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Green Function Approach to Interface States in Band-Inverted Junctions

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Narrow-gap semiconductor compounds like $Pb_{1-x}Sn_xTe$ and $Hg_{1-x}Cd_xTe$ present band inversion under compositional variation. In a band-inverted heterojunction the fundamental gap, defined as the difference between Γ_6 and Γ_8 energies, has opposite signs on each side [1]. Type III superlattices with band inversion of CdTe/HgTe and PbTe/SnTe have been successfully grown in the past [2, 3]. One of the most conspicuous characteristics of band-inverted heterojunctions is the existence of interface states lying within the fundamental gap, provided that the two gaps overlap [4 to 8]. In IV–VI compounds those interface states are properly described by means of a two-band model using the effective $\boldsymbol{k} \cdot \boldsymbol{p}$ approximation. On the contrary, the analysis is more complex in II–VI compounds due to mixing with heavy-hole states since non-centrosymmetry effects are not negligible in this case. The equation governing conduction- and valence-band envelope functions in a simple two-band model, neglecting far-band corrections, is a Dirac-like equation. Exact solutions can then be found in view of this analogy because one can use elaborated techniques like those related to supersymmetric quantum mechanics [7]. The aim of this note is to present an alternative way of solution based on the so-called *point interaction potentials* [9, 10] (any arbitrary sharply peaked potential approaching the δ-function limit) along with a Green function method. We believe that our treatment gives a very intuitive explanation of the origin of interface states, while other approaches may obscure the way how those states arise. Moreover, the effects of external electric and magnetic fields can be included in a straightforward fashion, as we will show later.

In the effective-mass approximation the electronic wave function is a sum of products of Bloch functions at the band edge with slowly varying envelope functions. The two-band model Hamiltonian in the absence of external fields is of the form

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

where the Z-axis is perpendicular to the heterojunction, $E_G(z)$ stands for the position dependent gap, α_y, α_z, and β are the usual 4×4 Dirac matrices, $v_\perp$ and v_z are interband matrix elements having dimensions of velocity. As usual, it is assumed that these matrix elements are constant through the whole heterostructure due to the similarity of the zone centre in both semiconductors. Since the gap depends only upon z, the transverse momentum is a constant of motion and we can set the Y-axis parallel to this component. In the two-band case there are four envelope functions including spin and we arrange them in a four-

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component vector $F(\boldsymbol{r})$. This vector satisfies the equation

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

where $V(z)$ gives the position of the gap centre. It is understood that the growth direction is [111]. The way $V(z)$ changes from one layer to another is not well understood but, assuming that the interface states spread over distances much larger than the interface region, we can confidently consider it as a step-like function. Accordingly we take

$$E_G(z) = E_{GL}\theta(-z) + E_{GR}\theta(z), \tag{3a}$$

$$V(z) = V_L\theta(-z) + V_R\theta(z), \tag{3b}$$

θ being the Heaviside step function. Here, the subscripts L and R mean left and right sides of the heterojunction, respectively.

As we have already mentioned above, the momentum perpendicular to the interface is conserved, and therefore we look for solutions of the form

$$F(\boldsymbol{r}) = F(z) \exp\left(\frac{i}{\hbar}\, \boldsymbol{r}_\perp \cdot \boldsymbol{p}_\perp\right) \tag{4}$$

to (2). The function $F(z)$ satisfies the following equation:

$$(\alpha_y v_\perp p_\perp + \alpha_z v_z p_z + \tfrac{1}{2}\beta E_G(z) - E + V(z))\, F(z) = 0. \tag{5}$$

A simple way to solve this equation is the Feynman-Gell-Mann *ansatz* [11]

$$F(z) = (\alpha_y v_\perp p_\perp + \alpha_z v_z p_z + \tfrac{1}{2}\beta E_G(z) + E - V(z))\, \chi(z). \tag{6}$$

After a little algebra we obtain

$$\left\{-\frac{d^2}{dz^2} + \frac{1}{\hbar^2 v_z^2}\left[\frac{1}{4}E_G^2(z) - [E - V(z)]^2 + v_\perp^2 p_\perp^2\right] - i\Delta\alpha_z(\beta - \lambda)\,\delta(z)\right\}\chi(z) = 0. \tag{7}$$

For brevity we have defined

$$\Delta = \frac{E_{GR} - E_{GL}}{2\hbar v_z}, \tag{8a}$$

$$\lambda = 2\,\frac{V_R - V_L}{E_{GR} - E_{GL}}, \tag{8b}$$

and we have used the relationships $d\theta(\pm z)/dz = \pm\delta(z)$. Note that in the case of a band-inverted heterojunction $E_{GR}E_{GL} < 0$.

It is worth mentioning that (7) is nothing but a Klein-Gordon equation with scalar-like and electrostatic-like terms depending on position (like a relativistic spinless particle with a position-dependent mass in an electric field as occurs in QED) plus a point interaction potential arising from the discontinuity of the gap and the gap centre. The occurrence of this short-range potential makes possible the existence of bound states deep in the gap. In order to find the bound states we use a Green function formalism, similar to that previously used in the case of the Dirac equation with point interaction potentials [12]. To this end,

let us consider the Green function associated to (7) without the point interaction potential,

$$\left\{-\frac{\partial^2}{\partial z^2}+\frac{1}{\hbar^2 v_z^2}\left[\frac{1}{4}E_G^2(z)-[E-V(z)]^2+v_\perp^2 p_\perp^2\right]\right\}G(z,z';E)=I_4\delta(z-z'), \tag{9}$$

where I_4 stands for the 4×4 unity matrix. Since we are interested in bound state levels, the boundary conditions read

$$\lim_{|z|,|z'|\to\infty} G(z,z';E)=0. \tag{10}$$

The Green function is a 4×4 matrix which permits the factorization $G(z,z';E)=g(z,z';E)\,I_4$, where $g(z,z';E)$ is a scalar function since the operator on the left-hand side of (9) is scalar.

The solution of (7) is then simply written as follows:

$$\begin{aligned}\chi(z) &= i\Delta\alpha_z(\beta-\lambda)\int_{-\infty}^{\infty} dz'\,G(z,z';E)\,\delta(z')\,\chi(z'),\\ &= i\Delta\alpha_z(\beta-\lambda)\,g(z,0;E)\,\chi(0).\end{aligned} \tag{11}$$

It is assumed that the envelope functions are continuous at the heterojunction so that the value $\chi(0)$ is defined without ambiguities; this is completely different from what is found in the Dirac equation for point interaction potentials (see [9] and references therein). Once the Green function is known, the 4-vector $\chi(z)$ can be obtained and using (4) and (6) the envelope functions are finally determined. Bound state levels can be computed taking the limit $z\to 0$ in (11). To obtain nontrivial solutions we require the 4×4 determinant to vanish. Thus, using the definitions of Δ and λ given in (8) we obtain

$$\frac{1}{\hbar^2 v_z^2}\left[\frac{1}{4}(E_{GR}-E_{GL})^2-(V_R-V_L)^2\right]=\left(\frac{1}{g(0,0;E)}\right)^2. \tag{12}$$

At this point we would like to stress that we just require the value of the Green function at the origin of the (X, X') plane if only the bound state levels are needed. In the absence of external fields, as we are considering here, this value is actually not difficult to obtain. Let u_+ and u_- be two independent, scalar solutions of the Sturm-Liouville problem (7) (dropping the point interaction term), vanishing at $+\infty$ and $-\infty$, respectively. Therefore, we can write

$$g(0,0;E)=\frac{u_+(0)\,u_-(0)}{W[u_+,u_-]}, \tag{13}$$

where $W[u_+,u_-]$ is the Wronskian of the two solutions. Defining two real parameters

$$\begin{aligned}K_L &= \frac{1}{\hbar v_z}\sqrt{\frac{1}{4}E_{GL}^2-(E-V_L)^2+v_\perp^2 p_\perp^2},\\ K_R &= \frac{1}{\hbar v_z}\sqrt{\frac{1}{4}E_{GR}^2-(E-V_R)^2+v_\perp^2 p_\perp^2},\end{aligned} \tag{14}$$

the two independent solutions are $u_+ = \exp(-K_R z)$ and $u_- = \exp(K_L z)$ so that $g(0, 0; E) = 2/(K_R + K_L)$. Using (12) one finally obtains

$$K_R + K_L = \frac{1}{\hbar v_z}\sqrt{\frac{1}{4}(E_{GR} - E_{GL})^2 - (V_R - V_L)^2}\,. \tag{15}$$

K_R and K_L should be real for obtaining exponentially decreasing envelope functions as $|z| \to \infty$ and then the gaps must overlap, i.e. $(E_{GR} - E_{GL})^2/4 > (V_R - V_L)^2$. This solution agrees with that previously proposed by Korenman and Drew [5]. The reader is referred to [5] for a full discussion of its physical implications. Here we stress the main advantages of using our method. First of all, we have restricted ourselves to the case of no external potentials. Nevertheless, it is clear that applied electric or magnetic fields can be easily handled with minor modifications of the equations. Note that the crucial point is that one assumes that the Klein-Gordon equation *without* the point interaction potential arising from the abrupt interface can be solved exactly and the corresponding Green function is explicitly written out. This is so for a large variety of electric and magnetic field configurations, as pointed out in [13]. Thus, for instance, it is possible to investigate Landau levels in band-inverted heterojunctions in a rather simple way, instead of using more elaborated mathematical treatments, as those recently carried out by Aggasi [14]. In addition, it is also possible to study the confined Stark effect, a topic which remains open in the literature. The second aspect we remark is the fact that there is no need to use an abrupt heterojunction model, simulated by a step potential. The only requirement is that K_R^{-1} and K_L^{-1} must be much larger than the interface itself, an implicit assumption when using the envelope-function formalism. Qualitatively the profile of the heterojunction is *soliton-like* [7] and, as a consequence, its derivative is a sharply peaked function. Thus the integral equation (11) can be solved by a limiting process, in analogous way to the Dirac equation for sharply peaked functions approaching the δ-function limit [12]. To conclude, we feel that the approach we developed holds valid in a large variety of cases of practical interest and it may help in a better understanding of interface states in band-inverted heterojunctions.

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