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Electronic states in graded-gap junctions with band inversion

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Abstract

We theoretically study electronic states in graded-gap junctions of IV–VI compounds with band inversion. Using a two-band model within the $\boldsymbol{k} \cdot \boldsymbol{p}$ approximation and assuming that the gap and the gap centre present linear profiles, we demonstrate the existence of a set of localized states along the growth direction with a discrete energy spectrum. The envelope functions are found to be a combination of harmonic oscillator eigenfunctions, and the corresponding energy levels are proportional to the square root of the quantum number. The level spacing can be directly controlled by varying the structure thickness.

Narrow-gap IV–VI compounds like $Pb_{1-x}Sn_xTe$ and $Pb_{1-x}Sn_xSe$ present band inversion under compositional variation. In a band-inverted heterojunction the fundamental gap has opposite signs on each side [1]. For instance, $Pb_{1-x}Sn_xSe$ undergoes band inversion as the Sn molar fraction is increased: At $x = 0.14$ the gap vanishes whereas the negative one reaches the magnitude of the PbSe gap at $x = 0.28$. Recently, such heterojunctions have received much attention because subbands of electron-like and hole-like localized interface states are formed with the energy lying within the fundamental gap [2–5], a particular feature not found in most common III–V heterojunctions. In those compounds the electronic states near the gap are properly described by means of a two-band model using the effective $\boldsymbol{k} \cdot \boldsymbol{p}$ approximation [2], where a quite strong coupling of host bands in the semiconductor occurs. The equation governing conduction- and valence-band envelope-functions in a simple two-band model, neglecting far-band corrections, is a Dirac-like equation. In view of the analogy existing between the two-band model and the Dirac equation, the exact solution can be found since one can use elaborated techniques like those related to supersymmetric quantum mechanics [6].

In this paper we exploit further such a formal similarity to demonstrate for the first time the existence of a new type of localized electronic states whose envelope functions resemble those of the harmonic oscillator but, unlike the case of the well-known parabolic quantum wells, there are no classical turning points. In the present structure, the confining potential leading to localized states enters in the equation of motion as a position-dependent mass term, whereas in the case of parabolic quantum wells the conduction-band modulation appears as an electrostatic-like interaction within the framework of a one-band model Hamiltonian. In our approach, we require a graded-gap structure with band inversion. An appropriate graded doping may create a modulation of both conduction- and valence-band with linear profiles, which manifest themselves through the occurrence of a linear scalar potential in the Dirac-like Hamiltonian. For our present purposes, we then take advantage of a number of linear potentials

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for which the Dirac equation reduces to Schrödinger-like harmonic oscillator equations [7], and then exact solutions can be found in a closed form.

The two-band model Hamiltonian in the absence of external fields is of the form

$$\mathcal{H} = \alpha_y v_\perp p_\perp + \alpha_z v_z p_z + \tfrac{1}{2}\beta E_g(z), \tag{1}$$

where the z axis is perpendicular to the heterojunction (it is assumed that the growth direction is [111]), $E_g(z)$ stands for the position dependent gap, α_y, α_z and β are the usual 4×4 Dirac matrices, $v_\perp$ and v_z have dimensions of velocity and they are related to the Kane matrix elements. As usual, it is assumed that these matrix elements are constant through the whole heterostructure. Since the gap and the gap centre depend only upon z, the transversal momentum is a constant of motion and we can set the y axis parallel to this component. In a graded-gap structure of thickness L with band inversion we have $E_g(z) = Kz$, where $K = (E_{gR} - E_{gL})/L$. Here $E_{gR} > 0$ ($E_{gL} < 0$) is the magnitude of the gap at z_R ($-z_L$) with $L = z_R + z_L$ and $E_{gR}/E_{gL} = -z_R/z_L$.

In the two-band model there are four envelope-functions including spin, and we arrange them in a four component spinor $F(\boldsymbol{r})$, whose upper and lower components give the coefficients of the L_6^- and L_6^+ parts of the wave function. This spinor satisfies the equation

$$\mathcal{H} F(\boldsymbol{r}) = [E - V(z)]\, F(\boldsymbol{r}), \tag{2}$$

where $V(z)$ gives the position of the gap centre. The way $V(z)$ changes from one material to another is not well understood, thus it is often considered that the misalignment follows the same profile of $E_g(z)$ [3]. Therefore $V(z) = (\frac{1}{2}\lambda)E_g(z)$ where $\frac{1}{2}\lambda = (V_R - V_L)/(E_{gR} - E_{gL})$, V_R and V_L being the gap centre at z_R and $-z_L$, respectively. We shall see below that the existence of localized states requires that $|\lambda| < 1$, namely the gaps must overlap (type I heterojunctions). The same condition is found for the existence of interface states in band inverted junctions [2]. As we have already mentioned, the momentum perpendicular to the interface is conserved, and therefore we look for solutions of the form $F(\boldsymbol{r}) = F(z)\exp(i\boldsymbol{r}_\perp \cdot \boldsymbol{p}_\perp/\hbar)$ to Eq. (2). The function $F(z)$ satisfies the following equation,

$$[\alpha_y v_\perp p_\perp + \alpha_z v_z p_z + \tfrac{1}{2}\beta E_g(z) - E + V(z)]F(z) = 0. \tag{3}$$

A simple way to solve this equation is the Feynman–Gell-Mann ansatz [8]

$$F(z) = [\alpha_y v_\perp p_\perp + \alpha_z v_z p_z + \tfrac{1}{2}\beta E_g(z) + E - V(z)]\chi(z). \tag{4}$$

After a little algebra we have

$$\left(\frac{d^2}{dz^2} + \frac{1}{\hbar^2 v_z^2}\{\tfrac{1}{4}E_g(z)^2 - [E - V(z)]^2 + v_\perp^2 p_\perp^2\} + M \right)\chi(z) = 0, \tag{5}$$

where the 4×4 constant matrix M is given by $M = -i(K/2\hbar v_z)\alpha_z(\beta - \lambda)$, whose eigenvalues $\pm\mu = \pm(K/2\hbar v_z)\sqrt{1-\lambda^2}$ are real since we take $|\lambda| < 1$. Setting $\chi(z) = f_\pm(z)\phi_\pm$, where $\phi_\pm$ are the eigenvectors corresponding to the eigenvalues $\pm\mu$, we obtain

$$\left(-\frac{d^2}{dz^2} + \mu^2 z^2 + \frac{\lambda K E}{\hbar^2 v_z^2} z \right) f_\pm(z) = \left(\frac{E^2 - v_\perp^2 p_\perp^2}{\hbar^2 v_z^2} \mp \mu \right) f_\pm(z), \tag{6}$$

which clearly reduces to a nonrelativistic oscillator equation by carrying out a suitable translation of the origin of coordinates (recall that $\mu^2 > 0$). Thus, inverting the various transforms necessary to arrive at (6), it is not difficult to demonstrate that envelope functions are simply combinations of Hermite polynomials times a decreasing exponential factor similar to that of the harmonic oscillator, provided that $f(z)$ vanishes at $|z| \to \infty$ in a suitable way. The corresponding bound levels can also be found in a simple fashion, and they are given by

$$E_n^2 = (1 - \lambda^2)(n\hbar v_z K\sqrt{1-\lambda^2} + v_\perp^2 p_\perp^2), \tag{7}$$

n being a positive integer. Notice that the energy levels increase as the square root of K and n, thus being no longer equally spaced. This behaviour is usually obtained in "relativistic-like" oscillator equations [9]. As an example, let us consider the case of selenides with symmetric band inversion, i.e., $-E_{gL} = E_{gR} = E_g$ and $V_L = V_R$ ($\lambda = 0$). Typical parameters are $E_g =$

0.15 eV, $\hbar w_z$ = 2.76 eV. For $L = 2z_R = 2z_L = 600$ Å and $p_\perp = 0$ we obtain four bound state levels with energy less than $\frac{1}{2}E_g$: $E_1 = 37.2$ meV, $E_2 = 52.5$ meV, $E_3 = 64.3$ meV and $E_4 = 74.3$ meV. Hence the level spacings are $E_2 - E_1 = 15.3$ meV, $E_3 - E_2 = 11.8$ meV, $E_4 - E_3 = 10.0$ meV, showing that the levels are not equally spaced but deviation from that behaviour is actually small.

To summarize, we have discussed in some detail the electronic structure of graded-gap heterojunctions of IV–VI compounds presenting band inversion. The theoretical analysis is based on the two-band model arising in the $\boldsymbol{k} \cdot \boldsymbol{p}$ approach which, neglecting far-band couplings, becomes completely analogous to a Dirac-like equation with linearly rising scalar- and electrostatic-like potentials. The Dirac Hamiltonian for linear potentials is exactly solvable, leading to envelope functions that can be expressed as a sum of harmonic oscillator functions. Therefore, carriers are spatially localized close to $z = 0$, i.e., the plane where band inversion occurs. However, notice that the maximum value of the envelope functions is located at $z_0 = -2\lambda E/K\sqrt{1-\lambda^2}$ since Eq. (6) is a harmonic oscillator equation centered at z_0. This is to be compared with interface states lying within the fundamental gap which, in absence of external fields, are centered at the crossing point of the L_6^- and L_6^+ bands [2]. In addition, we have found that the energy levels increase as the square root of the effective coupling K and the quantum number n. Let us stress that the level spacing and the spatial extend of the envelope functions depend on the value of K and, as a consequence, they can be controlled by varying the values of E_{gL} and E_{gR} as well as the thickness of the structure L. Finally, some words concerning the validity of the present model are in order. It is known that Hamiltonian (1) has limitations since it neglects far-band corrections. Those effects can be evaluated by means of the standard second-order perturbation theory [3], although we do not attempt to carry out such a computation here. However, we can confidently expect that our results are valid, at least qualitatively, since in most selenides such corrections only cause small deviations of the results predicted from (1). In fact, interface states lying within the fundamental gap remain even if far-band terms are included in the Hamiltonian, while only minor modifications of the dispersion relation are observed [3]. We hope that our results may encourage experimental effort in this field for two reasons. First, to validate or discard the existence of localized states in actual band-inverted junctions other than interface states. Second, the feature of having oscillator-like states along with their associated discrete spectrum may be the basis for designing new devices and applications.

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References

[1] K. Seeger, Semiconductor physics (Springer, Berlin, 1991).
[2] V. Korenman and H.D. Drew, Phys. Rev. B 35 (1987) 6446.
[3] D. Agassi and V. Korenman, Phys. Rev. B 37 (1988) 10095.
[4] D. Agassi, Phys. Rev. B 49 (1994) 10393.
[5] F. Domínguez-Adame, Phys. Status Solidi (b) 186 (1994) K49.
[6] O.A. Pankratov, Semicond. Sci. Technol. 5 (1990) S204.
[7] F. Domínguez-Adame and M.A. González, Europhys. Lett. 13 (1990) 193.
[8] R.P. Feynman and M. Gell-Mann, Phys. Rev. 109 (1958) 193.
[9] F. Domínguez-Adame and B. Méndez, Can. J. Phys. 69 (1991) 780.