РАЗДЕЛ I. ФИЗИКА

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 The dimensional quantization in a semiconductor with a complex zone

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Abstract

The problem of the energy spectrum and the wave function of electrons in subbands of the conduction band in n-GaP with allowance for the dimensional quantization was theoretically considered.

Key words: energy spectrum, quantum well, wave function, dimensional quantization.

Recently, optical transitions between levels in a dimensional quantized well (DQW), which are used in infrared photoconverters [1], have attracted considerable attention. For semiconductors with a simple zone, the calculation of interlevel transitions for an DQW of an arbitrary potential was carried out earlier in [2, 3]. At the same time, the interlevel optical transitions in the DQW of hole conduction are of interest because of the nonzero absorption for light of arbitrary polarization, which have practical application [4]. A theoretical research of this type of problem is made difficult by the complexity of the band structure of a semiconductor. In particular, in [5–7] such a problem was solved numerically in the case of a rectangular DQW with a fixed thickness. However, even a small variation of the thickness or depth of the DQW can greatly change the final result, which makes it difficult to analyze intermediate calculations. In [8], on the basis of the perturbation theory, analytical expressions were obtained [9]. The energy spectrum of the holes was studied, and the intersubband absorption of polarized radiation in an infinitely deep semiconductor quantum well was studied. The calculations were carried out in the Luttinger – Cohn approximation [10, 11] for semiconductors with a zinc blende lattice.

However, a theoretical research of dimensional quantization in a potential well grown on a semiconductor base with a complex zone, one subzone of which has a “hump-like structure” (for example, n-GaP or p-Te) remains open, which was researched in this work.

Note that the research of a number of phenomena, in particular optical or photovoltaic effects in a dimensionally quantized well, requires knowledge of the energy spectrum and wave functions of electrons.

For a quantum well with potential $U(z)$, we represent the effective Hamiltonian of electrons in n-GaP as

$$\hat{H} = \hat{H}_0 + \hat{R}_2 k_{\perp}^2, \quad (1)$$

where

$$\hat{H}_0 = \frac{\Delta}{2} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} - \begin{bmatrix} A_3 & 0 \\ 0 & A_1 \end{bmatrix} \frac{\partial^2}{\partial z^2} + U(z), \quad (2)$$

$$\hat{R}_2 = \begin{bmatrix} B_3 & D \sin \varphi \cos \varphi \\ D \sin \varphi \cos \varphi & B_1 \end{bmatrix},$$

$A_{3,1}, B_{3,1}, D, P$ are n-GaP band parameters, $k_{\perp}^2 = k_x^2 + k_y^2$, $\vec{k}_{\perp} = (k_x, k_y)$ (or $k_x = k_{\perp} \cos \varphi$, $k_y = k_{\perp} \sin \varphi$) is two-dimensional wave vector directed along the interface, $\vec{r}_{\perp} = (x, y)$. Below, we assume that the wave function of electrons in the DQW plane is $\Psi \propto \exp(i\vec{k}_{\perp} \vec{r}_{\perp})$.

The unperturbed energy levels $E_{\xi}(0)$ and the wave function of electrons $\psi_{\xi}^{(0)} = \begin{bmatrix} \psi_3^{(0)} \\ \psi_1^{(0)} \end{bmatrix}$ in the subbands of the conduction band $X_{\xi} (\xi = 3, 1)$ at n-GaP are determined from the following matrix differential equation $\hat{H}_0 \hat{\psi}_{\xi}^{(0)} = \hat{E}_{\xi} \hat{\psi}_{\xi}^{(0)}$, where $\hat{E}_{\xi} = \begin{bmatrix} \tilde{E}_3 & 0 \\ 0 & \tilde{E}_1 \end{bmatrix}$. Then we have

$$\left\{ \frac{\Delta}{2} \begin{bmatrix} \psi_3^{(0)} \\ -\psi_1^{(0)} \end{bmatrix} - \frac{\partial^2}{\partial z^2} \begin{bmatrix} A_3 \psi_3^{(0)} \\ A_1 \psi_1^{(0)} \end{bmatrix} + P \frac{\partial}{\partial z} \begin{bmatrix} -\psi_1^{(0)} \\ \psi_3^{(0)} \end{bmatrix} + U(z) \begin{bmatrix} \psi_3^{(0)} \\ \psi_1^{(0)} \end{bmatrix} \right\} = \begin{bmatrix} \tilde{E}_3 \psi_3^{(0)} \\ \tilde{E}_1 \psi_1^{(0)} \end{bmatrix}, \quad (3)$$

where the third term describes the transformation of an electron with mass $m_{1(3)}$ to mass $m_{3(1)}$.

Next, consider one of the possible cases. In this case, we will assume that the effective masses of the electrons in both subbands are the same, i.e. $A_3 = A_1 = A$. Then the last equation will be

$$\left\{ \frac{\Delta}{2} \begin{bmatrix} \psi_3^{(0)} \\ -\psi_1^{(0)} \end{bmatrix} - \frac{\partial^2}{\partial z^2} \begin{bmatrix} A \psi_3^{(0)} \\ A \psi_1^{(0)} \end{bmatrix} + P \frac{\partial}{\partial z} \begin{bmatrix} -\psi_1^{(0)} \\ \psi_3^{(0)} \end{bmatrix} + U(z) \begin{bmatrix} \psi_3^{(0)} \\ \psi_1^{(0)} \end{bmatrix} \right\} = \begin{bmatrix} \tilde{E}_3 \psi_3^{(0)} \\ \tilde{E}_1 \psi_1^{(0)} \end{bmatrix}, \quad (4)$$

Then we have a system of equations

$$\begin{cases} -\frac{\partial^2 \psi_3^{(0)}}{\partial z^2} - \frac{P}{A} \frac{\partial \psi_1^{(0)}}{\partial z} + \frac{1}{A} [U(z) - \tilde{E}_3] \psi_3^{(0)} + \frac{1}{A} \frac{\Delta}{2} \psi_3^{(0)} = 0, \\ -\frac{\partial^2 \psi_1^{(0)}}{\partial z^2} + \frac{P}{A} \frac{\partial \psi_3^{(0)}}{\partial z} + \frac{1}{A} [U(z) - \tilde{E}_1] \psi_1^{(0)} - \frac{1}{A} \frac{\Delta}{2} \psi_1^{(0)} = 0. \end{cases} \quad (5)$$

Next, we make the notation of type $\psi_3^{(0)} + i\psi_1^{(0)} = \zeta^{(0)}$ and assume that $\tilde{E}_3 = \tilde{E}_1 = \tilde{E} = E(k_{\perp}) - B k_{\perp}^2$. Then we get the equation for $\zeta^{(0)}$

$$\frac{\partial^2 \zeta_-}{\partial z^2} - i \frac{P}{A} \frac{\partial \zeta_-}{\partial z} - \frac{1}{A} [U(z) - \tilde{E}] \zeta_- + \frac{1}{A} \frac{\Delta}{2} \zeta_+ = 0, \quad (6)$$

If we assume that $U(z) = U_0 = \text{const}$ and make the following notation $\kappa_A^2 = \frac{1}{A} (U_0 - \tilde{E})$, $\kappa_{\Delta}^2 = \frac{1}{A} \frac{\Delta}{2}$, $2\chi = \frac{P}{A}$, then we will have

$$\frac{\partial^2 \zeta_-}{\partial z^2} - 2i\chi \frac{\partial \zeta_-}{\partial z} - \kappa_A^2 \zeta_- + \kappa_{\Delta}^2 \zeta_-^* = 0. \quad (7)$$

Solution (7) $\zeta_- = C \cdot \exp(\alpha z)$ is simplified if we assume that $\zeta_-(z)$ function is a real quantity, the characteristic equation for which has roots

$$\alpha_{\pm} = i\chi \pm \sqrt{-\chi^2 + 4 \left(\kappa_A^2 - \kappa_{\Delta}^2 \frac{C^*}{C} \right)} \quad (8)$$

To simplify the solution of the problem, we assume that $C = C^*$, $C -$ is a real quantity. Then

$$\alpha_{\pm} = i\chi \pm \sqrt{-\chi^2 + 4(\kappa_A^2 - \kappa_{\Delta}^2)} \quad (9)$$

and we have that

$$\zeta_{-}(z) = \exp(i\chi z) \left\{ C_{+} \cdot \exp\left(z\sqrt{-\chi^2 + 4(\kappa_A^2 - \kappa_{\Delta}^2)}\right) + C_{-} \cdot \exp\left(-z\sqrt{-\chi^2 + 4(\kappa_A^2 - \kappa_{\Delta}^2)}\right) \right\} \quad (10)$$

If $\kappa_A^2 < \kappa_{\Delta}^2$. Than

$$\zeta_{-} = \exp(i\chi z) \left[C_1 \cdot \cos\left(z\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) + iC_2 \sin\left(z\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right]. \quad (11)$$

Considering the boundary conditions of type $\zeta_{\pm}(z = -a/2) = 0$, $\zeta_{\pm}(z = +a/2) = 0$, if condition $\cos(a/2\chi) \pm i\sin(a/2\chi) \neq 0$ is satisfied, then the relationship between C_1 and C_2 is defined as $C_1 = \pm iC_2 \operatorname{tg}\left(a/2\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right)$. In this case, from the normalization condition

$$|C_1| = \left| \sin\left(\frac{a}{2}\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right|, \quad |C_2| = \left| \cos\left(\frac{a}{2}\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right|, \quad (12)$$

and the expression for $\zeta_{-}(z)$ is

$$\begin{aligned} \zeta_{-}(z) = \exp(i\chi z) \times \\ \times \left[\frac{1}{2} \left[\sin\left(\left(z + \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) - \sin\left(\left(z - \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right] + \right. \\ \left. + \frac{1}{2} \left[\sin\left(\left(z - \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) + \sin\left(\left(z + \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right] \right] \end{aligned} \quad (13)$$

whence the electron wave functions are determined by the ratios

$$\Psi_1 = \frac{1}{2} \left\{ [\cos(\chi z) - \sin(\chi z)] \cdot \sin\left(\left(z + \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) - \right. \quad (14)$$

$$\left. - [\cos(\chi z) + \sin(\chi z)] \cdot \sin\left(\left(z - \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right\},$$

$$\begin{aligned} \Psi_3 = -\frac{1}{2} \left\{ [\cos(\chi z) + \sin(\chi z)] \cdot \sin\left(\left(z + \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) + \right. \quad (15) \\ \left. + [\cos(\chi z) - \sin(\chi z)] \cdot \sin\left(\left(z - \frac{a}{2}\right)\sqrt{\chi^2 + 4(\kappa_{\Delta}^2 - \kappa_A^2)}\right) \right\}. \end{aligned}$$

At $\psi_3^{(0)}(z = \pm a/2) = 0, \psi_1^{(0)}(z = \pm a/2) = 0$, we obtain expressions for the energies of the dimensionally-quantized states of electrons at the point X of the Brillouin zone, i.e. with y

$$E = U_0 - \frac{\Delta}{2} - \frac{P^2}{16A} - A\pi^2 \frac{(2n+1)^2}{4} a^2, \quad E = U_0 - \frac{\Delta}{2} - \frac{P^2}{16A} - A\pi^2 n^2 a^2, \quad (16)$$

where the first ratio corresponds to even to the inversion of the coordinates of states, and the second to odd states, an integer.

Note that in the case when $4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2 > 0$, then the wave function can be represented as

$$\psi_3^{(0)}(z) = \exp(-z\chi) \cdot \left[\tilde{C}_1 \cos\left(z\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) + \tilde{C}_3 \sin\left(z\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) \right] \quad (17)$$

Then, from the normalization condition of the wave function, it is easy to obtain expressions for $\tilde{C}_1, \tilde{C}_3$ in the form

$$C_1^{-2} = \frac{sh(a\chi)}{2\chi \left[\chi^2 + 4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2 \right]} \times \left\{ 4(\kappa_A^2 - \kappa_\Delta^2) + \chi^2 \cdot \cos\left(a\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) + \right. \\ \left. + \chi \cdot \sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2} \cdot \sin\left(a\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) \right\}. \quad (18)$$

$$C_3^{-2} = \frac{sh(a\chi)}{2\chi \left[\chi^2 + 4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2 \right]} \times \left\{ -4(\kappa_A^2 - \kappa_\Delta^2) + \chi^2 \cdot \cos\left(a\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) + \right. \\ \left. + \chi \cdot \sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2} \cdot \sin\left(a\sqrt{4(\kappa_A^2 - \kappa_\Delta^2) - \chi^2}\right) \right\}. \quad (19)$$

Thus, it was shown that the dimensionally-quantized spectrum of electrons in a semiconductor, the conduction band of which consists of two subzones, between which there is an energy gap, consists of a set of dimensionally quantized levels that do not intersect each other due to the presence of an energy gap. Expressions are obtained for the wave functions and energy spectra of electrons for different cases, differing from each other by 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 conduction band.

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