Quantum theory of energy parameters of a two-well nanosystem as the main working element of a broadband photodetector of the far IR range

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For stable operation of quantum nanostructures, being the main elements of broadband photodetectors functioning in a very far infrared range, they should demonstrate peculiar characteristics: provide high detective properties over the whole width of the absorption band in the desired range of electromagnetic field energies at minimum dark current. Due to the significant mismatch in the size of the unit cells of anisotropic materials of quantum wells and barriers, it is difficult to produce stable high-quality photodetectors [1]. Therefore, intensive research is underway into such isotropic materials, whose quantum wells and barriers have well-matched unit cell sizes and, with the optimal geometric design, can meet these requirements for the successful operation of QWIPs[2].

In the proposed paper, a quantum mechanical calculation of the electron spectrum and wave functions is performed for a nanoheterostructure, which consists of two wide quantum wells, having an inverted internal structure of the potential profile. The binary QWIP, being a double quantum well with an extremely weak coupling between both of its wide wells is considered. It is assumed that the first well (1) contains an inner barrier and the second well (2) – an inner well with the same physical and geometric parameters (Fig. 1a, b).

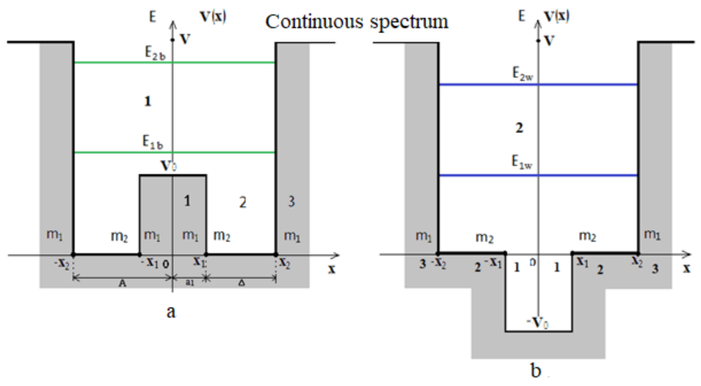

Fig. 1a, b. Potential profiles of the first and second quantum wells

To simplify the cumbersome analytical expressions, we assume that the distance between the wide wells is large enough to consider a structure of two uncoupling wells. At first, let us obtain the spectrum and wave functions of an electron in a wide QW with an internal barrier, Fig. 1a. The potential profile $V_b(x)$ and electron effective mass $m_b(x)$ are fixed by the expressions (1) and (2), respectively:

$$V_b(x)=\begin{cases} V_0, & 0\le|x|\le x_1 \\ 0, & x_1\le|x|\le x_1 \\ V, & x_2\le|x|\le\infty \end{cases} \quad (1) \qquad m_b(x)=\begin{cases} m_1, & 0\le|x|\le x_1 \\ m_2, & x_1\le|x|\le x_1 \\ m_3, & x_2\le|x|\le\infty \end{cases} \quad (2)$$

Solving the Schrödinger equation

$$\left[-\frac{\hbar^2}{2}\frac{d}{dx}\frac{1}{m_b(x)}\frac{d}{dx}+V_b(x)\right]\psi_b(x)=E_b\psi_b(x) \qquad (3)$$

it is clear that since the structure is symmetric, the solutions should be even (s-symmetric) and odd (a-antisymmetric). Considering the above-barrier region of energies ($0\le V_0\le E_b\le V$), for the even states, the wave functions are written in a symmetric form: (4)

$$\psi_b^s(x)=\begin{cases} \psi_{b_1}^s(x)=A_{b_1}^s\cos(k_1x), & 0\le|x|\le x_1 \\ \psi_{b_2}^s(x)=A_{b_2}^s\cos(k_2x)+B_2^s\sin(k_2x), & x_1\le|x|\le x_1 \\ \psi_{b_3}^s(x)=A_{b_3}^s e^{-\gamma|x|}, & x_2\le|x|\le\infty \end{cases}$$

while for odd states, the wave functions are written in an antisymmetric form: (5)

$$\psi_b^a(x)=\begin{cases} \psi_{b_1}^a(x)=A_{b_1}^a\sin(k_1x), & 0\le|x|\le x_1 \\ \psi_{b_2}^a(x)=A_{b_2}^s\cos(k_2x)+B_2^a\sin(k_2x), & x_1\le|x|\le x_1 \\ \psi_{b_3}^a(x)=A_{b_3}^a e^{-\gamma|x|}, & x_2\le|x|\le\infty \end{cases}$$

where

$$k_1=\sqrt{\frac{2m_1(E-V_0)}{\hbar^2}};\ k_2=\sqrt{\frac{2m_2E}{\hbar^2}};\ \gamma=\sqrt{\frac{2m_1(V-E)}{\hbar^2}}; \qquad (6)$$

These functions are continuous at the interfaces of the structure

$$\begin{cases} \psi_{b_1}^{s,a}(x_1)=\psi_{b_2}^{s,a}(x_1);\ \ \psi_{b_1}^{s,a}(x_2)=\psi_{b_2}^{s,a}(x_2); \\ \dfrac{1}{m_1}\dfrac{d\psi_{b_1}^{s,a}(x)}{dx}\Big|_{x=x_1}=\dfrac{1}{m_2}\dfrac{d\psi_{b_2}^{s,a}(x)}{dx}\Big|_{x=x_1} \\ \dfrac{1}{m_2}\dfrac{d\psi_{b_2}^{s,a}(x)}{dx}\Big|_{x=x_2}=\dfrac{1}{m_1}\dfrac{d\psi_{b_3}^{s,a}(x)}{dx}\Big|_{x=x_2} \end{cases} \qquad (7)$$

and satisfy the normality condition

$$\int_{-\infty}^{\infty}\left|\psi_b^{s,a}(x)\right|^2dx=\delta_{s,a} \qquad (8)$$

In an explicit form, the continuity conditions for the symmetric states produce four linear homogeneous equations

$$\begin{cases} A_{b_1}^s\cos(k_1x_1)=A_{b_2}^s\cos(k_2x_1)+B_{b_2}^s\sin(k_2x_1) \\ -\dfrac{k_1}{m_1}A_{b_1}^s\sin(k_1x_1)=-\dfrac{k_2}{m_2}A_{b_2}^s\sin(k_2x_1)+\dfrac{k_2}{m_2}B_{b_2}^s\cos(k_2x_1) \\ A_{b_2}^s\cos(k_2x_2)+B_{b_2}^s\sin(k_2x_2)=A_{b_3}^s e^{-\gamma x_2} \\ -\dfrac{k_2}{m_2}A_{b_2}^s\sin(k_2x_2)+\dfrac{k_2}{m_2}B_{b_2}^s\cos(k_2x_2)=-\dfrac{\gamma}{m_1}A_{b_3}^s e^{-\gamma x_2} \end{cases} \qquad (9)$$

Using it, the equation for the discrete energy spectrum of s-states in above-barrier region is written in a form of a determinant

$$\begin{vmatrix} \cos(k_1x_1) & -\cos(k_2x_1) & -\sin(k_2x_1) & 0 \\ -\dfrac{k_1}{m_1}\sin(k_1x_1) & \dfrac{k_2}{m_2}\sin(k_2x_1) & -\dfrac{k_2}{m_2}\cos(k_2x_1) & 0 \\ 0 & \cos(k_2x_2) & \sin(k_2x_2) & -e^{-\gamma x_2} \\ 0 & -\dfrac{k_2}{m_2}\sin(k_2x_2) & \dfrac{k_2}{m_2}\cos(k_2x_2) & \dfrac{\gamma}{m_1}e^{-\gamma x_2} \end{vmatrix}=0 \qquad (10)$$

Solving it, a compact analytical equation is obtained

$$tg(a_2k_2)=\frac{\dfrac{\gamma}{k_1}\cos(a_1k_1)-\sin(a_1k_1)}{\dfrac{m_bk_2}{m_wk_1}\cos(a_1k_1)+\dfrac{m_w\gamma}{m_bk_2}\sin(a_1k_1)}, \qquad (11)$$

here n=1,2,3,…max n is an index that sequentially numbers the solutions, which are the energies $(E_b^s(n))$ of symmetric states.

The similar calculations for antisymmetric states in the above-barrier part of the discrete energy spectrum brings to the following dispersion equation

$$tg(a_2k_2)=\frac{\dfrac{\gamma}{k_1}\sin(a_1k_1)+\cos(a_1k_1)}{\dfrac{m_bk_2}{m_wk_1}\sin(a_1k_1)-\dfrac{m_w\gamma}{m_bk_2}\cos(a_1k_1)}, \qquad (12)$$

from which the energies of a-states $(E_b^a(n))$ are obtained. All unknown coefficients $A^{a,s}$ and $B^{a,s}$ are found from the system (9) and condition (8). Setting them into (4) and (5), we get the exact analytical expressions for symmetric and antisymmetric wave functions.

The spectrum and wave functions of the electron for the case when a wide QW contains a narrow inner well with the parameters shown in Fig. 1b is obtained in a similar way. As a result, in the region $0\le E\le V$, the dispersion equation for the energies of s-states (E_w^s)

$$tg(\Delta k_2)=\frac{\dfrac{m_1\gamma}{m_3k_1}\cos(a_1k_1)-\sin(a_1k_1)}{\dfrac{k_2}{k_1}\cos(a_1k_1)+\dfrac{m_1\gamma}{m_3k_2}\sin(a_1k_1)}, \qquad (13)$$

as well as one for the energy levels of a-states (E_w^a)

$$tg(\Delta k_2)=\frac{\sin(a_1k_1)+\dfrac{m_3k_1}{m_1\gamma}\sin(a_1k_1)}{\dfrac{m_3k_2}{m_1\gamma}\sin(a_1k_1)-\dfrac{k_1}{k_2}\cos(a_1k_1)}, \qquad (14)$$

are obtained.

The developed theory makes it possible to control the values of optical parameters of QWIPs (positions of energy levels and half-widths of electromagnetic field absorption bands). These devices are function at the base of many nano elements, containing two wide quantum wells with identical potentials (V) and half-widths (A) but different inner wells or barriers, respectively. Inner wells and barriers are located in the centers of both wide QWs and have the same potentials (V_0) and half-widths (a_1). Wide QWs are far enough so as not to affect the spectrum of each other's quasiparticles.

Now, the task is to calculate the energy spectrum of electron (E_w, E_b) in QWs with an inner well (w) and inner barrier (b) as function of V_0 magnitude and geometric size ($A=a_1+\Delta$). Then, the average energy values $\hbar\tilde{\omega}=1/2[\Delta E_b(21)+\Delta E_w(21)]$ and the half-width $\hbar\Delta\tilde{\omega}=|\Delta E_b(21)+\Delta E_w(21)|$ of electromagnetic field absorption bands are obtained. Here $\Delta E_{(b,w)}(21)=E_{2(b,w)}-E_{1(b,w)}$ where $E_{2(b,w)}$ and $E_{1(b,w)}$ are the respective energies of the second (2) and first (1) energy levels in a QW with a barrier (b) and in a QW with a well (w), which is caused by the highest probability of a quantum transition from the ground to the first excited state of the system .

In order to reveal whether there are peculiarities in the formation of energy spectra, and, since, in QWIPs functioning depending on the relationship between the effective masses of electron in wells (m_w) and barriers (m_b), the calculations were performed for three types of nanostructures: a) absent (negligible) difference of masses $m_b=m_w$; b) masses are close ($m_b\ge m_w$), being typical to the experimental parameters; c) the mass in the barrier is bigger than the mass in the well ($m_b=2m_w$). We should note that energetic parameters as functions of V_0 and geometric sizes (a_1, Δ) are calculated for the region where the energies of the excited states E_{2b} and E_{2w} would not be much distant from each other and would not be significantly less than the potential (V) of the QW for good tunneling of the electron current-generated in the system.

The magnitudes V=300 meV and $m_w=m_b=0.075$ are taken as close to those studied experimentally. The potential V_0 and geometric parameters (a_1, Δ) are varied within such limits that the conditions $E_{1\,(b,w)}\ge V_0$ and $E_{2\,(b,w)}\le V$ are fulfilled. The necessary conditions for the operation of QWIPs in such energy interval $(\hbar\tilde{\omega}, \Delta\hbar\tilde{\omega})$ are strongly limited by the magnitudes of the potential (V) and the width (2A) of both QWs. The characteristics of the inner well and barrier (V_0, a_1, Δ) significantly affect the values of the average energy $(\hbar\tilde{\omega})$ and absorption band width $(\Delta\hbar\tilde{\omega})$, and therefore, the coefficient (k) of their ratio, which makes it possible to optimize the operation of QWIPs.

It is revealed that at $m_w=m_b$, regardless of values of V and A parameters for the wide QW and at any values of V_0, a_1, Δ of the inner well or barrier, $E_{1\,b}>E_{1\,w}$, and $E_{2\,b}>E_{2\,w}$ always. It means that due to the tunneling of an electron from the excited state (E_{2b}) of QW with an inner barrier into the excited state (E_{2w}) of QW with a shallow well, a current in corresponding direction will arise. If A, a_1, Δ magnitudes are fixed and the potential V_0 increases ($20\text{ meV}\le V_0\le 60\text{ meV}$), the values of the excited energies E_{2b}, E_{1b} only increase and E_{2w}, E_{1w}– decrease. However, when A is constant and a_1 increases, with respective decreases of Δ, the magnitudes $E_{2\,b}$ i $E_{2\,w}$ change at differently. Therefore, the optical parameters also change differently. If QW width (A) decreases $\hbar\tilde{\omega}$, $\Delta\hbar\tilde{\omega}$ values increase according to quantum mechanical considerations.

As a result, it turned out that in the structures with V=300 meV and if the effective masses in barriers and wells are equal (or very close), double QWIPs could work optimally with QWs of 5nm wide, with an internal barrier and a well with a potential of $V_0=60$ meV and a width of 4 nm. For bigger widths of QWs, it would be necessary to apply a large constant electric field to the structure, which leads to an increase in the dark current, i.e., worsens the sensitivity of the system.

An interesting and important condition for the practical implementation of QWIPs of type (b, c) is shown, in which the typical ratio between the effective masses ($m_w< m_b$) in wells and barriers is observed. The calculation shows that, unlike to the structures with $m_w=m_b$, in these systems, depending on V_0 and geometric parameters (A, a_1), the ratio between the values of the energies of excited states $E_{2b}< E_{2\,w}$ can change to the opposite. At the same time, in the structure where $m_b=2m_w=0.05$ at all values of A>3nm, the operation of QWIPs is impossible due to the large difference ($V-E_{2\,w}$), which complicates the tunneling of electrons between the wells. Only at A=2.5nm (a_1=2nm, Δ=0.5nm) the optimal functioning of QWIP is possible, because beyond these limits the value of $E_{2w}>V$, that is, this level falls into the continuous spectrum.

Analyzing the obtained data, it is clear that only if V_0=60 meV, A=2.5nm, at a_1=1nm or 2nm, the optimal functioning of binary QWIPs can occur.

Main results and conclusions

1. The theory of functioning of QWIPs, constructed of two wide QWs with inner barrier and well, respectively, is developed.
2. The energy spectrum of electron in such nanostructure is calculated and its properties are revealed depending on energetic and geometric parameters of typical QWIPs.
3. The limits of the varying geometric parameters of both wide QWs at which QWIPs operate in the optimal regime are established. When the first excited levels in both wide wells are sufficiently distant from each other (which ensures the required width of the absorption band of the electromagnetic field) and the upper level from both excited ones is located so close to the top of both QWs that provides good electron tunneling, the functioning of QWIP becomes optimal.

References

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