Energy spectrum of a new type of narrow-gap semiconductor heterostructures

A. V. Kolesnikov

L. D. Landau Institute of Theoretical Physics, Russian Academy of Sciences, 117940 Moscow, Russia

A. P. Silin

P. N. Lebedev Physical Institute, Russian Academy of Sciences, 117924 Moscow, Russia

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Semiconductor heterostructures are considered which consist of semiconductors with identical energy gaps and work functions, but different Kane matrix elements (effective masses). Energy quantization in such heterostructures arises only if the momenta associated with the free motion in the plane of the layers of the heterostructure are finite. The energy spectrum consists of a number of valleys, where the effective mass of the current carriers is different in each of them. Each valley, except for the main one, starts from a finite momentum. The correct conditions for joining wave functions for similar kinds of structures are obtained in the single-band approximation. © *1996 American Institute of Physics.* [S1063-7761(96)01506-5]

In semiconductor heterostructures consisting of narrow-gap semiconductors with different Kane matrix elements, it is possible to achieve energy quantization even without energy barriers and quantum wells, i.e., for identical energy gaps 2Δ and work functions of the components of the semiconductor heterostructure.

Wideband superlattices, similar to such heterostructures and formed by semiconductors with identical work functions but different effective masses, were considered in Refs. 1 and 2 in the one-dimensional, single-band approximation, i.e., without taking account of the free motion of the plane of the layers. As will be seen from what follows, this free motion of the current carriers leads to a number of interesting effects, in particular, the formation of bound states in such heterostructures. An attempt to allow for transverse motion was made in Ref. 3; however, the authors of that work limited themselves to a single-band description, valid only for wideband superlattices. In the present paper we consistently take into account the influence of the free transverse motion of the current carriers on the structure of the energy spectrum. Here we first solve the two-band problem for narrow-band semiconductor heterostructures. That done, the result for the wideband case is next obtained by taking the appropriate limit. The answer turns out to be different from the results of Ref. 3. The reason for this discrepancy can be found in the conditions of continuity at the boundary, which differ substantially from those commonly used.

To calculate the energy spectrum, we employ the two-band equation[4–6]

$$\begin{bmatrix} \Delta-E & p_ik-p_i\dfrac{d}{dz} \\ p_ik-p_i\dfrac{d}{dz} & -\Delta-E \end{bmatrix}\begin{Bmatrix}\psi\\ \chi\end{Bmatrix}=0. \qquad (1)$$

Here $\hbar=1$, $k=\sqrt{k_x^2+k_y^2}$ is the momentum of free motion in the plane of the layers of the heterostructure, and $\{{\psi \atop \chi}\}$ are the wave functions. For simplicity, let us consider a double hetero-transition, in which $p_i=p_0$ for $|z|<d/2$ (a "quantum well") and $p_i=p$ for $|z|>d/2$ (a "barrier"). The energy is reckoned from the middle of the forbidden band, and $p>p_0$.

We will restrict the discussion to bound states, i.e., those states for which the wave function falls off exponentially at infinity. In this case, the solution of Eq. (1) has the following form:

$$\begin{Bmatrix}\psi_1(z)\\ \chi_1(z)\end{Bmatrix}=Ne^{k_1z}\begin{Bmatrix}1\\ \beta\end{Bmatrix},\quad z<-\frac{d}{2},$$
$$\begin{Bmatrix}\psi_2(z)\\ \chi_2(z)\end{Bmatrix}=Ne^{-k_1z}\begin{Bmatrix}1\\ \gamma\end{Bmatrix},\quad z>\frac{d}{2}, \qquad (2)$$
$$\begin{Bmatrix}\psi_3(z)\\ \chi_3(z)\end{Bmatrix}=N\left[e^{ik_0z}\begin{Bmatrix}1\\ \beta_0\end{Bmatrix}+Re^{-ik_0z}\begin{Bmatrix}1\\ \gamma_0\end{Bmatrix}\right],\quad |z|<\frac{d}{2}.$$

Here N is a normalization constant, the constant R is determined from the matching conditions,

$$\beta=\frac{p(k+k_1)}{\Delta+E},\quad \gamma=\frac{p(k-k_1)}{\Delta+E},$$
$$\beta_0=\frac{p_0(k+ik_0)}{\Delta+E},\quad \gamma_0=\frac{p_0(k-ik_0)}{\Delta+E},$$
$$k_1=\frac{1}{p}\sqrt{p^2k^2-E^2+\Delta^2},\quad k_0=\frac{1}{p_0}\sqrt{E^2-\Delta^2-p_0^2k^2}.$$

In the new type of heterostructures which we consider here, the boundary conditions are far from ordinary. At the interfaces, the quantity

$$\sqrt{p_i}\begin{Bmatrix}\psi_i\\ \chi_i\end{Bmatrix}(i=1,2,3,\ p_{1,2}=p,\ p_3=p_0), \qquad (3)$$

must be continuous. One can easily convince oneself of this from the equation of continuity.[1)]

Matching the solutions of Eq. (1) at the boundaries $|z|=d/2$ leads to the transcendental equation

$$\cos(u\sqrt{x-1})=\frac{2x^2-x(\xi+1)^2+2\xi^2}{x(\xi-1)^2} \qquad (4)$$

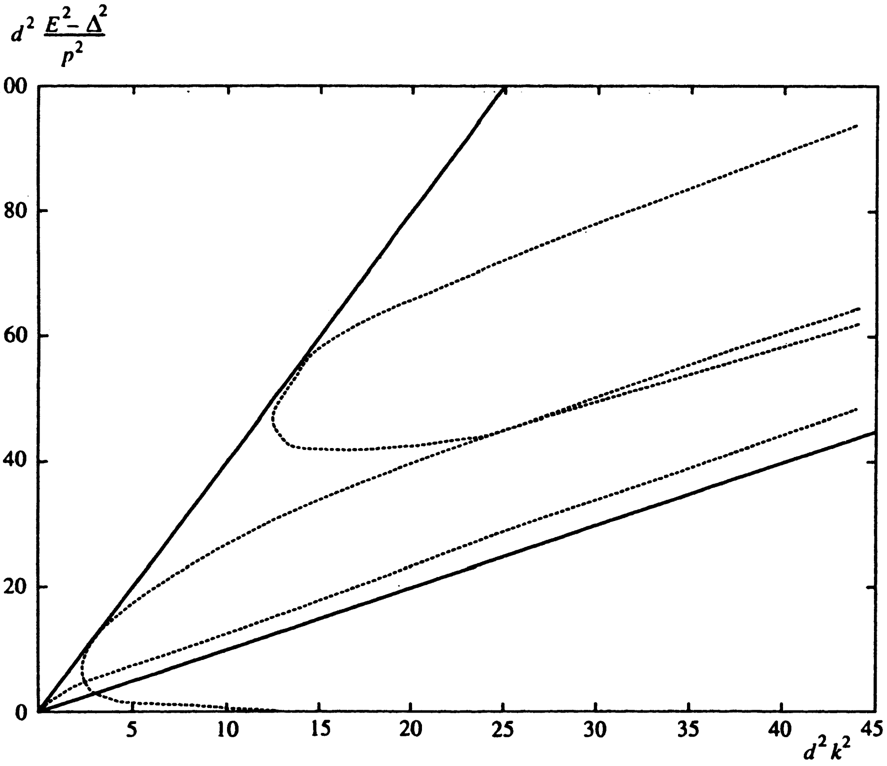

FIG. 1. The solid lines represent the spectrum of the bulk states in each of the semiconductors. The upper straight line overhangs the region of localized states; above it lie the states corresponding to free motion of the carriers. Physically the picture is obvious from its analogy with the Schrödinger problem for the potential $U_{\text{eff}}=(k^2/2)(1/m-1/m_0)$ (Ref. 7), where the latter depends on the momentum parallel to the layers. Therefore, for small k there is only one localized state, and with increasing k the depth of the well grows, as a result of which new levels of size quantization arise.

to determine the energy levels $E_i=\pm\Delta\sqrt{1+\lambda u^2x_i^2}$, $i=0,1,2,3,\ldots$. Here

$$\xi=\frac{p}{p_0},\quad u=2dk,\quad \lambda=\frac{p_0^2}{4d^2\Delta^2}. \tag{5}$$

The plus sign corresponds to electrons, and the minus sign, to holes. In what follows, for definiteness we will consider only electron states. Hole states are obtained by changing the sign of the energy. Since we restrict ourselves to bound states,

$$1<x<\xi^2.$$

Note that Eq. (4) depends only on the momentum k, the layer thickness, and the ratio of the Kane matrix elements, and does not depend on the width of the forbidden band. However, although for a wideband semiconductor the Dirac equation (1) reduces to the Schrödinger equation under the conditions

$$\frac{E-\Delta}{\Delta}\ll 1,\quad \frac{\Delta(E-\Delta)}{p_0^2}\gg k^2,$$

the solution (2) does not reproduce the corresponding energy quantization conditions for the Schrödinger equation even for small values of k. The explanation for this is that the correct condition for matching the wave functions of the Schrödinger equation (and this correct condition is obtained from the Dirac equation) is continuity of the wave function $\sqrt{p_i}\psi_i$ and the combination[8] $p_i^{3/2}(k+d/dz)\psi_i$, which follows directly from Eq. (3). If we take into account that in the case under consideration Δ is continuous and $m_i=\Delta/p_i^2$, then we find that $(1/m^{1/4})\psi_i$ and $(1/m_i^{3/4})(k+d/dz)\psi_i$, and not the usual ψ_i and $(1/m_i)(d/dz)\psi_i$, must also be continuous at the boundary.

Introducing the notation $y=\sqrt{(E^2-\Delta^2)/p_0^2-k^2}$, we can rewrite Eq. (4) in the form

$$\cos^2(yd)=\frac{(k^2(\xi-1)-y^2)^2}{k^2(\xi-1)^2(y^2+k^2)}. \tag{6}$$

The levels of size quantization of the energy E_i are connected with the values of y_i determined by relation (6) by the relation $E_i=\pm\sqrt{\Delta^2+k^2p_0^2+p_0^2y^2(k)}$.

We have analyzed Eq. (6) for the case $\xi=2$. A study of Eq. (6) shows that for any value $k\neq 0$ of the momentum of free motion and $\xi>1$, there is always at least one bound level. And if the conditions

$$k_n<k<k_{n+1},\quad n=1,2,3,\ldots,\quad k_n=\frac{n\pi}{4d\sqrt{\xi^2-1}},$$

are fulfilled, then there are $2n+1$ bound states. Analysis also shows that all the way to the momentum $2dk\leqslant 2.38$ there is only one bound state. It is interesting to note that the new bound states arise in pairs. Note also the presence of a state located in the forbidden bands of both semiconductors, where the exponent in the solution (2) is a real quantity for all values of z. This state is easily studied by a method analogous to that described above if we write down the analytic continuation of Eq. (6):

$$\cosh^2(yd)=\frac{(k^2(1-\xi)-y^2)^2}{k^2(\xi-1)^2(k^2-y^2)},\quad y^2=k^2+\frac{\Delta^2-E^2}{p_0^2}.$$

The given state is analogous to the near-boundary state that arises in semiconductor structures with mutually inverted bands.

The structure of the energy spectrum in the heterostructure considered here differs fundamentally from the energy spectrum of the usual quantum wells (see, e.g., Ref. 9), where there is a system of quantum levels with identical effective masses for the free motion of the current carriers in the plane of the layers. In our case, the energy spectrum consists of a system of energy valleys with different "effective masses"

$$m_i=\frac{m_0}{x_i^2}.$$

Note that the current carriers with $k=0$, strictly speaking, are not bound; since their wave function does not fall off exponentially at infinity, they do not feel such a heterostructure. All the valleys except the lowest ($i=0$) start from some boundary momentum of free motion.

Thus, when the current carriers pass through such a heterostructure, "hot" current carriers with large momenta of free motion in the plane of the layers of the heterostructure will be captured preferentially. This is because for "cold" current carriers bound states are absent.

Note that even simpler systems possess such properties. Thus, if we consider a single hetero-transition with $p_i=p_0$ for $z<0$ and $p_i=p \neq p_0$ for $z>0$, then it is easy to see that the coefficient R of reflection from this hetero-transition will tend to zero as k tends to zero:

$$R=\frac{4k^2(p-p_0)^2(E^2-\Delta^2)}{[k^2(p-p_0)^2+(\sqrt{E^2-\Delta^2-k^2p_0^2}+\sqrt{E^2-\Delta^2-k^2p^2})^2]^2},$$

i.e., such hetero-transitions transmit cold particles preferentially. The expression for R is symmetric under interchange of p_0 and p, i.e., such a hetero-transition identically reflects particles approaching from the right and from the left.

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