# Tunneling calculations for systems with singular coupling matrices: Results for a simple model

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The tight-binding approach has become one of the most common and useful methods for incorporating band-structure effects into the calculation of the tunneling resonances of resonant tunneling diodes, the energy levels of quantum wells, and other heterostructure properties. For several years now, numerical stabilization methods have allowed the use of tight-binding models for even very long structures ($\sim$3000 Å). These methods still, however, suffer from a common deficiency: the reliance on a transfer-matrix calculation to determine the boundary conditions. The difficulty is rooted in the fact that the mere generation of a transfer matrix requires a matrix inversion which may not always be possible. Recently, we have shown how to obtain the complex band structure in the case of singular coupling matrices, for which a transfer matrix does not exist. Here we study a simple model, deliberately constructed in such a way that a transfer matrix does not exist, and demonstrate that its tunneling properties are exactly what one anticipates from the bulk bands. [S0163-1829(96)00836-3]

Empirical tight-binding techniques have been employed for a number of years now in tunneling calculations for quantum heterostructures such as resonant tunneling diodes. They can provide a much more complete description of the bulk band structures of the constituent materials than can effective-mass approaches and they are well suited to handling heterointerfaces. Numerical stabilization methods[1–3] have permitted their use in modeling structures in excess of 3000 Å long. Despite these impressive achievements, tight-binding approaches still have one significant remaining problem, perhaps not as widely recognized as it should be: the reliance on transfer matrices.[4] In these methods a transfer-matrix equation yields the basis states in terms of which the boundary conditions are expressed. Furthermore, in Refs. 1 and 3, transfer matrices are used in the solution of the Schrödinger equation itself. The problem is quite simply that generating a transfer matrix requires inverting one or more submatrices which couple the various atomic planes to one another, and in many cases of interest these submatrices become singular, so that a transfer matrix does not exist. For example, in an [001]-oriented zinc-blende crystal described with the second-near-neighbor $sp^3$ model (which can correctly reproduce the $X$-valley transverse effective mass), at the interfacial wave vector $\mathbf{k}_\parallel = 2\pi/a\mathbf{e}_x$ (lattice constant is $a$), the transfer matrix does not exist.[5] This is a potentially fatal difficulty for the tight-binding method, since the above procedure is obviously of little use in treating indirect semiconductors having conduction-band minima which occur at the $X$ points. Using this procedure as the starting point in a calculation incorporating inelastic processes (which mix states of differing $\mathbf{k}_\parallel$) is likewise problematic. Difficulties will also arise when a set of tight-binding parameters renders the coupling matrices which one inverts to obtain the transfer matrix singular. Furthermore, the transfer matrix is most often computed numerically, so that even near-singular coupling matrices will result in a transfer matrix of poor quality, having inaccurate eigenvalues and eigenvectors. Thus one must determine the expansion states with a method applicable in the case of singular coupling matrices.

Because the real bands of a material are always available from the (well-behaved) bulk Hamiltonian, it seems more likely that the nonexistence of a transfer matrix under certain conditions is a defect of the method itself rather than an inherent physical property of the system. This is not to say that the nonexistence of a transfer matrix is without physical consequences: in our recent study of the complex bands of GaAs and AlAs in the second-near-neighbor $sp^3s^*$ model,[5] we have seen that it is indicative of evanescent states which grow and decay infinitely quickly. States with such properties obviously must be calculated by something other than the transfer-matrix method.[4] here we extend our previous work,[5] showing how it may be employed in tunneling calculations. To demonstrate its utility, we present a tunneling calculation for a single barrier/well heterostructure described using a second-near-neighbor two-band model having parameters deliberately chosen to give singular coupling matrices, so that a transfer matrix does not exist.

Our method is most easily introduced using a simple diatomic tight-binding model: one having an $s$-like orbital on each cation site and a $p_z$-like orbital on each anion site.[6,7] In order to illustrate the method in the case of singular coupling matrices, we include interactions up to second-near-neighbor; eventually we will set *one* of the second-near-neighbor parameters to zero in order to obtain singular coupling matrices. (Setting both to zero merely reduces the problem to the nearest-neighbor calculation, at which point the equations are easily rewritten in terms of nonsingular coupling matrices.) Because this model lacks $p_x$- and $p_y$-like orbitals, there is little point in including the dependence on $\mathbf{k}_\parallel = k_x\mathbf{e}_x + k_y\mathbf{e}_y$; therefore, we restrict $\mathbf{k}_\parallel = \mathbf{0}$. The Schrödinger equation in either the Bloch (now with $\mathbf{k} = k\mathbf{e}_z$) or planar-orbital bases (with $\mathbf{k}_\parallel = \mathbf{0}$) may be written down directly from its second-near-neighbor $sp^3$ form. It is, however, easier to recognize that for $\mathbf{k}_\parallel = \mathbf{0}$ the problem reduces to that of a linear chain of atoms and that the various interactions may be combined into intra- and inter-atomic layer couplings (Fig. 1). Taking the chain along the $z$ axis, with anion layers at positions $na/2$, cation layers at

 

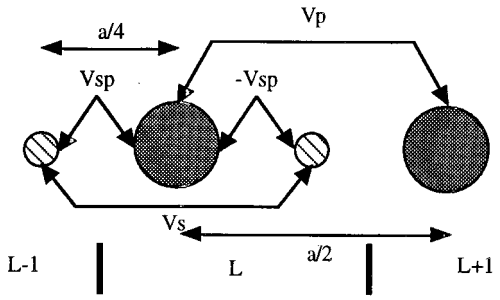


FIG. 1. Linear chain of atoms showing effective inter-atomic-layer matrix elements. Anions are large and shaded, cations are small and striped. A monolayer is $a/2$ long; monolayer $L$ is shown, along with the nearest-neighbor atoms of $L\pm1$.

$(na/2+a/4)$, $n\in J$, the bulk Hamiltonian is

$$\underline{\mathrm{H}}(k)=\begin{bmatrix} E_s+2V_s\cos\left(\frac{ka}{2}\right) & i2V_{sp}\sin\left(\frac{ka}{4}\right) \\ -i2V_{sp}\sin\left(\frac{ka}{4}\right) & E_p+2V_p\cos\left(\frac{ka}{2}\right) \end{bmatrix}, \quad (1)$$

where $E_s$ and $E_p$ are the same-layer interactions, $V_{sp}$ is the nearest-neighbor atomic layer interaction, and $V_s$ and $V_p$ are the second-near-neighbor atomic layer interactions. In this scheme the $L$th monolayer consists of the anion atomic layer at $La/2$ together with the cation atomic layer at $(La/2+a/4)$.

Writing the state in the planar orbital basis,

$$|\Psi\rangle=\sum_{n'}\left\{C^p_{n'}\left|za;\frac{n'a}{2}\right\rangle+C^s_{n'}\left|sc;\frac{n'a}{2}+\frac{a}{4}\right\rangle\right\}, \quad (2)$$

the Schrödinger equation yields pairwise equations:

$$V_pC^p_{n-1}+V_{sp}C^s_{n-1}+[E_p-E]C^p_n-V_{sp}C^s_n+V_pC^p_{n+1}=0, \quad (3)$$

$$V_sC^s_{n-1}-V_{sp}C^p_n+[E_s-E]C^s_n+V_{sp}C^p_{n+1}+V_sC^s_{n+1}=0, \quad (4)$$

where (3) and (4) are shown for bulk. As discussed in Ref. 5, the bulk eigenstates representing propagating (Bloch) and evanescent states are found for the solutions of the forward, (5), and reverse, (6), eigenproblems:

$$\lambda_+\underline{\mathrm{M}}_+\boldsymbol{X}_n=\underline{\mathbf{M}}_-\mathbf{X}_n, \quad (5)$$

$$\underline{\mathrm{M}}_+\boldsymbol{X}_n=\lambda_-\underline{\mathrm{M}}_-\mathbf{X}_n, \quad (6)$$

where

$$\underline{\mathrm{M}}_+\equiv\begin{bmatrix} V_p & 0 & 0 & 0 \\ V_{sp} & V_s & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix},$$

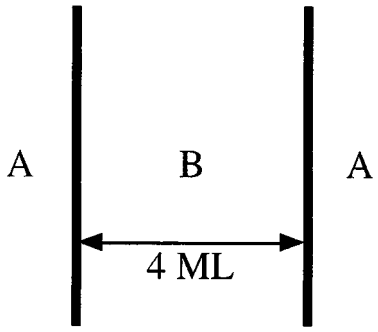


FIG. 2. Heterostructure for the tunneling problem.

$$\underline{\mathrm{M}}_-\equiv\begin{bmatrix} -[E_p-E] & V_{sp} & -V_p & -V_{sp} \\ V_{sp} & -[E_s-E] & 0 & -V_s \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \quad (7)$$

$$\mathbf{X}_m\equiv\begin{bmatrix}\mathbf{C}_m\\ \mathbf{C}_{m-1}\end{bmatrix}, \quad \mathbf{C}_m\equiv\begin{bmatrix}C^p_m\\ C^s_m\end{bmatrix}. \quad (8)$$

The eigenstates of (5) or (6) become the basis states in terms of which the boundary conditions in the left- and right-semi-infinite regions are expressed in the heterostructure tunneling problem. In Ref. 5 it is shown that although there appear to be two eigenproblems (for singular $\underline{M}_\pm$, $\lambda_\pm=\infty$ can be considered eignevalues, as well as the obvious $\lambda_\pm=0$), an implementation using EISPACK(Ref. 8) routines yields all eigenvalues in one diagonalization; we follow that procedure here. In addition, as expected from the discussion in Ref. 5, the characteristic polynomials of (5) and (6) are identical,

$$\begin{aligned}&\lambda^4_\pm V_pV_s+\lambda^3_\pm[(E_s-E)V_p+V^2_{sp}+(E_p-E)V_s]\\ &\quad+\lambda^2_\pm[(E_s-E)(E_p-E)+2V_pV_s-2V^2_{sp}]\\ &\quad+\lambda_\pm[(E_s-E)V_p+V^2_{sp}+(E_p-E)V_s]+V_pV_s=0, \end{aligned} \quad (9)$$

and it is seen that in the singular case (say $V_s=0$, $V_p\neq0$), (9) becomes a third-degree polynomial of the form $\lambda_\pm p(\lambda_\pm)$, where $p(\lambda_\pm)$ is a polynomial of degree 2 of which $\lambda_\pm=0$ is *not* a root.

We consider the simple single well/barrier tunneling problem depicted in Fig. 2; four monolayers of material B are sandwiched between two semi-infinite regions of material A. We take the structure to be unbiased and compute the transmission probability as a function of the energy of the incident particle. The eigenstates of the left-and right-semi-infinite regions, A, are thus identical. We express the boundary conditions in terms of the eigenstates of (5), (6), arranging the vectors as columns of a $4\times4$ matrix, $\underline{\mathrm{P}}$, which we write in terms of $2\times2$ blocks, $\underline{\mathrm{P}}_{i,j}$:

$$\underline{\mathrm{P}}\equiv[\mathbf{s}^{(f)}|\mathbf{b}^{(f)}|\mathbf{s}^{(r)}|\mathbf{b}^{(r)}]=\begin{bmatrix}\underline{\mathrm{P}}_{1,1} & \underline{\mathrm{P}}_{1,2}\\ \underline{\mathrm{P}}_{2,1} & \underline{\mathrm{P}}_{2,2}\end{bmatrix}, \quad (10)$$

where $\mathbf{s}^{(f)}$ and $\mathbf{s}^{(r)}$ are, respectively, forward- and reverse-decaying (surface) states and $\mathbf{b}^{(f)}$ and $\mathbf{b}^{(r)}$ are, respectively,

TABLE I. Tight-binding parameters for materials A and B; units are eV.

| Parameter | A | B |
|---|---|---|
| $E_s$ | 0.5 | 0.3 |
| $E_p$ | −0.6 | −0.2 |
| $V_{sp}$ | 0.5 | 0.3 |
| $V_s$ | 0.0 | 0.0 |
| $V_p$ | 0.1 | 0.05 |

forward- and reverse- propagating (Bloch) states. Note that in the case of singular $\underline{M}_{\pm}$, $\mathbf{s}^{(r)} \in \mathrm{Ker}(\underline{M}_{+})$ and $\mathbf{s}^{(f)} \in \mathrm{Ker}(\underline{M}_{-})$.

The most natural method for solving the tunneling problem without generating a transfer matrix (except to obtain the basis states) is that of Ting, Yu, and McGill;[2] we employ it here, but modify it by obtaining the basis states from the generalized eigenproblem (5) or (6) instead of computing and diagonalizing a transfer matrix. Since these states are used in formulating the boundary conditions, we discuss only that part of the method of Ref. 2 here. In the left-semi-infinite region that total state consists of a unit amount of the forward-propagating eigenstate and as yet unknown amounts of reverse-decaying and reverse-propagating eigenstates:

$$\begin{bmatrix} \mathbf{C}_0 \\ \mathbf{C}_{-1} \end{bmatrix} = \begin{bmatrix} \underline{P}_{1,1} & \underline{P}_{1,2} \\ \underline{P}_{2,1} & \underline{P}_{2,2} \end{bmatrix} \begin{bmatrix} \mathbf{I} \\ \mathbf{r} \end{bmatrix}, \quad \mathbf{I} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \mathbf{r} = \begin{bmatrix} r_s \\ r_b \end{bmatrix}, \tag{11}$$

where the reflection coefficient is $|r_b|^2$ and, from (11),

$$\mathbf{r} = \underline{P}_{1,2}^{-1}[\mathbf{C}_0 - \underline{P}_{1.1}\mathbf{I}], \tag{12}$$

$$\mathbf{C}_{-1} - \underline{P}_{2,2}\underline{P}_{1,2}^{-1}\mathbf{C}_0 = [\underline{P}_{2,1} - \underline{P}_{2,2}\underline{P}_{1,2}^{-1}\mathbf{P}_{1,1}]\ \mathbf{I}. \tag{13}$$

In the right semi-infinite region the state consists of as yet unknown amounts of forward-propagating and forward-decaying eigenstates:

$$\begin{bmatrix} \mathbf{C}_6 \\ \mathbf{C}_5 \end{bmatrix} = \begin{bmatrix} \underline{P}_{1,1} & \underline{P}_{1,2} \\ \underline{P}_{2,1} & \underline{P}_{2,2} \end{bmatrix} \begin{bmatrix} \mathbf{t} \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{t} = \begin{bmatrix} t_s \\ t_b \end{bmatrix}, \tag{14}$$

where the transmission coefficient is $|t_b|^2$, and, from (14),

$$\mathbf{t} = \underline{P}_{2,1}^{-1}\mathbf{C}_5, \tag{15}$$

$$\mathbf{C}_6 - \underline{P}_{1,1}\underline{P}_{2,1}^{-1}\mathbf{C}_5 = \mathbf{0}. \tag{16}$$

Because we consider only unbiased structures and there are only either two (or zero) Bloch states at a given energy, the speeds of all propagating states are identical and thus all velocity factors become unity. Equations (13) and (16) express the boundary conditions for the entire structure and the Schrödinger equation as written using the method of Ref. 2 results in a $16\times16$ banded matrix. We take the A-B interface to occur at an anion plane; for the same-plane interface parameter we take $E_p = \frac{1}{2}(E_p^{(A)} + E_p^{(B)})$ and for the second-nearest-neighbor interactions we take $V_p = \frac{1}{2}(V_p^{(A)} + V_p^{(B)})$ and $V_s = \frac{1}{2}(V_s^{(A)} + V_s^{(B)})$. Since our purpose here is to demonstrate our method rather than model a specific heterostructure, we select the interface parameters on the basis of convenience. With regard to equations (11)–(16), we emphasize that we are *not* inverting coupling matrices; indeed for there to be a basis, the columns of (10) must be linearly independent. In addition, we stress that the eigenstates of (5), (6) are used in formulating the boundary conditions in *exactly* the same manner as are the transfer-matrix eigenstates in the original method of Ting, Yu, and McGill.[2] With this modification to their method, it is no longer necessary to deal with transfer matrices and thus the presence of eigenstates of (5), (6) corresponding to infinite or zero eigenvalues presents no problem.

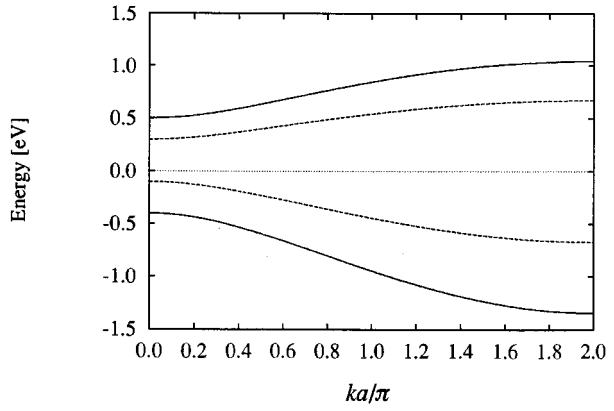


FIG. 3. Real bands of materials A (solid lines) and B (dashed lines) as produced by the parameters of Table I.

As indicated in the discussion of (10)–(16) above, one formulates the boundary conditions for the tunneling problem in terms of the eigenstates of (5), (6) regardless of whether or not the matrices $\underline{M}_{\pm}$ are singular. What may come as a surprise is that the transmission and reflection coefficients in the case of singular $\underline{M}_{\pm}$ behave *exactly* as one would expect based on the band structures of the constituent materials. We demonstrate this by constructing a deliberately singular case, the parameters of which are listed in Table I. Since our purpose here is to demonstrate the utility of this method the parameters are not chosen to mimic some particular materials, rather they are selected to best show the current approach. In Fig. 3, we graph the bands of A (solid lines) and B (dashed lines) produced by these parameters. Since $V_s = 0$ for both materials, it is readily apparent that the

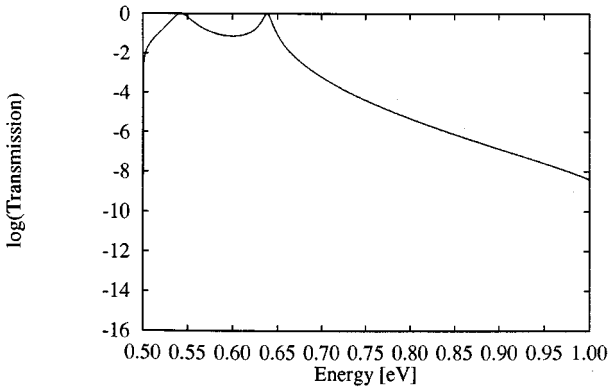


FIG. 4. Base-10 logarithm of the transmission-versus-energy curve of the single well/barrier heterostructure of Fig. 2, with materials A and B described by the parameters of Table I.

matrices $\underline{M}_{\pm}$ for both are singular. In particular, this means that there is no transfer matrix for either material and the eigenstates of material A used in formulating the boundary conditions cannot be calculated in the usual manner.

We calculate the transmission-versus-energy curve of the structure of Fig. 2 using the modified method of Ref. 2 discussed above; the results are plotted in Fig. 4. The energy resolution for this curve is 1 meV and for *all* points flux conservation was excellent: $R+T=1.0\pm\delta,\ 0\leqslant\delta<10^{-10}$. Furthermore, Fig. 4 displays exactly the behavior we expect from the bands of Fig. 3. There, notice that the carriers incident from the conduction band of A initially tunnel *over* a quantum well made of material B, until they reach an energy of about 0.67 eV, at which point they are above the conduction-band maximum of B so that the well becomes a barrier. Correspondingly in Fig. 4, we observe an initially high transmission with two shallow resonances at about 0.543 and 0.638 eV which then falls above this final resonance. The resonances, too, exhibit the proper physics: comparing the deBroglie wavelengths of the incident particles ($\lambda=2\pi/k_{\mathrm{inc}}$), we find that at the lower-energy resonance almost exactly two half wavelengths fit in the well while at the higher almost exactly three half-wavelengths fit in the well. Thus, we see that even in the case of singular coupling matrices, we can accurately calculate heterostructure tunneling properties.

We have demonstrated that it is possible to accurately calculate the transmission properties of a heterostructure described with a tight-binding model even in cases in which the matrices coupling the various atomic planes are singular. By removing the necessity of dealing with transfer matrices in formulating the boundary conditions, we have resolved a major problem of tight-binging approaches. Our simple, deliberately singular example displays the intuitively expected transmission behavior and we find that flux conservation is excellent. This method should be generalizable to more complete tight-binding models to enable the calculation of transmission properties and energy levels of heterostructures in situations for which a transfer matrix does not exist (e.g., certain $\mathbf{k}_{\|}$ or parameter sets). This should increase the utility of tight-binding methods when employed as parts of calculations for indirect semiconductors and/or incorporating inelastic processes.

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