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Establishment of an effective-mass Hamiltonian for abrupt heterojunctions

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For an abrupt heterojunction between two otherwise uniform semiconductors in one dimension we suggest using the effective-mass Hamiltonian $H=-\frac{1}{2}\hbar^2[m(z)]^\alpha\nabla[m(z)]^\beta\nabla[m(z)]^\alpha+V(z)$ with $2\alpha+\beta=-1$ and where $m(z)$ is the position-dependent effective mass and $V(z)$ is the position-dependent conduction band edge. The wave-function matching conditions across the heterojunction are continuity of $m^\alpha\phi$ and $m^{\alpha+\beta}\nabla\phi$. By imposing a simple physical criterion on the solution, ϕ, of the eigenvalue problem for H we find an experssion for β involving the underlying Bloch functions appropriate to the two-component semiconductors, evaluated at the heterojunction. In a model calculation we estimate $\beta\approx 0$ for GaAs-$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$, independent of x.

I. INTRODUCTION

Calculations of physical quantities relevant to semiconductors are often done using effective-mass theory (EMT). For homogeneous semiconductors EMT is well established via the Wannier-Slater theorem.[1] For graded, mixed semiconductors, however, the theory is on a weaker foundation. One of the features of graded, mixed semiconductors that has given difficulty in attempts to derive or justify an EMT is the fact that the effective mass of the charge carriers depends on position. This property leads to complications in defining the kinetic energy operator in the effective-mass Hamiltonian.

In recent years there have been several attempts[2] to establish an EMT—the extended Wannier-Slater theorem—for *slowly* graded, mixed semiconductors; a concensus has not yet been reached, however. For *abrupt* heterojunctions little work has been done in deriving an EMT but some restrictions[3] have been placed on the form the kinetic energy operator can take.

A related problem in the abrupt case is the determination of the matching conditions on the effective-mass wave function and its derivative across the heterojunction. This problem has been addressed in the literature;[4–8] we briefly review the results below after we have established our notation.

Of course, if the Hamiltonian were known everywhere, including the heterojunction, the matching conditions would be readily available. In the absence of knowledge of the Hamiltonian or common agreement on the matching conditions the default matching conditions commonly assumed in applications,[9,10] are continuity of the wave function and of the current. Frequently even the discontinuity in the effective mass across the heterojunction is ignored.[11]

Our earlier work[3] suggests that a kinetic energy operator of the form[12] $\frac{1}{2}[m(z)]^\alpha\hat{p}[m(z)]^\beta\hat{p}[m(z)]^\alpha$, with the (real) parameters α and β unspecified except for the constraint $2\alpha+\beta=-1$, is a prime candidate for constructing a proper effective-mass Hamiltonian:

$$H=-\tfrac{1}{2}\hbar^2[m(z)]^\alpha\nabla[m(z)]^\beta\nabla[m(z)]^\alpha+V(z)\ . \qquad (1)$$

Here $V(z)$ tracks the bottom of the conduction bands—for type-1 heterojunctions, to which we restrict our attention—and so is constant except for a finite discontinuity across the heterojunction. In applications, a slowly varying potential, $W(z)$, due to a shallow impurity or some external influence, would commonly be added to Eq. (1). Such a potential is of no interest to us in the present work and so is ignored.

Notice that away from the heterojunction, in regions where m and V are constant, the Hamiltonian of Eq. (1) reduces to the conventional and required form

$$H=-\frac{\hbar^2}{2m}\nabla^2+V(z)\ , \qquad (2)$$

where m and V are appropriate to the region in which z lies. Thus, in practice, the eigenvalue problem for H is solved by using Eq. (2) and by applying the matching conditions derived from the Hamiltonian of Eq. (1) to the solution ϕ, across the heterojunction. These conditions are continuity[3] of $m^\alpha\phi$ and $m^{\alpha+\beta}\nabla\phi$.

In the Hamiltonian of Eq. (1) the effective mass (m), the conduction-band offset in the potential (V), and the parameter β are all EMT quantities to be specified either through calculations in a more fundamental (e.g., band theory) model or through measurement. Both m and V have been reasonably well determined by experiment; β has not.

We can look to prior model calculations[4–8] of matching conditions to shed some light on the preferred value of β. White and Sham,[4] using a three-band $\mathbf{k}\cdot\mathbf{p}$ approach (conduction, light-hole and heavy-hole bands) to heterojunctions, deduced that the envelope functions, which modulate the Bloch functions appropriate to each semiconductor, must be continuous and their normal derivatives must be discontinuous across the heterojunction. This result coupled with their calculation of the bound states of a sandwich heterostructure leads us to conclude that their EMT comes closest to our $\beta=-1$ case.

Zhu and Kroemer,[5] using Wannier functions as crystalline basis functions in a tight-binding approximation, deduced an effective-mass Hamiltonian that contains a kinetic energy operator like that in Eq. (1) with $\beta=0$ and a potential energy term that incorporates a Dirac delta function at the junction in addition to the band offset. Their matching conditions contain an unknown parameter, S, to be determined empirically just as our β must be. Apparently their $S=1$ case corresponds to our $\beta=0$ case.

Ando and Mori[6] introduce a 2×2 transfer matrix connecting ϕ and $\nabla\phi$ across the heterojunction. These are more general matching conditions than in our model. Nevertheless, in a tight-binding calculation applicable to a chain of atoms having a single s orbital, they deduce a form of the transfer matrix that encompasses our $\beta=0$ case.

Ishibashi *et al.*[7] extended the approach of Ando and Mori[6] to situations in which the band offset is not small and thereby determined a transfer matrix appropriate to nonparabolic bands. Since their transfer matrix involves band-gap energies as well as effective masses their model cannot be directly compared with ours.

Kahen and Leburton,[8] using a hybrid band-structure technique applied to superlattices, determined matching conditions appropriate to our $\beta=-1$ case. Their result incorporates band nonparabolicity through energy-dependent effective masses.

It is thus apparent that there is no universal agreement in the literature as to the correct EMT Hamiltonian nor the correct wave function matching conditions. It does appear that, in the context of our model, the choices $\beta=0$ or $\beta=-1$ are somewhat favored. Doubtless experiment will have to answer the question as to what value of β, if any, is correct.

In the present paper we pursue another approach to the determination of β and express this parameter in terms of Bloch functions appropriate to the two semiconductors, evaluated at the heterojunction. Subject to our approximations, we find that β does not depend on the *size* of the change in chemical composition across the heterojunction but, rather, depends on the *rates* of change of various quantities with respect to chemical composition. This implies, for example, that GaAs-$\mathrm{Al}_x\mathrm{Ga}_{1-x}$As will have one x-independent value of β while InP-$\mathrm{Al}_x\mathrm{In}_{1-x}\mathrm{P}$ will have another. That is, we will show under our criterion, that β depends on the *type* of compound semiconductor but not on the relative amounts of the components mixed in the semiconductor—at least to the extent that crystal parameters depend *linearly* on chemical composition.

Our procedure, used by White and Sham[4] and also suggested by Ando and Mori,[6] for determining β is very simple. We recognize that the eigensolutions of H of Eq. (1) describe scattering states wherein a "free" electron in component semiconductor scatters from the heterojunction, being partially reflected and partially transmitted in the process. If EMT is to be correct we suggest that the reflection and transmission amplitudes calculated from Eq. (1) should be the same as those calculated from a more fundamental approach—one that involves Bloch functions and explicitly incorporates the underlying periodic crystalline potentials. By adopting this criterion we find an expression for β valid for low-energy electrons and small conduction-band offsets, necessary limitations of conventional EMT. By resorting to a model calculation, using a Kronig-Penney–type model with δ-function potentials, we are able to express β in terms of other EMT parameters with the result that, for typical semiconductors $\beta\approx0$. This is in agreement, or at least consistent, with some previous estimates.[5,6]

In Sec. II we set up the problem in the Bloch function formalism; in Sec. III we implement the approach described above and give expressions for β in terms of the underlying Bloch functions; in Sec. IV we describe our model calculation; and in Sec. V we discuss our results.

II. BLOCH FORMALISM

In the one-electron approximation the Hamiltonian for a graded, mixed semiconductor in one dimension is given by

$$\mathscr{H}=-\frac{\hbar^2}{2m}\nabla^2+\mathscr{V}(z,\mathscr{L}(z)) , \tag{3}$$

where m is the free-electron mass, $\mathscr{V}(z,\mathscr{L}(z))$ is the quasi-periodic semiconductor potential in the virtual-crystal approximation, and $\mathscr{L}(z)$ is the grading function that describes the mixing of the components present in the compound semiconductor.

In a situation where the compound semiconductor consists of two components, such as GaAs and AlAs, it is common to let $\mathscr{L}(z)$ be the fraction of AlAs present and to write

$$\mathscr{V}(z,\mathscr{L}(z))=\mathscr{V}_{\mathrm{GaAs}}(z)+\mathscr{L}(z)[\mathscr{V}_{\mathrm{AlAs}}(z)-\mathscr{V}_{\mathrm{GaAs}}(z)] . \tag{4}$$

We elect not to be so specific at this stage and simply model an abrupt heterojunction by choosing

$$\mathscr{L}(z)=\begin{cases}L_1 \text{ for } z<0 ,\\ L_2 \text{ for } z>0 ,\end{cases} \tag{5}$$

so that the quasiperiodic potential in Eq. (3) becomes

$$\mathscr{V}(z,\mathscr{L}(z))=\begin{cases}\mathscr{V}(z,L_1) \text{ for } z<0 ,\\ \mathscr{V}(z,L_2) \text{ for } z>0 .\end{cases} \tag{6}$$

We make the further simplifying assumption that

$$\mathscr{V}(-z,L_i)=\mathscr{V}(z,L_i) . \tag{7}$$

This latter condition leads to certain symmetry conditions on the Bloch functions that simplify some of our final expressions.

We now seek solutions of

$$\mathscr{H}\Psi(z)=\mathscr{E}\Psi(z) , \tag{8}$$

where

$$\mathscr{H}=\begin{cases}-\dfrac{\hbar^2}{2m}\nabla^2+\mathscr{V}(z,L_1) \text{ for } z<0 ,\\ -\dfrac{\hbar^2}{2m}\nabla^2+\mathscr{V}(z,L_2) \text{ for } z>0 ,\end{cases}$$

and where the matching conditions across $z=0$ are continuity of Ψ and $\nabla\Psi$.

The eigenfunctions of Eq. (8) are not pure Bloch states; more properly they are scattering states, $\Psi_{k_i}^{(i)}$, which may be constructed from Bloch states, $\psi_k(z)$, belonging to the separate regions $z<0$ and $z>0$. Thus

$$\Psi_{k_1}^{(1)}(z)\equiv\begin{cases}\psi_{k_1}(z)+\mathcal{R}^{(1)}\psi_{-k_1}(z) \text{ for } z<0\ ,\\ \mathcal{T}^{(1)}\psi_{k_2}(z) \text{ for } z>0\ ,\end{cases}$$

$$\Psi_{k_2}^{(2)}(z)\equiv\begin{cases}\mathcal{T}^{(2)}\psi_{-k_1}(z) \text{ for } z<0\ ,\\ \psi_{-k_2}(z)+\mathcal{R}^{(2)}\psi_{k_2}(z) \text{ for } z>0,\end{cases} \tag{9}$$

and k_i is positive and less than π/a_i where a_i is the appropriate lattice constant.

Appendix A contains a short summary of the properties of the Bloch functions $\psi_k(z)$ appropriate to a periodic, symmetric potential $\mathcal{V}(z)$. These will be useful later. Note also that we are neglecting the band index as a label in writing down the scattering states in Eq. (9) and in subsequent equations. This does not constitute an approximation, however; Eq. (9) is the most general solution of Eq. (8) for given energy.

The connection between $\mathcal{E}$ and k_i is given by a dispersion relation $\mathcal{E}=\mathcal{E}^{(i)}(k_i)$ which, for k_i near the assumed band minimum at $k_i=0$, may be written

$$\mathcal{E}=\mathcal{E}^{(i)}(k_i)\approx\mathcal{E}^{(i)}(0)+\frac{\hbar^2k_i^2}{2m_i}\ . \tag{10}$$

Thus, the k_1 and k_2 appearing on the right-hand sides of Eq. (9) in the definitions of $\Psi_{k_1}^{(1)}(z)$ and $\Psi_{k_2}^{(2)}(z)$ are not independent but are each determined by the energy. Of course, if $\Psi_{k_1}^{(1)}(z)$ and $\Psi_{k_2}^{(2)}(z)$ belong to different energies then the k_i associated with the former are independent of the k_i associated with the latter.

$\Psi_{k_i}^{(i)}$ with $i=1$ (2) represents the state in which a right (left) traveling electron is incident on the heterojunction from the region $z<0$ ($z>0$) with wave number k_1 (k_2). $\Psi_{k_i}^{(i)}(z)$ therefore exists only if $k_i\geq 0$. The normalization of these states can be shown to be

$$(\Psi_{k_i}^{(i)},\Psi_{k_j'}^{(j)})=\delta_{ij}\delta(k_i-k_j') \tag{11}$$

where $\Psi_{k_i}^{(i)}(z)$ and $\Psi_{k_i'}^{(i)}(z)$ belong to different energies unless $k_i=k_i'$. It is apparent from Eq. (11) that the subscript k_i in $\Psi_{k_i}^{(i)}(z)$ is a continuous variable that uniquely distinguishes states belonging to the same i but different energies from each other. The totality of states in a given band thus consists of $\Psi_{k_1}^{(1)}(z)$ with $0<k_1<\pi/a_1$ and $\Psi_{k_2}^{(2)}(z)$ with $0<k_2<\pi/a_2$, k_1 and k_2 ranging independently of each other.

The reflection and transmission amplitudes, $\mathcal{R}^{(i)}$ and $\mathcal{T}^{(i)}$ are determined by matching $\Psi_{k_i}^{(i)}(z)$ and $\nabla\Psi_{k_i}^{(i)}(z)$ at $z=0$. The result, in a form that will be useful later, is

$$\frac{1+\mathcal{R}^{(1)}}{\mathcal{T}^{(1)}}=\frac{\mathcal{T}^{(2)}}{1+\mathcal{R}^{(2)}}=\frac{\psi_{k_2}(0)}{\psi_{k_1}(0)}\ ,$$

$$\frac{1-\mathcal{R}^{(1)}}{\mathcal{T}^{(1)}}=\frac{\mathcal{T}^{(2)}}{1-\mathcal{R}^{(2)}}=\frac{\psi_{k_1}(0)}{\psi_{k_2}(0)}\frac{\partial\mathcal{E}^{(2)}/\partial k_1}{\partial\mathcal{E}^{(1)}/\partial k_1}\ . \tag{12}$$

In deriving Eq. (12) we have exploited the assumed symmetry of the potentials, Eq. (7), by making use of Eqs. (A7) and (A8) at $z=0$. We have also used Eqs. (A10) and (A13) to simplify the results.

In writing the expressions for $\Psi_{k_i}^{(i)}(z)$ in Eq. (9) we implicitly assumed that the energy $\mathcal{E}$ was in an allowed band for electrons in both the $z<0$ and the $z>0$ regions. This will not always be the case for there are energies that lie in an allowed band on one side of the heterojunction but in a band gap on the other side. To appropriately modify the expressions in Eq. (9) to cover such a case it is only necessary to analytically continue the given expressions in $\mathcal{E}$ and reject any terms that diverge with increasing values of $|z|$. For example, suppose that the energy is in an allowed band for $z<0$ but in a forbidden band for $z>0$. We should reject $\Psi_{k_2}^{(2)}(z)$ and replace k_2 by $i\kappa_2$ (κ_2 real and positive) in $\Psi_{k_1}^{(1)}(z)$. This leads to $\Psi_{k_1}^{(1)}(z)$ decreasing exponentially as $z\to+\infty$, i.e., the transmitted wave is damped out as required physically.

III. DETERMINATION OF β

We next seek solutions of the EMT eigenvalue equation

$$H\Phi=E\Phi\ , \tag{13}$$

where H is given by Eq. (1) with

$$V(z)=\begin{cases}\mathcal{E}^{(1)}(0) \text{ for } z<0\ ,\\ \mathcal{E}^{(2)}(0) \text{ for } z>0\ ,\end{cases} \tag{14}$$

and we note that $V(z)$ tracks the bottom of the conduction band and contains the discontinuity of the band edge across the heterojunction.

The solutions of Eq. (13) are scattering states, $\Phi_{k_i}^{(i)}(z)$, and may be constructed from plane-wave states belonging to the separate regions $z<0$ and $z>0$:

$$\Phi_{k_1}^{(1)}(z)\equiv\begin{cases}e^{ik_1z}+\mathcal{R}^{(1)}e^{-ik_1z} \text{ for } z<0\ ,\\ \mathcal{T}^{(1)}e^{ik_2z} \text{ for } z>0\ ,\end{cases}$$

$$\Phi_{k_2}^{(2)}(z)\equiv\begin{cases}\mathcal{T}^{(2)}e^{-ik_1z} \text{ for } z<0\ ,\\ e^{-ik_2z}+\mathcal{R}^{(2)}e^{ik_2z} \text{ for } z>0\ .\end{cases} \tag{15}$$

In accordance with the criterion proposed in the Introduction we have used the same reflection and transmission amplitudes in Eq. (15) we used in Eq. (9).

We now impose on the solutions in Eq. (15) the matching conditions appropriate to the Hamiltonian of Eq. (1) or Eq. (13), namely continuity[3] of $m^{\alpha}\Phi_{k_i}^{(i)}(z)$ and $m^{\alpha+\beta}\nabla\Phi_{k_i}^{(i)}(z)$ across the heterojunction at $z=0$, and use the reflection and transmission amplitudes of Eq. (12) to obtain

$$\alpha = \left[\ln \frac{1+\mathscr{R}^{(1)}}{\mathscr{T}^{(1)}} \right] \Big/ \ln \frac{m_2}{m_1} \left[\ln \frac{\psi_{k_2}(0)}{\psi_{k_1}(0)} \right] \Big/ \ln \frac{m_2}{m_1} ,$$

$$\beta = \left[\ln \left[\frac{k_1}{k_2} \frac{1-\mathscr{R}^{(1)}}{1+\mathscr{R}^{(1)}} \right] \right] \Big/ \ln \frac{m_2}{m_1}$$

$$= \left[\ln \left[\frac{\psi_{k_1}(0)^2}{\psi_{k_2}(0)^2} \frac{k_1 \partial \mathscr{E}^{(2)}/\partial k_2}{k_2 \partial \mathscr{E}^{(1)}/\partial k_1} \right] \right] \Big/ \ln \frac{m_2}{m_1} . \tag{16}$$

These values of α and β will not yield an entirely acceptable effective-mass Hamiltonian since they are energy dependent. However, we can extract acceptable expressions by recognizing that in EMT energies must be near the bottom of the conduction bands. We begin by simplifying β of Eq. (16) for small values of k_1 and k_2 in the parabolic band approximation to obtain

$$\beta = \left[\ln \frac{\psi_{k_1}(0)^2}{\psi_{k_2}(0)^2} \frac{m_1}{m_2} \right] \Big/ \ln \frac{m_2}{m_1} \tag{17}$$

and, incidentally, find $2\alpha+\beta=-1$ to be automatically satisfied.

To proceed further let us take the band discontinuity $\mathscr{E}^{(2)}(0)-\mathscr{E}^{(1)}(0)$ to be small or, more properly, $\Delta\mathscr{L} \equiv L_2 - L_1$ to be small. Then we can expand m_2 and $\psi_{k_2}(0)$ in Taylor series in Δ:

$$m_2 = m_1 + \frac{\partial m}{\partial \mathscr{L}} \Delta\mathscr{L} ,$$

$$\psi_{k_2}(0) = \psi_{k_1}(0) + \frac{\partial \psi_k}{\partial \mathscr{L}} \Delta\mathscr{L} , \tag{18}$$

which yields

$$\beta = -1 - 2 \left[\frac{1}{\psi_0(0)} \frac{\partial \psi_0(0)}{\partial \mathscr{L}} \right] \Big/ \left[\frac{1}{m} \frac{\partial m}{\partial \mathscr{L}} \right] \tag{19}$$

and, of course, $\alpha = -(1+\beta)/2$.

This shows that β depends on the *rates* of change of quantities with respect to the grading function but not on the *size* of the changes. Thus β for, say, a GaAs-$\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As}$ heterojunction (with $x \equiv \mathscr{L}$) is *independent* of x—to the extent that our approximations are valid.

Equation (19) constitutes our primary result: an expression for the EMT parameter β in terms of underlying band theory quantities. It is thus on the same footing as two other EMT parameters—the effective mass and the conduction-band offset.

In order that our EMT Hamiltonian of Eq. (1) be useful in calculations we must obtain a value for β. We therefore turn to a model calculation of this parameter in the next section.

IV. MODEL CALCULATION

In order to obtain an estimate of β for use in EMT we resort to a simplified Kronig-Penney calculation. For the heterojunction potential of Eq. (6) we choose

$$\mathscr{V}(z,\mathscr{L}(z)) = \begin{cases} V_1 a \sum\limits_{n=0}^{\infty} \delta[z+(2n+1)a/2] & \text{for } z<0 \\ V_2 a \sum\limits_{n=0}^{\infty} \delta[z-(2n+1)a/2] & \text{for } z>0 \, . \end{cases} \tag{20}$$

This is a series of δ-functions located at $z=\pm a/2$, $\pm 3a/2$, $\pm 5a/2, \ldots$, where the potential strengths are different in the $z<0$ and $z>0$ regions.

The desired Bloch functions to be used in Eq. (9) are readily found to be, for $-a/2<z<a/2$,

$$\psi_{k_i} = C(k_i) e^{ik_i z} \left[e^{i(K-k_i)z} \sin \left[\frac{K+k_i}{2} a \right] + e^{-i(K+k_i)z} \sin \left[\frac{K-k_i}{2} a \right] \right] , \tag{21}$$

where

$$C(k_i) = \left[\sin^2 \left[\frac{K+k_i}{2} a \right] + \sin^2 \left[\frac{K-k_i}{2} a \right] + 2 \sin \left[\frac{K-k_i}{2} a \right] \sin \left[\frac{K+k_i}{2} a \right] \frac{\sin(Ka)}{Ka} \right]^{-1/2} \times (2\pi)^{-1/2} ,$$

and where K is defined by $\mathscr{E} \equiv \dfrac{\hbar^2 K^2}{2m}$.

The solution in, say, the interval $(2n-1)a/2<z<(2n+1)a/2$ is found by using the actual value of z in the external phase ikz but by using the value $(z-na)$ in the term in the square brackets of Eq. (21). That is, the value used for z in the latter term must lie between $-a/2$ and $a/2$. This guarantees the translation invariance property, Eq. (A4): $u(z+a)=u(z)$.

Let us now evaluate the EMT parameter β using Eq. (16). From Eqs. (12), (A10), (A13), and (21) we find

$$\frac{1-\mathscr{R}^{(1)}}{1+\mathscr{R}^{(1)}} = \frac{\psi_{k_1}(0)^2}{\psi_{k_2}(0)^2} \frac{\partial \mathscr{E}^{(2)}/\partial k_2}{\partial \mathscr{E}^{(1)}/\partial k_1}$$

$$= \frac{\psi_{k_1}(0) \nabla \psi_{k_2}(0)}{\psi_{k_2}(0) \nabla \psi_{k_1}(0)}$$

$$= \frac{\cos(k_1 a/2) \sin(k_2 a/2)}{\sin(k_1 a/2) \cos(k_2 a/2)} . \tag{22}$$

We now wish to use this result in Eq. (16) to find β. In doing so we must limit ourselves to "small" values of k_1 and k_2. For the sake of definiteness let us take the conduction-band discontinuity

$$\Delta\mathscr{E} \equiv \mathscr{E}^{(2)}(0) - \mathscr{E}^{(1)}(0) > 0$$

and let $k_2 \to 0$. Then k_1 may be determined from Eq. (10)

$$\frac{\hbar^2 k_1^2}{2m_1} = \Delta\mathscr{E} . \tag{23}$$

We then have, from Eqs. (22) and (23), as $k_2 \rightarrow 0$

$$\frac{k_1}{k_2}\frac{1-\mathscr{R}^{(1)}}{1+\mathscr{R}^{(1)}} \rightarrow (k_1 a/2)\frac{\cos(k_1 a/2)}{\sin(k_1 a/2)} \rightarrow 1-\tfrac{1}{12}k_1^2 a^2$$

$$\approx 1-\Delta\mathscr{E}\frac{m_1 a^2}{6\hbar^2} = 1-\frac{m_1 a^2}{6\hbar^2}\frac{\partial\mathscr{E}}{\partial\mathscr{L}}\Delta\mathscr{L} \qquad (24)$$

and so, using Eqs. (18) and (24) in Eq. (16),

$$\beta \approx -\frac{m^2 a^2}{6\hbar^2}\frac{\partial\mathscr{E}/\partial\mathscr{L}}{\partial m/\partial\mathscr{L}} \; . \qquad (25)$$

This expression is entirely in terms of EMT parameters which are known experimentally. For a GaAs-A1_xAs heterojunction Casey and Panish[13] give $E_{\text{gap}} = (1.424 + 1.247x)$ eV for $0 < x < 0.45$, $m = (0.067 + 0.083x)m_0$ where m_0 is the free-electron mass, and $a \approx 5.60$ A. Miller *et al.*[10] estimate the shift of the conduction-band edge with changing chemical composition to be 57% of the shift of the band gap, so that $\Delta = 0.57(1.247x)$ eV. Using these parameter values we find $\beta \approx -0.03$. Even a Si-Ge heterojunction yields a β of the same order of magnitude. This would suggest that $\beta = 0$ might be a reasonable value for many heterojunctions, thus giving the matching conditions across the junction as continuity of $\phi/m^{1/2}$ and $\nabla\phi/m^{1/2}$.

V. SUMMARY

For an abrupt heterojunction between two otherwise homogeneous semiconductors we suggest using the effective-mass Hamiltonian

$$H = -\tfrac{1}{2}\hbar^2[m(z)]^{\alpha}\nabla[m(z)]^{\beta}\nabla[m(z)]^{\alpha} + V(z) \; , \qquad (1)$$

with $2\alpha+\beta=-1$ and where $V(z)$ denotes the bottom of the conduction band appropriate to the semiconductor at the point z. By adopting a simple physical criterion we were able to find an expression for β in Eq. (19) in terms of the Bloch functions of the two semiconductors, evaluated at the heterojunction. The physical criterion we adopted was that the reflection and transmission amplitudes describing the scattering of electrons from the heterojunction and calculated from EMT are the same as those calculated in a more fundamental approach using Bloch functions. Since these amplitudes serve to define basis functions in the two approaches [Eqs. (15) and (9), respectively] physical quantities calculated in EMT and calculated using the Bloch formalism should agree.

By resorting to a simple Kronig-Penney—type model we found an expression for β, Eq. (25), entirely in terms of EMT parameters. Commonly used heterojunctions appear to require $\beta \approx 0$ which, in turn, requires continuity of $\phi/m^{1/2}$ and $\nabla\phi/m^{1/2}$ across the heterojunction. This result is consistent with some previous determinations[5,6] of matching conditions; it does not agree with others,[4,7,8] some of which[4,8] favor $\beta = -1$.

Several simplifying assumptions (some basic to all EMT models) were involved in our derivation: (a) there is an abrupt change in the underlying crystalline properties at the heterojunction, with no band curvature, (b) the underlying crystalline potentials are spatially symmetric, (c) the junction is located one-half of a respective lattice constant from the nearest lattice points, (d) the conduction-band discontinuity across the junction is small, (e) electrons have energies near the bottoms of the conduction bands, (f) the bands are parabolic, and (g) the problem is one-dimensional. In applications not consistent with our approximations we cannot put great faith in the value $\beta=0$. However, we do feel that Eq. (1) for the EMT Hamiltonian has merit even in these situations if β is viewed as a parameter to be determined by fits to experimental data, just as m and V are.

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APPENDIX: PROPERTIES OF BLOCH FUNCTIONS

An electron of mass m in a periodic one-dimensional, symmetric potential, $\mathscr{V}(z) = \mathscr{V}(-z)$ with lattice constant a is governed by the Schrödinger equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi + \mathscr{V}(z)\psi = \mathscr{E}\psi \; , \qquad (\text{A1})$$

which is satisfied by Bloch functions

$$\psi_{nk}(z) = e^{ikz}u_{nk}(z) \; , \qquad (\text{A2})$$

where n is the band index and where the crystal momentum, k, is limited to the first Brillouin zone: $|k| < \pi/a$.

The functions $u_{nk}(z)$ satisfy

$$\nabla^2 u_{nk} + 2ik\nabla u_{nk} - \frac{2m}{\hbar^2}\mathscr{V}(z)u_{nk} = (k^2 - 2m\mathscr{E}/\hbar^2)u_{nk} \qquad (\text{A3})$$

and

$$u_{nk}(z+a) = u_{nk}(z) \; . \qquad (\text{A4})$$

These conditions yield a dispersion relation connecting $\mathscr{E}$ and k which we acknowledge in the following by treating $\mathscr{E}$ as a function of k. Our normalization will be

$$\int_0^a dz\, u_{nk}^*(z)u_{n'k}(z) = \frac{a}{2\pi}\delta_{nn'} \; , \qquad (\text{A5})$$

giving

$$(\psi_{nk}, \psi_{n'k'}) \equiv \int_{-\infty}^{+\infty} dz\, \psi_{nk}^*(z)\psi_{n'k'} = \delta(k-k')\delta_{nn'} \; . \qquad (\text{A6})$$

From Eqs. (A1)—(A4) it is possible to show that the functions $u_{nk}(z)$ are such that

$$\psi_{nk}(z) = \psi_{n-k}^*(z) = \psi_{nk}^*(-z) \; , \qquad (\text{A7})$$

and, therefore, that

$$\nabla\psi_{nk}(z) = \nabla\psi_{n-k}^*(z) = -\nabla\psi_{nk}^*(-z) \; . \qquad (\text{A8})$$

With these symmetry properties the conserved current

$$j_{nk}(z) \equiv \frac{\hbar}{2mi}[\psi_{nk}^*(z)\nabla\psi_{nk}(z) - \psi_{nk}(z)\nabla\psi_{nk}^*(z)] \; , \qquad (\text{A9})$$

takes a simple form when evaluated at $z=0$:

$$j_{nk}(0)=\frac{\hbar}{mi}\psi_{nk}(0)\nabla\psi_{nk}(0)\ . \tag{A10}$$

Another useful expression for $j_{nk}(0)$ can be derived from Eq. (A1) and its complex conjugate. We let ψ_{nk} and $\psi_{n'k'}$ be solutions belonging to energies $\mathcal{E}$ and $\mathcal{E}'$, respectively. Then

$$\psi^*_{nk}\nabla^2\psi_{n'k'}-\psi_{n'k'}\nabla^2\psi^*_{nk}=-\frac{2m}{\hbar^2}(\mathcal{E}'-\mathcal{E})\psi^*_{nk}\psi_{n'k'}$$

or

$$\nabla(\psi^*_{nk}\nabla\psi_{n'k'}-\psi_{n'k'}\nabla\psi^*_{nk})=-\frac{2m}{\hbar^2}(\mathcal{E}'-\mathcal{E})\psi^*_{nk}\psi_{n'k'} \tag{A11}$$

We integrate Eq. (A11) over z from 0 to a and use the symmetry property, Eq. (A4), to obtain

$$(e^{i(k'-k)a}-1)[\psi^*_{nk}(0)\nabla\psi_{n'k'}(0)-\psi_{n'k'}(0)\nabla\psi^*_{nk}(0)]$$
$$=-\frac{2m}{\hbar^2}(\mathcal{E}'-\mathcal{E})\int_0^a dz\,\psi^*_{nk}(z)\psi_{n'k'}(z)\ . \tag{A12}$$

Finally we take $n'=n$, and let $k'\rightarrow k$, $\mathcal{E}'\rightarrow\mathcal{E}$ and use Eqs. (A5), (A7), (A8), and (A10) to obtain from Eq. (A12)

$$j_{nk}(0)=\frac{1}{2\pi\hbar}\frac{\partial\mathcal{E}}{\partial k}\ . \tag{A13}$$

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