

# Ballistic hot-electron transport in nanoscale semiconductor heterostructures: Exact self-energy of a three-dimensional periodic tight-binding Hamiltonian

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As the length scale for semiconductor heterostructures approaches the regime of the lattice constant, our current theory for calculating ballistic hot-electron transport becomes inapplicable. In this case, a method such as the Green's function formalism should be used to calculate ballistic electron transmission functions from the exact, periodic lattice potential. We present a method for directly calculating the exact surface Green's function for three-dimensional periodic leads which is necessary for such a scheme. Except in cases of high crystal symmetry, the method is limited by the difficulty to solve a nonsymmetric matrix Riccati equation.

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## I. INTRODUCTION

Ballistic hot-electron transport in semiconductor heterostructures has been the subject of much research for decades. This research has been enabled especially by the development of devices such as the solid-state hot-electron transistor<sup>1</sup> and the tunneling hot-electron transfer amplifier.<sup>2,3</sup> Furthermore, local scale study of buried semiconductor heterostructures has been made possible by the application of ballistic electron emission spectroscopy,<sup>4-6</sup> a scanning tunneling probe technique.

Regardless of the method, the mechanism for hot-electron generation via tunnel-junction emission in all cases is essentially identical. Hot electrons are injected through a base material, over a barrier, and into a semiconductor collector. A heterostructure can be placed in the base itself<sup>7</sup> or in the collector,<sup>8</sup> close to the base-collector interface. Much work in this field has focused on ballistic transport through single barriers,<sup>9</sup> double resonant barriers,<sup>10</sup> quantum dots,<sup>11</sup> and superlattices.<sup>12-14</sup> A well-developed theory has been implemented to predict the observed voltage-current relation to the actual transmission function through the structure by making use of the bulk conduction-band offsets and effective masses.<sup>15-17</sup>

Despite the agreement of the current theory with observed transport features, it is still quite impossible to correctly predict the results of ballistic electron transmission through planar heterostructures with extremely small length scales within these schemes. This is because when the discrete translational symmetry of the bulk semiconductor lattice is broken by heterostructure boundaries after only a few unit cells, *electronic band structure* of the thin layer has little meaning. In order to calculate the transmission function through such a heterostructure, the system must be treated exactly, with a realistic *three-dimensional* potential modeling the actual periodic landscape the electrons travel in, rather

than one-dimensional models with bulk approximations for each layer and band offset relations for each boundary. This task requires a powerful method capable of transmission function calculation, such as the Green's function Fisher-Lee formalism.<sup>18-20</sup> Of course, the true potential must take into account the many-body effects of electron-electron interaction. For simplicity, and to focus on the impact of periodicity, in this work we assume that these interactions can be treated as an effective potential.

## II. FORMALISM

The basic idea behind this method is that the transmission coefficient can be calculated from a Green's function  $G = (E - H)^{-1}$ , where  $H$  is the Hamiltonian operator and  $E$  is the electron kinetic energy. Of course, the Hamiltonian for the "open" systems used in scattering calculations has infinite extent in real space, so the explicit manipulation of this Green's function is impossible. Therefore, we break the problem into manageable parts, treating the finite heterostructure itself explicitly in the real-space basis, and finding an "analytic" self-energy to account for the effect of the semi-infinite leads which couple propagating electron states to the heterostructure "conductor."<sup>21</sup> Once this self-energy is known, the transmission function can be calculated using the well-known Fisher-Lee relation:

$$T = \text{Tr}[\Gamma_p G \Gamma_q G^\dagger],$$

where

$$\Gamma = i[\Sigma - \Sigma^\dagger]$$

and the subscripts  $p$  and  $q$  denote the incoming and outgoing leads, respectively.  $\Sigma$  represents the self-energy.

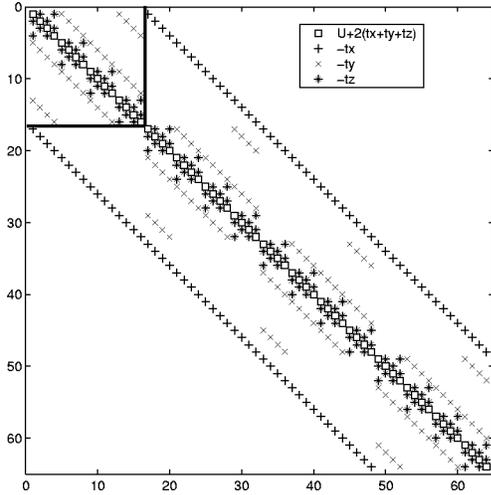


FIG. 1. Schematic view of a  $4 \times 4 \times 4$  3D space-basis Hamiltonian matrix operator. The 2D surface submatrix is shown boxed in the upper-left corner.

### III. BASIS

Because we are segregating portions of the Hamiltonian spatially, we use the space basis for our calculation. In the space basis, the Hamiltonian operator is discretized on a spatial lattice. The potential-energy operator is diagonal, but the kinetic-energy operator is not. We can use the discrete second derivative to express the one-dimensional (1D) kinetic-energy operator in this basis,

$$\frac{-\hbar^2}{2m} \frac{d^2 f_i}{dx^2} = \frac{-\hbar^2 (f_{i+1} - 2f_i + f_{i-1}))}{2ma^2},$$

where  $a$  is the lattice resolution. Because of the form of this representation, in one dimension the Hamiltonian operator has tridiagonal symmetry. In three dimensions, the Hamiltonian has *block* tridiagonal symmetry, as shown schematically for a finite 3D Hamiltonian of a unit cell discretized into  $4 \times 4 \times 4$  elements in Fig. 1.

In order to find the self-energy,

$$\Sigma = -t^2 g,$$

[where  $t = -\hbar^2/2ma^2$  and  $g$  is the surface submatrix of the semi-infinite  $(E-H)^{-1}$  matrix] of three-dimensional semi-infinite “leads,” we must therefore invert a semi-infinite matrix with block tridiagonal symmetry to determine the surface elements which couple the leads to the heterostructure. The calculation of these surface self-energy elements of 3D periodic Hamiltonians is the ultimate subject of the present work.

### IV. METHOD

#### A. One-dimensional constant potential

To illustrate the method for the three-dimensional case, we begin first with the trivial one-dimensional lead with a constant potential. In this case we have a system which can

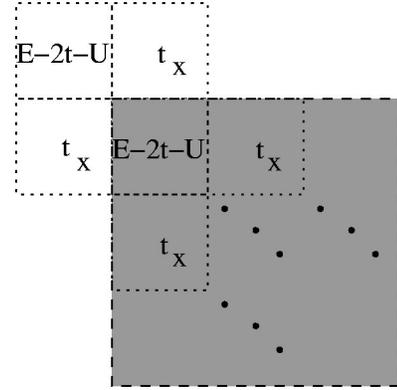


FIG. 2. In the space-basis nearest-neighbor approximation, the semi-infinite matrix  $E-H$  can be collapsed into a finite matrix by absorbing the self-energy into the first element.

be solved efficiently by conventional methods. However, it is instructive to examine how the theory works for this trivial example because it provides a convenient touchstone for our method.

The fundamental concept in the method is that the semi-infinite periodic matrix we wish to invert can be collapsed into a finite matrix by the very self-energy it is used to calculate. Refer to Fig. 2. Because of the semi-infinite nature of the matrix, the shaded portion is identical to the entire matrix. Therefore, the effect it has on the first element is the same as the self-energy we wish to calculate. We can construct a self-consistent equation for the inverse by adding the unknown self-energy to this first element:

$$g = (E - H + \Sigma)^{-1},$$

$$g = (E - 2t - U - t^2 g)^{-1}$$

or

$$-t^2 g^2 + (E - 2t - U)g - 1 = 0.$$

This can, of course, be solved using the quadratic formula

$$g = \frac{2t + U - E \pm \sqrt{(2t - U - E)^2 - 4t^2}}{-t^2}. \quad (1)$$

#### B. One-dimensional periodic potential

From the derivation above, we see that the surface Green's function  $g$  is the first element of the inverse of  $E - H - t^2 g$ , where  $H$  is the Hamiltonian of one unit cell of the potential. In the previous case the unit cell was one element, but when discrete translational periodicity is present, the potential is not the same everywhere, so we have a more complicated task. However, the form of the Hamiltonian allows us to use a simple variation on the concept used in the constant potential case above.

The convenient inversion method we use in this case is the Cramer's rule, which asserts that the first element of the

inverse of a matrix is the *determinant* of the minor matrix (excluding the first row and column) divided by the *determinant* of the entire matrix.<sup>22</sup>

We have seen that in the one-dimensional tight-binding nearest-neighbor approximation, the Hamiltonian is tridiagonal. Therefore, we can use a recursion relation to separate out the undetermined  $g$  and recover a quadratic equation similar to the one in the previous simplification. If the determinant of a square minor matrix from the  $i$ th diagonal element to the  $j$ th (for  $i < j$ ) is written  $D(i, j)$ , we have

$$D(i, j) = D(i, j-1)D(j, j) - t^2 D(i, j-2). \quad (2)$$

In this notation, Cramer's rule looks like

$$g = \frac{D(2, N)}{D(1, N)}, \quad (3)$$

where  $N$  is the size of the unit cell. Combining Eq. (2) and Eq. (3), we have

$$g = \frac{D(2, N-1)(E-2t-U_N-t^2g) - t^2 D(2, N-2)}{D(1, N-1)(E-2t-U_N-t^2g) - t^2 D(1, N-2)}. \quad (4)$$

Now, if we denote the determinants of the finite matrix (without the self-energy term) as  $D'(i, j)$ , we see that by applying the recursion relation again, we can separate out the unknown  $g$  in the above equation in order to solve for it,

$$g = \frac{D'(2, N) - t^2 D'(2, N-1)g}{D'(1, N) - t^2 D'(1, N-1)g},$$

or,

$$\begin{aligned} -t^2 D'(1, N-1)g^2 + [D'(1, N) + t^2 D'(2, N-1)]g \\ - D'(2, N) = 0. \end{aligned} \quad (5)$$

Again, the quadratic formula can be used to find the exact solution.

### C. Three-dimensional potential with longitudinal translational symmetry

Since the surface of a 3D unit cell is two-dimensional, we are now looking not for a scalar self-energy, but a matrix. Correspondingly, instead of solving the scalar quadratic equations of the 1D examples, we must solve a quadratic *matrix equation*. We have essentially the same equation as the 1D constant potential, except that all variables are matrices,

$$-t^2 g^2 + (EI - H_{2D})g - I = 0.$$

Fortunately, the only coefficient of this quadratic matrix equation which is not proportional to the identity matrix is the coefficient linear in  $g$ . We can easily diagonalize this matrix by transforming the equation using the diagonalizing matrix  $S$  and inserting  $I = SS^{-1}$ ,

$$-t^2 S^{-1}gSS^{-1}gS + S^{-1}(EI - H_{2D})SS^{-1}gS - I = 0.$$

Then, we change variables to  $g' = S^{-1}gS$ ,

$$-t^2 g'^2 + S^{-1}(EI - H_{2D})Sg' - I = 0.$$

This matrix equation can be solved using the scalar quadratic formula since every matrix is diagonal. Our solution  $g$  is easily recovered by transforming back from the diagonalizing basis,

$$g = Sg'S^{-1} = \frac{A + S\sqrt{A'^2 - 4t^2IS^{-1}}}{2t^2},$$

where

$$A = EI - H_{2D}$$

and

$$A' = S^{-1}AS.$$

### D. Three-dimensional periodic potential with transverse translational symmetry

When we impose periodicity along the transport direction, we must make use of an inversion method similar to Cramer's rule for the 1D periodic case. However, we have a matrix equation and we are not only interested in calculating the first element of the inverse, but the entire block corresponding to the 2D surface of the unit cell. Cramer's rule *does* work for tridiagonal block matrices, but now we must be careful because, in general, matrices do not commute. The definition of the *block determinant* then involves the order in which the sub-blocks are multiplied: the topmost 2D block [i.e., closest to the (1,1) element] is always multiplied on the left. We can also make use of the recursion relation used in the 1D case. With these things in mind, we repeat the procedure for the 1D case, and Eq. 3 becomes

$$g = D(2, N)(D(1, N))^{-1}. \quad (6)$$

Using the recursion relation, Eq. (2), we have

$$\begin{aligned} g(D(1, N-1)(E-2t-U_N-t^2g) - t^2 D(1, N-2)) \\ = D(2, N-1)(E-2t-U_N-t^2g) - t^2 D(2, N-2), \end{aligned}$$

and, by implementing Eq. (2) again, we get an equation similar to the scalar Eq. (5),

$$gAg + gB + Cg + D = 0, \quad (7)$$

where

$$A = -t^2 D'(1, N-1),$$

$$B = D'(1, N),$$

$$C = t^2 D'(2, N-1),$$

and

$$D = -D'(2, N).$$

This is a nonsymmetric Riccati equation (NSRE),<sup>23–26</sup> for which there is no exact solution in the general case. However, in the case that the potential has full translational symmetry in the direction parallel to the surface, each of the blocks in the Hamiltonian has constant diagonal components. This essentially means that our solution  $g$  will commute with  $A$ ,  $B$ ,  $C$ , and  $D$ . It also means that  $A^{-1}$  diagonalizes  $B$ ,  $C$ , and  $D$ . We can then use the quadratic formula to find a solution, proceeding in a similar fashion as in the 1D periodic and 3D constant potential case,

$$g = \frac{-F + S\sqrt{F'^2 - 4S^{-1}DA^{-1}SS^{-1}}}{2}, \quad (8)$$

where  $S$  is the matrix that diagonalizes  $F = (B + C)A^{-1}$  and  $F' = S^{-1}(B + C)A^{-1}S$ .

### E. Full three-dimensional periodic potential

As stated previously, the case of a random unit-cell potential with no special symmetry, leading to the unsimplified NSRE, is an unsolved problem. However, the solution of this problem can be approximated by an iterative procedure. One such method utilizes Eq. (6) explicitly.

The first step to this method is choosing an initial guess for  $g$  and self-consistently iterating the equation to generate a new  $g$ ,

$$\begin{aligned} g_{i+1} = & [D(2, N-1)(EI - 2tI - U_N - t^2 g_i) - t^2 D(2, N-2)] \\ & \times [D(1, N-1)(EI - 2tI - U_N - t^2 g_i) \\ & - t^2 D(1, N-2)]^{-1}. \end{aligned} \quad (9)$$

For convergence to the proper *complex* and *symmetric* solution, we add a small imaginary component,  $-10^{-6}i$ , to the energy.<sup>27</sup> We use  $g_0 = \hat{0}$  for the first energy but thereafter we use the approximated solution from the previous energy. This perturbative method accelerates the iteration process since the energies at which the transmission function is calculated are usually spaced closely and so successive solutions should be relatively similar.

For subsequent calculations, the iteration is terminated when the maximum element of

$$gAg + gB + Cg + D$$

is less than  $5 \times 10^{-4}$ .

## V. RESULTS

### A. 1D calculations

We can now apply the Fisher-Lee formalism to calculate the transmission function of a few one-dimensional potentials.

Figure 3 shows a comparison of calculated transmission functions of different numbers of 1-eV high, 2-Å wide barriers separated by 2 Å with constant potential ( $U=0$ ) leads and 1 Å discretization [using Eq. (1)], and the case where not only the conductor is made up of a superlattice of barriers,

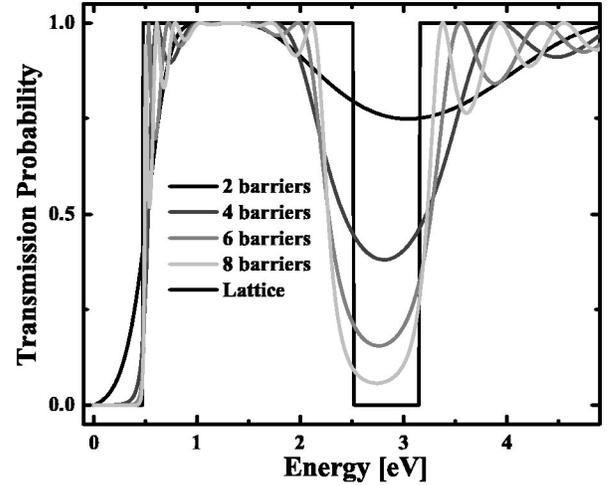


FIG. 3. Comparison of transmission functions of multibarrier conductors with constant leads and an infinite crystal of identical barriers. Dips in transmission develop into band gaps.

ers, but the leads themselves have the same periodicity [using the solution to Eq. (5)]. This is the case of an infinite 1D crystal. The dips in transmission develop into *band gaps* between which the transmission is unity. In other words, when there is a state in the crystal, we can expect it to exist everywhere with the same amplitude because it is an eigenfunction of the crystal Hamiltonian. Therefore, the probability flux at one extreme is the same as the other, and there is perfect transport. When there are no states, as in the band gap, there can of course be no transport.

Figure 4 shows a comparison of this behavior with an independently calculated band structure.<sup>28</sup> The band gaps in the band structure clearly align with the regions of zero transmission, as expected.

### B. 3D calculations

The case of 3D transverse translational symmetry, when the potential is constant in planes perpendicular to the trans-

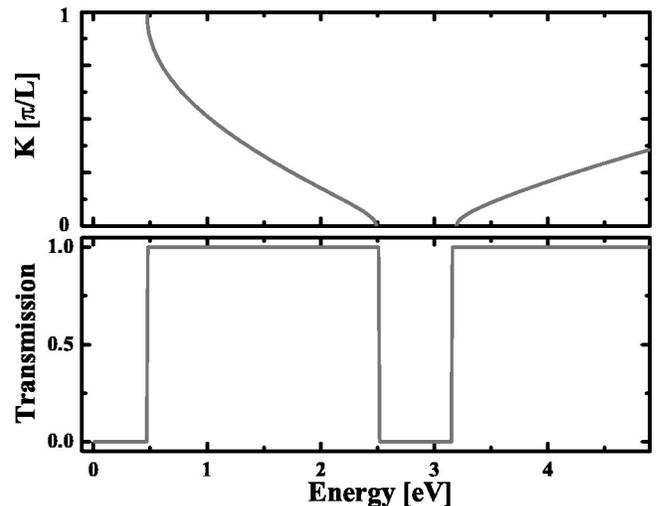


FIG. 4. Comparison of transmission function and independently calculated band structure for a 1D crystal of square barriers. Note the alignment of  $T=0$  regions with band gaps.

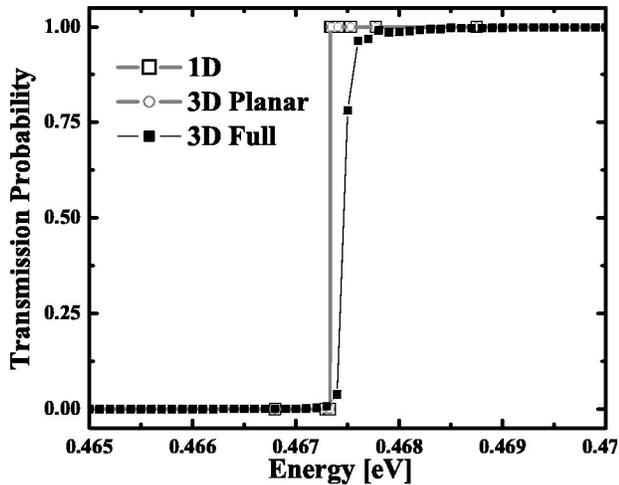


FIG. 5. Comparison of transmission functions calculated using the 1D exact and 3D exact (“Planar”) and approximated (“Full”) frameworks for equivalent lattices periodic along the transport direction.

port direction, is equivalent to a 1D periodic system. It provides us with a means to check our general 3D iterative solution method, Eq. (9). Figure 5 shows a comparison of calculated transmission functions using exact methods of calculating the surface Green’s function for 3D and 1D Hamiltonians of the infinite crystal of 2-Å wide, 1-eV high barriers spaced 2 Å apart, using 1 Å lattice resolution (the 3D unit cell has  $4 \times 4 \times 4$  discretization), as used previously. We also compare the results of the general iterative 3D method with these two methods. We see that the two exact methods (“1D” and “3D Planar”) coincide exactly, showing a first band edge consistent to five digits (0.467 33 eV). The solution obtained using Eq. (9) (“3D Full”) differs slightly and is

not identically 1 or 0 in the band-edge region as for the exact methods. Using a smaller imaginary part of the energy, the band edge can be made sharper. However, the convergence of the solution becomes slower. The value used here ( $-10^{-6}i$ ) gives  $\approx 0.1$  meV resolution, which is usually sufficient.

## VI. CONCLUSION

To accurately calculate the transmission function of hot ballistic electrons through semiconductor heterostructures, a method which treats the system explicitly as a periodic crystalline lattice must be used, such as the Fisher-Lee Green’s function method. Toward this end, we have derived a Riccati matrix equation for the surface Green’s function of periodic leads. In cases of high symmetry, this equation can be solved exactly, but in the general case, a numerical algorithm such as iteration must be used. Once the surface Green’s function is known, it can be used to find the transmission function for systems with arbitrary conductors.

This framework can be incorporated into another which can realistically model the electron potential within semiconductors. Density-functional theory calculations are well suited for this purpose.<sup>29–31</sup> It may be necessary to include more self-energy terms,<sup>32</sup> as the electron-electron interaction is not explicitly accounted for in the theory presented here. This will allow for a significantly useful application of *ab initio* theory to actual nanoscale device modeling.

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