are band parameters of *p-Te*, $\vec{k}_\perp = k_\perp(\sin\varphi, \cos\varphi)$ is two-dimensional wave vector directed along the interface.

The wave functions in the upper valence bands ($M_1^{'}$ and $M_2^{'}$) are a superposition of states with the projection of the angular momentum on the axis Z $(m_z = \pm 3/2)$

$$\Psi_{M_1^{'}} = \sum_{m_z=\pm 3/2} C_{m_z}^{(l)} \mid m_z \rangle , \qquad (2)$$

where $C_{3/2}^{(1)} = C_{-3/2}^{(2)} = C_1 = \sqrt{(1+\eta)/2}$, $C_{-3/2}^{(1)} = -C_{3/2}^{(2)} = = C_2 = \sqrt{(1-\eta)/2}$, $\eta = \beta k_z (\Delta^2 + \beta^2 k_z^2)^{-1/2}$.

The spectrum of holes in the valence band in a bulk gyrotropic crystal has the form

$$E_l(k_x, k_y, k_z) = Ak_\perp^2 + Bk_z^2 - (-1)^{-l}\left(\Delta^2 + \beta^2 k_z^2\right)^{1/2} \quad (l = 1,2). \qquad (2')$$

Here $A = \hbar^2/(2m_\perp), B = \hbar^2/(2m_{||})$, $m_\perp$ and $m_{||}$ are the transverse and longitudinal effective masses of holes in the subbands $M_1^{'}$ and $M_2^{'}$, which are equal with the opposite sign to the effective masses of electrons.

Then choosing the dimensionally quantization axis Oz and assuming that $k_z = \frac{1}{i}\frac{\partial}{\partial z}$ from (1) we have

$$\widehat{H} = \widehat{H}_0 + \widehat{R}_2 k_\perp^2 , \qquad (3)$$

where

$$\widehat{H}_0 = \Delta\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} - B\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\frac{\partial^2}{\partial z^2} - i\beta_V \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\frac{\partial}{\partial z} + U(z),$$

$$\widehat{R}_2 = A\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}k_\perp^2 , \qquad (4)$$

III. Hole states in a tellurium quantum well

The unperturbed energy levels $E_\xi(0)$ and the wave function of electrons $\psi_\xi^{(0)} = \begin{bmatrix} \psi_2^{(0)} \\ \psi_1^{(0)} \end{bmatrix}$ in the subbands M_ξ' $(\xi = 2,1)$ the conduction band of $p-Te$ are determined from the following matrix differential equation with band parameters A, B:

$$\widehat{H}_0 \bar{\psi}_\xi^{(0)} = \widehat{E}_\xi \bar{\psi}_\xi^{(0)} , \qquad (5)$$

where $\widehat{E}_\xi = \begin{bmatrix} \tilde{E} & 0 \\ 0 & \tilde{E} \end{bmatrix}$. Then we have

$$\left\{\frac{\Delta}{2}\begin{bmatrix} \psi_2^{(0)} \\ -\psi_1^{(0)} \end{bmatrix} - \frac{\partial^2}{\partial z^2}\begin{bmatrix} A_3\psi_2^{(0)} \\ A_1\psi_1^{(0)} \end{bmatrix} + U(z)\begin{bmatrix} \psi_2^{(0)} \\ \psi_1^{(0)} \end{bmatrix}\right\} = = \begin{bmatrix} \tilde{E}\psi_2^{(0)} \\ \tilde{E}\psi_1^{(0)} \end{bmatrix}, \qquad (6)$$

To simplify the problem, we assume that $U(z) = U_0 = const$. Then the last equation will look like

$$\begin{cases} \dfrac{\partial^2\psi_2^{(0)}}{\partial z^2} - \dfrac{1}{B}\left[U(z) - \tilde{E}\right]\psi_2^{(0)} + i\dfrac{\beta_V}{B}\dfrac{\partial\psi_2^{(0)}}{\partial z} - \dfrac{\Delta}{B}\psi_1^{(0)} = 0, \\ \dfrac{\partial^2\psi_1^{(0)}}{\partial z^2} - \dfrac{1}{B}\left[U(z) - \tilde{E}\right]\psi_1^{(0)} - i\dfrac{\beta_V}{B}\dfrac{\partial\psi_1^{(0)}}{\partial z} - \dfrac{\Delta}{B}\psi_2^{(0)} = 0 \end{cases} \qquad (7)$$

or

$$\frac{\partial^2\psi_+^{(0)}}{\partial z^2} - \kappa_E^2\psi_+^{(0)} + i\kappa_{\beta_V}\frac{\partial\psi_-^{(0)}}{\partial z} - i\kappa_\Delta^2\psi_-^{(0)} = 0, \qquad (8)$$

where $\kappa_E^2 = \frac{1}{B}\left(U_0 - \tilde{E}\right)$, $\kappa_\Delta^2 = \frac{\Delta}{B}$, $\kappa_{\beta_V} = \frac{\beta_V}{B}$, $\psi_\pm^{(0)} = \psi_2^{(0)} \pm i\psi_1^{(0)}$.

We will seek solution (8) in three approximations, which we analyze in more detail below.

1. Approximation. From (8) it is easy to obtain the following system of equations

$$\begin{cases} \dfrac{\partial^2 \psi_+^{(0)}}{\partial z^2} - \kappa_E^2 \psi_+^{(0)} = 0, \\ \dfrac{\partial \psi_-^{(0)}}{\partial z} + \dfrac{\kappa_\Delta^2}{\kappa_{\beta_V}} \psi_-^{(0)} = 0, \end{cases} \quad (9)$$

whose solution we write in the form

$$\psi_\pm^{(0)} = D_\pm \exp(\kappa_\pm z) + C_\pm \exp(-\kappa_\pm z), \quad (10)$$

where $\kappa_+ = \kappa_E$, $\kappa_- = \kappa_\Delta$, unknown quantities $D_\pm$, C_1 are determined from the boundary conditions of the problem, which will be discussed further. Note that κ_- the real value, κ_+ parameter can be both real (at $U_0 \rangle \tilde{E}$) and imaginary (at $U_0 \langle \tilde{E}$) values. Then the wave function $\psi_+^{(0)}$ in the first case will be exponential, and in the second case it will be trigonometric. If $\kappa_\pm$ the value is real, then we can assume that $D_\pm = 0$. This means that current carriers (holes in *p-Te*) with energy $\tilde{E} \langle U_0$ will behave like a de Broglie (plane wave), but in other cases they will not.

Further, we assume that the holes are in the potential well. Then

$$\psi_+^{(0)} = D_+ \exp(i\kappa z) + C_+ \exp(-i\kappa z),$$

$$\psi_-^{(0)} = C_1 \exp\left(-\frac{\kappa_\Delta^2}{\kappa_{\beta_V}} z\right), \quad (11)$$

where it is taken into account that $U_0 = 0$, $\kappa_+ = i\sqrt{\tilde{E}/B} = i\kappa$. Then, from the conditions of orthonormality and finiteness of the wave functions of holes at the interfaces of the well, we have that

$$\psi_+^{(0)}(z) = 2\kappa^{1/2} \frac{\cos(\kappa z)}{\left[2\kappa a + \sin(2\kappa a)\right]^{1/2}}. \quad (12)$$

From the boundary condition of the problem, we obtain expressions for the size-quantized energy spectrum of holes

$$\tilde{E} = B \frac{(2n+1)^2}{4a^2} \pi^2 \quad (n = 0,1,2,...) \quad (13)$$

2. Approximation. Now we look for the solution of equation (8) in the form

$$\psi_+^{(0)} = D \exp(\kappa z) \quad \psi_-^{(0)} = D^* \exp(\kappa^* z), \quad (14)$$

where κ^* and D^* are the complex conjugate wave vector and a parameter whose analytical form can be determined from the above boundary conditions. Then it is easy to obtain the following relations, useful for further calculations

$$D_{im} = i \cdot \frac{\left[\left(-\kappa^2 + \kappa_E^2\right) + i\left(-\kappa^* \kappa_{\beta_V} + \kappa_\Delta^2\right)\right]^2}{\left(-\kappa^2 + \kappa_E^2\right)^2 + \left(-\kappa^* \kappa_{\beta_V} + \kappa_\Delta^2\right)^2} D_{re}, \quad (15)$$

where D_{re} and D_{im} are the real and imaginary values of the quantity. It can be seen from (15) that the form of the wave function (14) depends on the physical nature of the wave vector. Therefore, consider the following cases:

a) let the wave vector be a real value, then

$$D_{im} = -2 \frac{\varsigma_{re}}{\varsigma_{re}^2 + 1} D_{re}, \quad (16)$$

where $\varsigma_{re} = \left(-\kappa^2 + \kappa_E^2\right) / \left(-\kappa \kappa_{\beta_V} + \kappa_\Delta^2\right)$. Then the wave functions of holes take the form

$$\psi_\pm^{(0)}(z) = \frac{\varsigma_{re}^2 + 1 \mp 2i\varsigma_{re}}{\varsigma_{re}^2 + 1} D_{re} \exp(\kappa z). \quad (17)$$

Then the energy spectrum of current carriers is determined from the following transcendental equation

$$\left(\frac{\tilde{E}}{B}\right)_\pm = \frac{\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_{\beta_V} \pm$$

$$\pm \left[\left(\frac{\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_{\beta_V}\right)^2 + 4\left(\frac{\tilde{E}^2}{B^2} - \frac{2\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_\Delta^2\right)\right]^{1/2}. \quad (18)$$

It can be seen from (18) that the energy spectrum takes real values when the following inequalities are fulfilled

$$\tilde{E} \rangle \frac{B}{2}\left[\frac{2\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_\Delta^2 - \left(\frac{\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_{\beta_V}\right)^2\right]^{1/2},$$

$$\frac{2\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_\Delta^2 \rangle \left(\frac{\varsigma_{re}}{\varsigma_{re}^2 + 1} \kappa_{\beta_V}\right)^2; \quad (19)$$

b) let the wave vector be an imaginary quantity, then the relationship between the quantities D_{im} and D_{re} is described as

$$D_{im} = -2 \frac{\varsigma_{im}}{\varsigma_{im}^2 + 1} D_{re}, \quad (20)$$

and the wave functions of holes are determined by

$$\psi_+^{(0)}(z)=\frac{2D_{re}}{1+b_2^2}(1+ib_2)\exp(\kappa z),$$

$$\psi_-^{(0)}(z)=D_{re}\left(1-\frac{(1+ib_2)^2}{b_2^2}\right)\exp(\kappa z), \quad (21)$$

where $\varsigma_{im}=\left(\kappa^2+\kappa_E^2-\kappa\kappa_{\beta_V}\right)/\kappa_\Delta^2$. $b_2=\dfrac{\kappa_\Delta^2-\kappa^*\kappa_{\beta_V}}{\kappa_E^2-\kappa^2}$.

Now let's try to solve the system of equations (7) in general form. To do this, after transforming in (7), it is easy to obtain the Schrödenger equation in the form

$$\frac{\partial^4\psi_2^{(0)}}{\partial z^4}-\frac{1}{B}\left(U_0-\tilde{E}-\frac{\beta_V^2}{B}\right)\frac{\partial^2\psi_2^{(0)}}{\partial z^2}-$$

$$-\frac{1}{B^2}\left\{\Delta^2-\left(U_0-\tilde{E}\right)^2\right\}\psi_2^{(0)}=0. \quad (22)$$

Consider the following cases:

a) for holes located in the well $(U_0=0)$, equation (22) takes the form

$$\frac{\partial^4\psi_2^{(0)}}{\partial z^4}+\aleph_1^2\frac{\partial^2\psi_2^{(0)}}{\partial z^2}-\aleph_0^4\psi_2^{(0)}=0, \quad (23)$$

whose solution we seek in the form

$$\psi_2^{(0)}=B_2\cdot e^{-\alpha_1\cdot z}+B_2\cdot e^{\alpha_2\cdot z}+B_3\cdot e^{-\alpha_2\cdot z}, \quad (24)$$

where $\aleph_1^2=B^{-1}\left(\tilde{E}+B^{-1}\beta_V^2\right)$, $\aleph_0^4=B^{-2}\left(\Delta^2-\tilde{E}^2\right)$, $\alpha_1=\aleph_-$, $\alpha_2=i\aleph_+$, $\aleph_\pm=\sqrt{\frac{1}{2}\left[\pm\left(\aleph_1^2\right)+\sqrt{\left(\aleph_1^2\right)^2+4\aleph_0^4}\right]}$

and, in what follows we will take into account that $\left(\aleph_1^2\right)\langle\sqrt{\left(\aleph_1^2\right)^2+4\aleph_0^4}$. Then, from the conditions of finiteness of the wave functions at the interface boundaries, we have

$$\psi_2^{(0)}(z)=\frac{B_2}{2}\left[\frac{e^{(2i\aleph_-+\aleph_+)a}-e^{-\aleph_+\cdot a}-2i\sin(\aleph_-\cdot a)}{ch(\aleph_+\cdot a)-\cos(\aleph_-\cdot a)}\cdot\left(e^{-\aleph_+\cdot z}-e^{-i\aleph_-\cdot z}\right)+2\left(e^{i\aleph_-\cdot z}-e^{-\aleph_+\cdot z}\right)\right]. \quad (25)$$

where B_2 is determined from the normalization condition of $\psi_2^{(0)}(z)$.

The energy spectrum of holes in a potential well is determined by the relation

$$\sin(\aleph_-\cdot a)-cos(\aleph_-\cdot a)+\frac{\aleph_-}{\aleph_+}exp(-\aleph_+\cdot a)=0. \quad (26)$$

b) for holes outside the well $(U_0\neq 0)$, the wave function of holes is determined by expression (25) and the energy spectrum by relation (26), but the following substitutions must be made: $\aleph_1\leftrightarrow\wp_1$, $\aleph_0\leftrightarrow\wp_0$, where $\wp_0^4=\frac{1}{B^2}\left\{\Delta^2-\left(U_0-\tilde{E}_2\right)^2\right\}$, $\wp_1^2=\frac{1}{B}\left(U_0-\tilde{E}-\frac{\beta_V^2}{B}\right)$;

c) in case of resonance, i.e. when the energy of holes is numerically equal to the height of the potential barrier, then the wave function of holes is determined by expression (25) and the energy spectrum by relation (26), but the following substitutions must be made: $\aleph_1^2\leftrightarrow\aleph_{01}$, $\aleph_0\leftrightarrow\aleph_{00}$, where $\aleph_{01}=\frac{\beta_V}{B}$, $\aleph_{00}^4=B^{-2}\left(\Delta^2-\tilde{E}^2\right)$

It can be seen from relation (22) that the wave function of holes in the potential well has two terms, one of which is exponentially decaying, and the rest are oscillating.

Conclusion

Thus, it was shown that the dimensionally-quantized spectrum of holes in gyrotropic crystals has a complex form and depends on the ratio of the hole energy to the potential barrier height. In particular, the energy spectrum of holes in the well consists of a set of dimensionally-quantized levels that do not intersect with each other due to the presence of an energy gap between the sus M_1' and M_2'.

Expressions are obtained for the wave functions and energy spectra of electrons for various cases, differing from each other in the relations for the characteristic wave vectors, which, in turn, depend on the band parameters of the semiconductor and on the energy gap between the subbands of the valence band of a gyrotropic crystal.

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