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Boundary conditions for tunneling through potential barriers in nonparabolic semiconductors

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A wave equation is formulated by using the energy-wave-vector relation for nonparabolic bands and it is shown that the resultant boundary condition is in agreement with the condition of the continuity of probability current density. The condition is shown to involve the velocity effective mass with the derivatives of the wave function, in place of the energy effective mass, used earlier. Calculated results are also presented for the probability of tunneling through a single rectangular barrier in the $Ga_{0.47}In_{0.53}As/InP/Ga_{0.47}In_{0.53}As$ system, which show that the nonparabolicity reduces significantly the value of the probability from those estimated by using the energy effective mass in the boundary condition.

Tunnel devices and narrow quantum wells have been extensively studied in recent years. The energy of the electrons in these systems is such that the effect of the nonparabolicity of the energy bands cannot be considered negligible. Calculations have been reported for the probability of tunneling through single and double barriers and for the energy eigenvalues in narrow quantum wells,[1–3] in which the energy bands have been taken to be nonparabolic. The nonparabolic dispersion relation, however, admits consideration of three different effective masses, namely, the energy effective mass m_e^*, the velocity effective mass m_v^*, and the acceleration effective mass m_a^*. These are given, respectively, by $(\hbar^2k^2/2E)$, $(\hbar^2k/\nabla_k E)$, and $(\hbar^2/\nabla_k^2 E)$; E and $\mathbf{k}$ are, respectively, the itenerant energy and the wave vector. The three effective masses have the same value for parabolic bands, but the values are significantly different for nonparabolic bands.

The effective mass enters the analysis of quantum devices when k is evaluated from a given E and also when the derivatives of the wave function are matched at the potential discontinuities. It is confusing to find that different effective masses have been used by different authors for the calculation of the same parameter. That m_e^* should be used to obtain k from E cannot be debated, although some authors[4] have used m_v^* and even m_a^*.[5] On the other hand, the confusion about which mass should be used in the boundary condition for the derivatives of the wave functions remains unresolved. The purpose of this letter is to discuss this boundary condition.

The equation for the wave function ψ is written in the effective mass approximation[6] as

$$E(-i\nabla)\psi - E\psi = 0, \tag{1}$$

where E is the energy of the electron measured from the conduction band edge, and the operator $E(-i\nabla)$ is obtained from the $E-k$ relation by substituting $-i\nabla$ for k. For the parabolic dispersion relation, $E=\hbar^2k^2/2m^*$, $E(-i\nabla) = -(\hbar^2/2m^*)\nabla^2$. The equation takes the following form for electrons with zero itinerant energy in quantum systems:

$$(\hbar^2/2m_i^*)\partial_z^2\psi_i + (E - V_i)\psi_i = 0, \tag{2}$$

where $\partial_z = \partial/\partial z$, and the subscript i is the index of the layer in the tunneling structure, assumed to be grown in the z direction. The material is taken to be uniform between the discontinuities. E is measured from the lowest conduction band edge in the structure and V_i is the difference between the conduction band edge energy in the ith layer and this minimum energy.

Problems of quantum devices are solved by first finding the solution of (2) for the constituent layers and then matching the solutions at the interface between ith and the $j(=i+1)$th layer with the boundary conditions:

$$\text{(i)}\,\psi_i = \psi_j; \quad \text{(ii)}\,(i/m_i^*)\partial_z\psi_i = (i/m_j^*)\partial_z\psi_j. \tag{3}$$

The first condition follows from the postulates of wave mechanics. The second condition is postulated as the continuity of the derivatives of the wave functions when transmission of free electrons is considered through potential discontinuities. The energy-wave-vector dispersion relations of superlattices and energy levels in quantum wells were evaluated in the early studies by assuming that the derivatives are continuous, as in the free electron problem.[7] This simplification worked for the $GaAs/Ga_xAl_{1-x}As$ system, apparently because m_i^* and m_j^* approach each other when nonparabolicity is included and become nearly equal. It was, however, concluded by Bastard[8] from k.p analysis that the boundary condition as given in (3) should be used, since m_i^* and m_j^* are different. It was also shown that m_i^* and m_j^* should be the corresponding energy effective masses, m_e^*'s, for nonparabolic energy bands. Currently, this is the most accepted boundary condition. It has been used to compute the energy eigenvalues in quantum wells[3] and also the tunneling probability for barriers.[1] The nonparabolicity parameter has also been obtained from such studies.[1] It has also been concluded that the effect of nonparabolicity is not very significant on energy levels in quantum wells.[3]

It should be noted, however, that for parabolic bands, the condition given by Bastard[8] is the same as that obtained earlier by Ben Daniel and Duke[9] from the condition of continuity of probability current density, which must be obeyed in the steady state. This condition is not, however, satisfied for nonparabolic bands if the energy effective mass is used in (3). This inconsistency has been explained for single quantum wells by stating that no current flows in such wells.[10] On the other hand, it has been argued for tunneling[1] that the condition matches the phase velocity since $\hbar k/m_e^*$ is proportional to $E/\hbar k$ and the requirement of matching the group velocities is met when contributions are summed for electrons with different energies. These arguments, however, cannot be accepted for clarifying the issue, since the boundary condition should not depend on the problem.

A solution to this inconsistency is, however, obtained if the effective-mass equation for nonparabolic semiconductors is formulated by using the corresponding $E-k$ relation to obtain the operator $E(-i\nabla)$.

Nonparabolic isotropic energy bands may be represented, in general, by the dispersion relation:

$$E=V_i+\left(\frac{\hbar^2}{2m_i^*}\right)\sum_{r=1}^{n} a_{ri}k_i^{2r}, \tag{4}$$

where $a_1=1$, the a_{ri}'s are constants dependent on the material, and m_i^* is the band-edge mass.

By using the corresponding expression for $E(-i\nabla)$, Eq. (2) is modified to

$$-\left(\frac{\hbar^2}{2m_i^*}\right)\sum_{r=1}^{n}(-1)^r a_{ri}\partial_z^{2r}\psi_i+(E-V_i)\psi_i=0. \tag{5}$$

Multiplying (5) by ψ_i^*, the corresponding equation for ψ_i^* by ψ_i, and taking the difference of the two equations we obtain

$$\left(\frac{\hbar^2}{2m_i^*}\right)\sum_{r=1}^{n}(-1)^r a_{ri}(\psi^*\partial_z^{2r}\psi_i-\psi\partial_z^{2r}\psi_i^*)=0. \tag{6}$$

But,

$$\begin{aligned}\psi_i^*\partial_z^{2r}\psi_i-\psi_i\partial_z^{2r}\psi_i^* &=\partial_z(\psi_i^*\partial_z^{2r-1}\psi_i-\psi_i\partial_z^{2r-1}\psi_i^* \\ &\quad-\partial_z\psi_i^*\partial_z^{2r-2}\psi_i+\partial_z\psi_i\partial_z^{2r-2}\psi_i^* \\ &\quad+\cdots+\partial_z^{r-1}\psi_i^*\partial_z^r\psi_i-\partial_z^{r-1}\psi_i\partial^r\psi_i^*).\end{aligned} \tag{7}$$

It may be easily shown by using the above expansion that

$$\psi^*\partial_z^{2r}\psi-\psi\partial_z^{2r}\psi^*=\partial_z[(ik)^{2(r-1)}r(\psi^*\partial_z\psi-\psi\partial_z\psi^*)]. \tag{8}$$

Equation (8) hence gives

$$\left(\frac{\hbar^2}{2m_i^*}\right)\sum_{r=1}^{n} r a_{ri}k_i^{2(r-1)}(\psi_i^*\partial_z\psi_i-\psi_i\partial_z\psi_i^*)=\text{constant}. \tag{9}$$

Considering that,

$$\left(\frac{1}{m^*}\right)\sum_{r=1}^{n} r a_r k^{2(r-1)}=\left(\frac{1}{\hbar^2 k}\right)\nabla_k E=\left(\frac{1}{m_v^*}\right), \tag{10}$$

we obtain for the boundary condition,

$$(-i\hbar/2m_{vi}^*)(\psi_i^*\partial_z\psi_i-\psi_i^*\partial_z\psi_i^*)=\text{constant}, \tag{11}$$

which is the condition for the continuity of probability current density. This condition when combined with the condition $\psi_i=\psi_j$ gives for the derivatives at the interface,

$$(1/m_{vi}^*)\partial_z\psi_i=(1/m_{vj}^*)\partial_z\psi_j. \tag{12}$$

Equation (5) also gives the assumed dispersion relation (4) so that k_i is required to be evaluated by using the relation

$$k_i^2=(2m_{ei}^*/\hbar^2)(E-V_i), \tag{13}$$

where

$$\left(\frac{1}{m_{ei}^*}\right)=\left(\frac{2}{\hbar^2}\right)(E-E_c)\left(\sum_{r=1}^{n} a_{ri}k_i^{2(r-1)}\right)^{-1}. \tag{14}$$

Consistent conditions are thus obtained from the formulated wave equation since the wave vector is given by the assumed dispersion relation and the boundary condition for the derivative satisfies the probability current continuity condition. It should, however, be mentioned that a wave equation for nonuniform materials is not required for solving the quantum device problems involving sharp potential discontinuities, as solutions of such problems may be worked out by matching the conditions at the boundaries with solutions for uniform materials, as discussed above. A wave equation for nonuniform materials for which a_r's are dependent on z would be required for special kinds of wells, e.g., parabolic wells or when an electric field is applied. However, the present formulation can be applied also for solving such problems by discretizing such nonuniform materials into uniform sections and then using the method of matching the solutions at the boundaries. The results of the present analysis can therefore be considered generally applicable to the problems involving uniform as well as nonuniform semiconductors with nonparabolic energy bands.

It is of interest to examine if the use of the velocity effective mass in the boundary condition has any significant effect on the final calculated results. The probability of tunneling through a barrier has been calculated for the purpose by using the physical constants of $Ga_{0.47}In_{0.53}As/InP/Ga_{0.47}In_{0.53}As$ system. Values of constants were taken as follow:

$$m_E^*=0.042m_0,\quad m_B^*=0.079m_0,\quad V_B=300\ \text{meV},$$

$$m_0=9.1\times10^{-31}\ \text{kg}.$$

Subscript E indicates $Ga_{0.47}In_{0.53}As$ (emitter), while B indicates InP (barrier).

The dispersion relation was taken as

$$E=V_i+(\hbar^2k^2/2m_i^*)[1-\alpha_i(\hbar^2k^2/2m_i^*)], \tag{15}$$

with $\alpha_E=1.167\ (\text{eV})^{-1}$, $\alpha_B=0.83\ (\text{eV})^{-1}$.

The probability of tunneling, T^*T, for a barrier width of d is given by

$$T^*T=(\cos^2 k_Bd+\gamma^2\sin^2 k_Bd)^{-1}, \tag{16}$$

$$\gamma=(\tfrac{1}{2})(1/r+r);\quad r=k_Em_{vB}^*/k_Bm_{vE}^*, \tag{17}$$

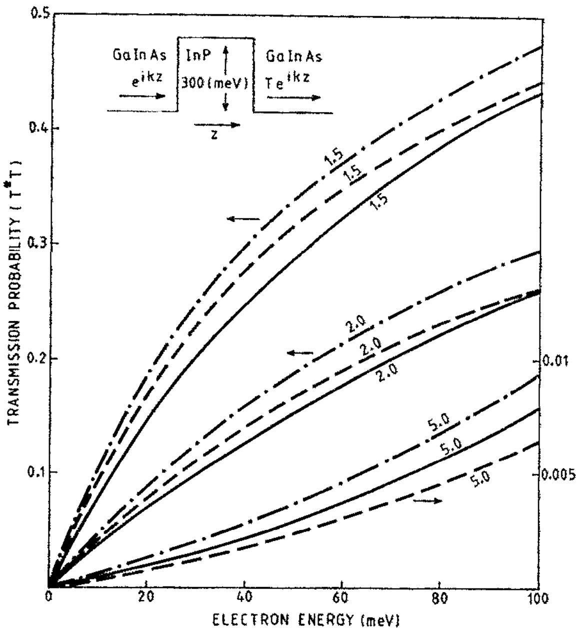

FIG. 1. Transmission probability through a rectangular barrier in the $Ga_{0.47}In_{0.53}As/InP/Ga_{0.47}In_{0.53}As$ system. Full line: present analysis; dashed line: parrabolic band; dashed-dotted line: nonparabolic band using energy effective mass in the boundary condition for the derivative of the wave function. Numbers on the curves indicate the width of the barrier in nm and the arrows point to the reference vertical scale.

$$m^*_{vi}=m^*_i(1-2\alpha_i\hbar^2k_i^2/2m^*_i), \qquad (18)$$

$$k_i^2=(2m^*_i/\hbar^2)\{1/2\alpha_i-(1/2\alpha_i) \times[1-4\alpha_i(E-V_i)]^{1/2}\}. \qquad (19)$$

Calculated values of T^*T are presented in Fig. 1 for the barrier widths of 1.5, 2, and 5 nm. Results for the width of 5 nm are presented in an extended scale to emphasize the differences, as T^*T has small values for this width. Results are shown also for parabolic bands i.e., taking $\alpha_E=\alpha_B=0$, and also when m^*_{vi} is replaced by

$$m^*_{ei}=m^*_i(1-\alpha_i\hbar^2k^2/2m^*_i)^{-1}. \qquad (20)$$

It is seen that the effect of the energy band nonparabolicity is significant and the effect increases with increase in the barrier width. Also, values obtained by using m^*_{vi} in the boundary condition are significantly lower than those for m^*_{ei} and the fractional difference increases with barrier width. A rough calculation for the current density indicates that it may differ by more than 50% for barrier widths of 5 nm.

In conclusion, it may be noted that the analysis presented in this letter shows that the velocity effective mass is required to be used for matching the derivatives of the wave functions at the potential discontinuities. The use of this mass causes a significant reduction in the calculated values of the transmission probability for single barriers. The results on tunneling, analyzed earlier by using the energy effective mass, are therefore required to be reanalyzed to examine if the values of the nonparabolicity parameter, as derived from such study, is altered. Similar reanalysis is also required for examining the conclusion reached earlier that the energy eigenvalues in quantum wells are not much affected by the energy band nonparabolicity.

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