Generalized Bloch theorem for complex periodic potentials: A powerful application to quantum transport calculations

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Band-theoretic methods with periodically repeated supercells have been a powerful approach for groundstate electronic structure calculations but have not so far been adapted for quantum transport problems with open boundary conditions. Here, we introduce a generalized Bloch theorem for complex periodic potentials and use a transfer-matrix formulation to cast the transmission probability in a scattering problem with open boundary conditions in terms of the complex wave vectors of a periodic system with absorbing layers, allowing a band technique for quantum transport calculations. The accuracy and utility of the method are demonstrated by the model problems of the transmission of an electron over a square barrier and the scattering of a phonon in an inhomogeneous nanowire. Application to the resistance of a twin boundary in nanocrystalline copper yields excellent agreement with recent experimental data.

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I. INTRODUCTION

Two typical problems of quantum transport of electrons in meso- and nanoscale devices are illustrated schematically in Fig. 1. The problems of finding the conductance either through the molecular junction, Fig. 1(A), attached at both ends to two metal electrodes, or through a thin film tunnel junction, Fig. 1(B), have been traditionally formulated using scattering theory in which electrons are coming from a reservoir at $+\infty$ and either get through the "scattering region," ending up in a reservoir at $-\infty$, or get scattered back into the original reservoir.^{1,2} Such a system is commonly referred to as "open," in contrast to isolated finite systems (molecules, nanoparticles) or crystals that are referred to as "closed." Green's functions have been the natural mathematical machinery for open systems.^{3–10}

More recently, a different method has been proposed that maps the open system onto a closed system by using boundary conditions equivalent to a "source" and a "sink."¹¹ This formulation allows the direct application of quantum chemistry methods normally applicable to molecules and nanoparticles to the quantum transport problem. An obvious alternative approach would be to map an open system onto periodically repeated *supercells*, which has been proven to be a very powerful concept that is widely used in the study of equilibrium systems, both molecules and solids.

In this paper, we develop a mapping of an open system onto a system of periodically repeated supercells. Though the relevant mathematical derivations appear somewhat complicated, the end result is an exact and simple expression for the tunneling conductance. The task is accomplished by repeating the molecular or tunnel junction shown in Fig. 1 and inserting "absorbing layers" between adjacent junctions, as shown schematically in Fig. 2(A). It is important to note that, without absorbing regions [Fig. 2(B)], the resulting wave functions would have multiple internal reflections that change the physics of the problem in an unacceptable way. Similarly, vacuum regions [Fig. 2(C)] cannot serve as absorbing layers because the resulting wave functions contain multiple reflections from the free surfaces. We will show that a suitable absorbing layer can be defined by adding an imaginary term to the usual crystalline potential of the electrodes. In order to obtain a suitable description of the resulting periodic supercell structure, we invoke two generalizations of the Bloch theorem:

(a) We cast the usual Bloch theorem in terms of a set of equations that yield not only the usual Bloch functions with real wave vectors but also solutions with imaginary wave vectors. The latter are not allowed by the usual Born–von Karman (BvK) boundary conditions which require identical normalization in each BvK cell, corresponding to an infinite perfect crystal. By viewing a thin crystalline layer as a single BvK cell, however, we can remove the condition of identical normalizations and obtain Bloch solutions with imaginary wave vectors. This generalization of the Bloch theorem has been done before in the context of particular basis sets.^{10,12}



FIG. 1. (Color online) Schematics of the quantum transport problem. (A) A molecule connected to metal electrodes. (B) A thin film tunnel junction.



FIG. 2. (Color online) Schematics of possible approaches to compute quantum conductance. A periodic array of molecules with parts of the electrodes attached, (A) with absorbing layers inserted into the electrodes to damp out the resonances, (B) without the absorbing layers, and (C) with free surfaces.

Here, we present a formulation that is independent of the choice of basis set. The solutions with imaginary wave vectors are known as "evanescent states" and have been used in the past to describe tunneling through insulating junctions. In the usual formulation, which focuses on evanescent states in the region of an insulator's energy gap, one can only get the exponential decay rates of the electron wave functions in the tunnel junction.^{13–18} In the present formulation, we get evanescent states at all energies *even in the absence of an energy gap*, which enables us to calculate the resistance of the entire junction, including the contact resistance, and a wider spectrum of systems such as junctions without an energy gap.

(b) We allow the periodic crystal potential to have an imaginary component, which results in all Bloch states being evanescent, i.e., there are no propagating Bloch waves, which is precisely what is needed to properly treat absorbing layers.

The present formulation relies on the concept of transfer matrices. They are employed here in a different way and allow us to derive the transmission probability and hence the conductance of a junction in terms of the complex wave vectors of the supercell structure with absorbing layers. Our method leads to an exceedingly simple formula for computing the transmission probability [see Eqs. (53) and (54) below] that is, in principle, exact. In essence, we will solve the Green's function for the scattering problem by hand, as presented in this paper, resulting in a straightforward complex band structure calculation to be implemented numerically. In this sense, our method is completely equivalent to a Green's function based method within the linear response theory discussed here.

In the next section, we first summarize the principle of the generalized Bloch theorem, which is the foundation of the subsequent discussion. Then, in Sec. III, we introduce the absorbing layers with imaginary potentials and construct a periodic reference system consisting of the electrodes and the absorbing layers. The transmission and reflection probabilities are derived in Sec. IV. We then demonstrate the accuracy and the flexibility of the method in three examples, two model problems in Sec. V, electron transmission over a square barrier and phonon transmission in an inhomogeneous nanowire, and finally, a real application in Sec. VI, where we calculate the resistance of a twin boundary in a metal.

II. GENERALIZED BLOCH THEOREM

The Bloch theorem is a consequence of the translational invariance of the Hamiltonian for an infinite periodic crystalline solid. The Hamiltonian commutes with the translation operator $P_{\mathbf{R}}$ associated with a lattice vector \mathbf{R} ,

$$[H, P_{\mathbf{R}}] = 0. \tag{1}$$

Consequently, any eigenstate of *H* is also an eigenstate of $P_{\mathbf{R}}$. One first shows that the eigenvalue equation for $P_{\mathbf{R}}$ can be written in the form

$$P_{\mathbf{R}}\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{R}}\phi_{\mathbf{k}}(\mathbf{r}), \qquad (2)$$

so that the wave vector \mathbf{k} labels the eigenvectors and eigenvalues of H, i.e.,

$$H\phi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\phi_{\mathbf{k}}(\mathbf{r}). \tag{3}$$

Finally, one shows that Eq. (2) requires that $\phi_{\mathbf{k}}(\mathbf{r})$ must have the form $\phi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$, where $u_{\mathbf{k}}(\mathbf{r})$ has the full crystal periodicity, i.e., $P_{\mathbf{R}}u_{\mathbf{k}}(\mathbf{r}) = u_{\mathbf{k}}(\mathbf{r})$.

One normally introduces BvK boundary conditions, large periodic cells of volume L^3 , in which the Bloch functions $\phi_{\mathbf{k}}(\mathbf{r})$ are normalized to unity. It is this identical normalization in every BvK cell that imposes the usual requirement that \mathbf{k} is real.

In quantum transport calculations illustrated in Fig. 1, the direction in which the current flows is treated differently than the other directions. The thin film or molecule in the junction is localized between the two electrodes. Thus, we can treat that region as a single BvK cell of an infinite periodic system and relax the usual condition of requiring the same normalization in every BvK cell. As a result, we can obtain Bloch solutions with both real and complex wave vectors. We will show later in this section that an infinite number of evanescent waves, which decay or grow exponentially along the direction of the current, are obtained.

The Schrödinger equation and the generalized Bloch theorem can be combined into a single "transfer-matrix equation" which allows evanescent solutions. This result has been derived in previous works for various forms of the Hamiltonian, namely, for pseudopotentials,⁹ for the layer Korringa-Kohn-Rostoker (KKR) method,¹⁰ and for tight-binding Hamiltonians.¹² Here, we provide a general derivation that is valid independently of the choice of Hamiltonian or basis set.

We begin by rewriting the periodic Hamiltonian H in Eq. (3) for an infinite crystalline solid in the form

$$H = H_0 + V_1(\mathbf{r}) + V_2(\mathbf{r}),$$
(4)

where V_1 and V_2 are potentials with the same periodicity. V_1 will be used to construct a set of complete basis functions. A special case would be $V_1=0$ and the basis functions would be the plane waves. In general, V_1 can be a reference periodic

potential that is otherwise arbitrary. At this point, both V_1 and V_2 are real potentials. Later, when we consider a single BvK cell embedded between two electrodes, we will make V_2 complex. There are no additional restrictions.

We now define a set of complete basis functions, $\xi_{nq}(\mathbf{r})$, that satisfy the BvK periodic boundary condition and the Schrödinger equation,

$$[H_0 + V_1(\mathbf{r})]\xi_{n\mathbf{q}}(\mathbf{r}) = E_{n\mathbf{q}}\xi_{n\mathbf{q}}(\mathbf{r}), \qquad (5)$$

where *n* is the band label and **q** is the wave vector and is real. We are interested in the wave functions traveling in (or opposite to) the direction of the current, which is defined as the *x* direction. Along this direction, we separate the leftgoing and right-going wave functions, $\xi_{m\mathbf{q}'L}(\mathbf{r})$ and $\xi_{n\mathbf{q}R}(\mathbf{r})$, respectively, according to the sign of the *x* component of the group velocities, $\partial E_{n\mathbf{q}}/\partial q_x$. For nonparabolic bands, the group velocity may be in a different direction than the wave vector **q**.

Now, we consider the wave functions for the full Hamiltonian H,

$$H\phi_{\mathbf{k}}(\mathbf{r};E) = E\phi_{\mathbf{k}}(\mathbf{r};E).$$
(6)

Note that we have labeled the wave functions in an unconventional way. The conventional form for the wave functions is $\phi_{n\mathbf{k}}$, where *n* is the band label and **k** is the (real) Bloch wave vector. The corresponding eigenenergy would be labeled as $E_{n\mathbf{k}}$. Here, we remove the band label and use an unlabeled *E* to highlight the fact that at each energy, there are a number of possible Bloch wave vectors **k** for which there are solutions to Eq. (6). This notation enables us to naturally account for possible solutions with energy *E* and complex wave vector *k* if we release the BvK requirement of unit normalization in each BvK cell (see below). Although an additional band label is needed if there is degeneracy, such as the degeneracy that often occurs along high symmetry directions, for the time being, we consider only nondegenerate bands. Generalization to degenerate bands is straightforward.

Before we proceed to expand the wave function in terms of the basis functions $\xi_{nq}(\mathbf{r})$, we break up the potential V_2 into layers using the BvK cells along the yz plane,

$$V_2(\mathbf{r}) = \sum_J V_J(x - x_J, y, z).$$
(7)

Here, V_J is nonzero only within a single layer of unit cells, which spans $x_J < x < x_J + a$, with x_J as the origin of the layer, *a* being the period in the *x* direction, and *J* denoting the layers. We allow the normalization of the $\phi_{\mathbf{k}}$ to be different in different BvK cells so that the wave vectors **k** can be complex. For complex **k**, the expansion coefficients are different in different layer cells. We, therefore, label the expansion coefficients with the layer index *J*,

$$\phi_{\mathbf{k}}(\mathbf{r} \in J; E) = \sum_{m\mathbf{q}'} C_{\mathbf{k}m\mathbf{q}'L}^{J}(E)\xi_{m\mathbf{q}'L}(\mathbf{r}) + \sum_{n\mathbf{q}} C_{\mathbf{k}n\mathbf{q}R}^{J}(E)\xi_{n\mathbf{q}R}(\mathbf{r}).$$
(8)

In order to find an equation for the coefficients C^J , we consider the Hamiltonian,

$$H_0 + V_1(\mathbf{r}) + V_J(x - x_J, y, z),$$
 (9)

where outside the layer *J*, the Hamiltonian is H_0+V_1 , and within layer *J*, there is an additional scattering potential V_J . The scattered wave function for a single incident beam of $\xi_{nqR}(\mathbf{r})$ can be obtained from the Lippmann-Schwinger equation,

$$\psi_{n\mathbf{q}R}^{J}(\mathbf{r}) = \xi_{n\mathbf{q}R}(\mathbf{r}) + \int d^{3}\mathbf{r}_{J}^{\prime}G_{1}(\mathbf{r},\mathbf{r}^{\prime})V_{J}(x^{\prime}-x_{J},y^{\prime},z^{\prime})\psi_{n\mathbf{q}R}^{J}(\mathbf{r}^{\prime}),$$
(10)

where the Green's function satisfies

$$E - H_0 - V_1(\mathbf{r})]G_1(\mathbf{r}, \mathbf{r}') = \delta(\mathbf{r}, \mathbf{r}').$$
(11)

The range of integration for \mathbf{r}' in Eq. (10) is over the layer J. For \mathbf{r} outside this range, the following linear combination of the basis functions solves the equation for G_1 :

$$G_{1}(\mathbf{r},\mathbf{r}') = \begin{cases} \sum_{m\mathbf{q}'} F_{m\mathbf{q}'}^{L}(\mathbf{r}')\xi_{m\mathbf{q}'L}(\mathbf{r}), & x < x_{J} \\ \sum_{n'\mathbf{q}''} F_{n'\mathbf{q}''}^{R}(\mathbf{r}')\xi_{n'\mathbf{q}''R}(\mathbf{r}), & x > x_{J} + a. \end{cases}$$
(12)

Substituting this back into Eq. (10), we find

$$\psi_{n\mathbf{q}R}^{J}(\mathbf{r}) = \begin{cases} \xi_{n\mathbf{q}R}(\mathbf{r}) + \sum_{m\mathbf{q}'} r_{m\mathbf{q}'n\mathbf{q}}\xi_{m\mathbf{q}'L}(\mathbf{r}), & x < x_{J} \\ \sum_{n'\mathbf{q}''} t_{n'\mathbf{q}''n\mathbf{q}}\xi_{n'\mathbf{q}''R}(\mathbf{r}), & x > x_{J} + a, \end{cases}$$
(13)

where

$$r_{m\mathbf{q}'n\mathbf{q}} = \int d^3 \mathbf{r}' F^L_{m\mathbf{q}'}(\mathbf{r}') V_J(\mathbf{r}') \psi^J_{n\mathbf{q}R}(\mathbf{r}')$$
(14)

and

$$t_{n'\mathbf{q}''n\mathbf{q}} = \delta_{nn'} \,\delta_{\mathbf{q}\mathbf{q}''} + \int d^3 \mathbf{r}' F_{n'\mathbf{q}''}^R(\mathbf{r}') V_J(\mathbf{r}') \psi_{n\mathbf{q}R}^J(\mathbf{r}') \quad (15)$$

are the reflection and transmission coefficients, respectively, of layer J. A similar equation can be written for the leftgoing wave function $\psi_{mq'L}^{J}(\mathbf{r})$ which is the scattered wave function from an incident wave function from the right, $\xi_{mq'L}(\mathbf{r})$. These scattering solutions allow us to rewrite the left-going term in Eq. (8) at $x=x_J$ as an exit wave function due to scattering by V_J from two incident wave functions. The first incident wave function is the second term of Eq. (8), $\sum_{nq} C_{knqR}^{J}(E)\xi_{nqR}(\mathbf{r})$, which produces a reflected wave, $\sum_{nqm'q'} C_{knqR}^{J}(E)\xi_{mq'L}(\mathbf{r})$. The second incident wave is the left-going wave function for layer J+1, $\sum_{mq'} C_{kmq'L}^{J+1}(E)\xi_{mq'L}(\mathbf{r})$, which produces a transmitted wave, $\sum_{mq'm'q''} C_{kmq'L}^{J+1}(E)t_{m'q''mq'}\xi_{m'q''L}(\mathbf{r})$. Summing these waves together, we find

$$\phi_{\mathbf{k}}(x_J, y, z; E) = \sum_{m\mathbf{q}'} \left[\sum_{n\mathbf{q}} C^J_{\mathbf{k}n\mathbf{q}R}(E) r_{m\mathbf{q}'n\mathbf{q}} + \sum_{m'\mathbf{q}''} C^{J+1}_{\mathbf{k}m'\mathbf{q}''L}(E) t_{m\mathbf{q}'m'\mathbf{q}''} \right] \xi_{m\mathbf{q}'L}(\mathbf{r}) + \sum_{n\mathbf{q}} C^J_{\mathbf{k}n\mathbf{q}R}(E) \xi_{n\mathbf{q}R}(\mathbf{r}).$$
(16)

Comparing Eqs. (8) and (16), we relate the expansion coefficients of neighboring layers,

$$C_{kL}^{J} = r_{LR}C_{kR}^{J} + t_{LL}C_{kL}^{J+1},$$
(17)

and a similar equation for layer J+1,

$$C_{\mathbf{k}R}^{J+1} = t_{RR}C_{\mathbf{k}R}^{J} + r_{RL}C_{\mathbf{k}L}^{J+1}, \qquad (18)$$

where $C_{kL(R)}^{J}$ are column vectors containing expansion coefficients, $C_{kmqL}^{J}(E)$ and $C_{knq'R}^{J}(E)$, of the wave function. We have collected the transmission coefficients for all rightgoing waves, $t_{n'q'nq'}$, into a transmission matrix t_{RR} and similarly collected all reflection coefficients, $r_{mq'nq}$, into a reflection matrix r_{LR} . For the left-going wave functions, the transmission and reflection matrices are t_{LL} and r_{RL} , respectively. In matrix form, the above two equations are combined as

$$\begin{pmatrix} I & -r_{LR} \\ 0 & t_{RR} \end{pmatrix} \begin{pmatrix} C_{kL}^J \\ C_{kR}^J \end{pmatrix} = \begin{pmatrix} t_{LL} & 0 \\ -r_{RL} & I \end{pmatrix} \begin{pmatrix} C_{kL}^{J+1} \\ C_{kR}^{J+1} \end{pmatrix},$$
(19)

where I is a unit matrix. We define the transfer matrix for a single layer of thickness a as

$$M_a = \begin{pmatrix} t_{LL} & 0 \\ -r_{RL} & I \end{pmatrix}^{-1} \begin{pmatrix} I & -r_{LR} \\ 0 & t_{RR} \end{pmatrix}.$$
 (20)

Then, Eq. (19) becomes

$$M_a |\phi_{\mathbf{k}}^J(E)\rangle = |\phi_{\mathbf{k}}^{J+1}(E)\rangle, \qquad (21)$$

with the wave function

$$|\phi_{\mathbf{k}}^{J}(E)\rangle = \begin{pmatrix} C_{\mathbf{k}L}^{J} \\ C_{\mathbf{k}R}^{J} \end{pmatrix}$$
(22)

expressed on any complete basis $\xi_n(\mathbf{r})$. Invoking the generalized Bloch theorem, Eq. (2), which now states $|\phi_{\mathbf{k}}^{J+1}\rangle = e^{ik_x a} |\phi_{\mathbf{k}}^J\rangle$, where k_x is the *x* component of the wave vector of the wave function $\phi_{\mathbf{k}}(\mathbf{r})$, we finally obtain

$$M_a |\phi_{\mathbf{k}}^J(E)\rangle = e^{ik_x a} |\phi_{\mathbf{k}}^J(E)\rangle, \qquad (23)$$

which is the transfer matrix form of the Schrödinger equation.

Equation (23) has the same form as Eq. (2), but its meaning is different. The transfer matrix M_a depends on the potential and the energy, while the translation operator $P_{\mathbf{R}}$ is independent of both. On the other hand, Eq. (23) is different than the eigenvalue problem of the Schrödinger equation in the sense that it solves for the eigenstates at a fixed energy. An interesting corollary follows. The number of Bloch eigenstates at a fixed energy, N_b , is a physical quantity that should be independent of the basis. On the other hand, the



FIG. 3. (Color online) Reference system containing only the electrodes and the absorbing layers. (A) A single absorbing layer with electrodes. (B) A periodic array of supercells.

number of eigenstates of Eq. (23) at each energy is equal to the total number of basis functions, N, used in the calculation. Usually, $N \ge N_b$. Therefore, Eq. (23) yields $N - N_b$ additional eigenstates of the translation operator which are not Bloch eigenstates. These additional solutions are evidently the evanescent wave functions. In principle, convergence is reached when $N \rightarrow \infty$. This result also proves that there is an infinite number of evanescent solutions.

The discussion in this section is general and applies to complex periodic potentials as well. We will use this result in the next section. For a complex periodic potential and a real energy, no solution with a real wave vector is possible. Therefore, every solution has a complex wave vector.

III. ABSORBING LAYERS INSERTED IN A PERFECT CRYSTALLINE ELECTRODE

We consider the scattering properties of the absorbing layers. Within a single absorbing layer [Fig. 3(A)] of thickness *d* inserted between $x=x_0$ and $x=x_0+d$ of a perfect electrode, we introduce a uniform small imaginary potential in addition to the electrode Hamiltonian $H^{(0)}$,

$$H^{(0)}\psi(x) - i\eta(x)\psi(x) = E\psi(x), \qquad (24)$$

with

$$\eta(x) = \begin{cases} \eta_0 & \text{for } x_0 < x < x_0 + d \\ 0 & \text{otherwise} \end{cases}$$
(25)

For free electron electrodes, an incident electron with wave vector k yields transmission probability

$$T_d = |t_d|^2 \approx e^{-\eta_0 d} \tag{26}$$

and reflection probability

$$R_d = |r_d|^2 \approx \frac{\eta_0^2}{4k^2 + \eta_0^2} \tag{27}$$

by solving the square barrier with a constant imaginary potential in the limits $\eta_0 \ll k_0$ and $\eta_0 d \gg 1$. Such scaling with η_0 also holds for electrodes with Bloch electrons. Therefore, if the imaginary part of the potential is small and the thickness of the absorbing layer is large, both transmission and reflection probabilities are small, i.e., $T_d = |t_d|^2 \ll 1$ and $R_d = |r_d|^2 \ll 1$. This requirement cannot be satisfied by real potentials in the absorbing layers (e.g., a vacuum barrier) because they always produce finite reflection probabilities.

The constant imaginary potential η_0 inside the absorbing layers does not affect the real part of the energy dispersion relation, E_{nk} . Therefore, there is no band mismatch at the interface between the electrode and the absorbing layer. The matching of the band structure between the electrode and the absorbing layer will be used below to reduce the complexity of the transfer matrix for the absorbing layer.

More generally, various forms of complex absorbing potentials with nonuniform imaginary potentials have been developed that can efficiently absorb the wave function in the asymptotic regions.^{19,20} In particular, we adopt the form suggested in Ref. 20. For a position *x*, the complex potential's value $-i\eta(x)$ is determined by the following procedure. Let

$$\alpha(x) = \begin{cases} \frac{2(x-x_0)c}{d}, & x_0 < x < x_0 + d/2\\ \frac{2(x_0+d-x)c}{d}, & x_0+d/2 < x < x_0+d \end{cases}$$
(28)

and

$$\beta(x) = \frac{4}{[c - \alpha(x)]^2} + \frac{4}{[c + \alpha(x)]^2} - \frac{8}{c^2},$$
 (29)

where *c* is a parameter that determines the strength of the imaginary potential. These values of $\alpha(x)$ and $\beta(x)$ are then used to compute the complex potential value for this position,

$$-i\eta(x) = \frac{-i\hbar^2}{2m} \left(\frac{4\pi}{d}\right)^2 \beta(x).$$
(30)

The wave function at $x=x_0$ on the left surface of an absorbing layer can be related to the wave function at $x=x_0$ +*d* on the right surface of the absorbing layer through a transfer matrix,

$$\psi(x_0 + d) = M_d \psi(x_0). \tag{31}$$

Because of the exact matching of the real part of the band structure between the absorbing layer and the electrode, transmission and reflection coefficients are diagonal in band indices. Therefore, the transmission and reflection matrices in Eq. (20) are all scalars, $t_{RR} = t_d^*$, $r_{LR} = r_d^*$, $t_{LL} = t_d$, and $r_{RL} = r_d$. Substituting t_d and r_d into Eq. (20) for M_d , we find

$$M_d = \frac{1}{t_d} \begin{pmatrix} 1 & -r_d^* \\ r_d & |t_d|^2 - |r_d|^2 \end{pmatrix}.$$
 (32)

Next, we consider the periodic reference system depicted in Fig. 3(B). The period of this supercell structure is a_0 . We apply the generalized Bloch theorem, Eq. (2), to this system which has a complex potential and a complex wave vector k_0 ,

$$\psi_{k_0}(x-a_0) = e^{-\iota k_0 a_0} \psi_{k_0}(x). \tag{33}$$

By combining Eqs. (31) and (33), we can relate the wave function of a generalized Bloch eigenstate at two ends of the same supercell between two absorbing layers in the form

$$\psi_{k_0}(x_0 + d - a_0) = e^{-ik_0 a_0} M_d \psi_{k_0}(x_0).$$
(34)

This wave function can be expanded in terms of the Bloch wave functions within the region between two absorbing layers,

$$\psi_{k_0}(x) = A\xi_L(x, E) + B\xi_R(x, E).$$
(35)

Here, for simplicity, we assume that there is a single leftgoing (ξ_L) and a single right-going (ξ_R) Bloch wave. If there are more Bloch waves in each direction, then both the basis $\xi_{L(R)}$ and the coefficients *A* and *B* should be viewed as vectors. The coefficients *A* and *B* form the eigenvector of Eq. (34),

$$\binom{A}{B} = \frac{e^{-ik_0 a_0}}{t_d} \binom{1}{r_d} - \binom{-r_d^*}{|t_d|^2 - |r_d|^2} \binom{A}{B},$$
(36)

and we used Eq. (32). The exponential factor is decaying for Im $k_0 < 0$, i.e., for left-going waves. It will be useful to rewrite the equation with a decaying exponential factor for right-going waves, Im $k_0 > 0$, by inverting the matrix on the right-hand side of Eq. (36),

$$\binom{A}{B} = \frac{e^{ik_0 a_0}}{t_d^*} \binom{|t_d|^2 - |r_d|^2 \quad r_d}{-r_d^* \quad 1} \binom{A}{B}.$$
 (37)

In an actual three-dimensional system, Eqs. (36) and (37) will be complicated by the transverse wave vector \mathbf{k}_{\parallel} which is perpendicular to the direction of the current. Although in that case we may view Eqs. (36) and (37) as a set of equations with an implicit index \mathbf{k}_{\parallel} , these equations are, in principle, coupled between \mathbf{k}_{\parallel} and $\mathbf{k}_{\parallel}+\mathbf{G}_{\parallel}$, where \mathbf{G}_{\parallel} is a two-dimensional reciprocal lattice vector. We note, however, that for the evanescent waves considered here, the exponential decay is faster for wave functions with a larger transverse wave vector. Thus, all \mathbf{k}_{\parallel} except those inside the two-dimensional first Brillouin zone can be neglected.

IV. TRANSMISSION AND REFLECTION PROBABILITIES IN TERMS OF COMPLEX WAVE VECTORS

Now, we are ready to consider the periodic system containing the actual device. We place the device into this system midpoint between two adjacent absorbing layers, in the configuration shown in Fig. 2(A). The transmission and reflection coefficients of the device are t and r. In the electrode region, instead of using the wave functions $\xi_L(x;E)$ and $\xi_R(x;E)$, it is more convenient to use the scattering wave functions in the electrode region of an electrode-moleculeelectrode assembly, $\chi_L(x)$ and $\chi_R(x)$, defined as

$$\chi_R(x) = \xi_R(x;E) + r\xi_L(x;E) \tag{38}$$

on the left of the device and

$$\chi_R(x) = t\xi_R(x;E) \tag{39}$$

on the right of the device. The form of $\chi_L(x)$ is similar but with the left and right sides interchanged. Now, we can expand the eigenstate wave function of the periodic system in the form

$$\psi_{k_1}(x) = C\chi_L(x) + D\chi_R(x), \tag{40}$$

where the subscript k_1 indicates the complex wave vector. Using Eqs. (38) and (39), we find

$$\psi_{k_1}(x) = (Ct^* + Dr^*)\xi_L(x;E) + D\xi_R(x;E)$$
(41)

on the left of the device and

$$\psi_{k_1}(x) = C\xi_L(x;E) + (Cr + Dt)\xi_R(x;E)$$
(42)

on the right. We also have the Bloch boundary condition for this system similar to Eq. (33),

$$\psi_{k_1}(x-a) = e^{-ik_1a}\psi_{k_1}(x), \tag{43}$$

where a is the period of the supercell and k is the complex wave vector. Similar to Eq. (31), between two absorbing layers, we still have

$$\psi_{k_1}(x_0 + d - a) = e^{-ika} M_d \psi_{k_1}(x_0), \tag{44}$$

where M_d is the same transfer matrix for the absorbing layer as in the reference system, Eq. (31). Substituting the expansion of the wave function, Eq. (42), into Eq. (44), we arrive at the following generalized eigenvalue problem:

$$\binom{t^* \ r^*}{0 \ 1} \binom{C}{D} = \frac{e^{-ik_1 a}}{t_d} \binom{1 \ -r_d^*}{r_d \ |t_d|^2 - |r_d|^2} \binom{1 \ 0}{r \ t} \binom{C}{D}.$$

$$(45)$$

For left-going waves, we drop all high order terms of t_d and r_d in Eqs. (36) and (45). Thus, B=0 in Eq. (36) and D=0 in Eq. (45). Comparing the two equations, we find

$$t^* = e^{i(k_1 a - k_0 a_0)}.$$
 (46)

Likewise, for right-going waves, we invert the matrix in Eq. (45) to obtain

$$\binom{1 \quad 0}{r \quad t} \binom{C}{D} = \frac{e^{ik_1 a}}{t_d^*} \binom{|t_d|^2 - |r_d|^2 \quad r_d}{-r_d^* \quad 1} \binom{t^* \quad r^*}{0 \quad 1} \binom{C}{D}.$$

$$(47)$$

Then, we drop all high order terms of t_d and r_d in Eqs. (37) and (47). We get A=0 and C=0 and

$$t = e^{i(k_0 a_0 - k_1 a)}.$$
(48)

In this manner, the problem of finding the transmission coefficient *t* in a scattering problem is converted into a problem of finding complex wave vectors k_0 and k_1 . The decay parameter λ for the scattering region is

$$\lambda = \left| \operatorname{Im} k_1 a - \operatorname{Im} k_0 a_0 \right|. \tag{49}$$

The transmission probability is then given by $T = \exp(-2\lambda)$.

The same procedure can be followed but without the imaginary potential in the absorbing layers, as in the con-

figuration of Fig. 2(B), to find the reflection probability. In this case, $r_d=0$ and $t_d=\exp(ik'_1d)$, where k'_1 is the complex wave vector of the periodic system, and the phase factor is to account for the thickness of the absorbing layer but now with only the real potential. Applying these values of t_d and r_d to Eqs. (45) and (47), we find

$$|r|^{2} = 1 + |t|^{2} - 2 \operatorname{Re}[te^{-ik_{1}'(a-d)}].$$
(50)

This seems to be a trivial result because for real potentials, $|r|^2 + |t|^2 = 1$ and Eq. (50) leads to Re $[te^{-ik_1'(a-d)}] = |t|^2$, which is redundant. However, if the device region contains a complex potential, then $|r|^2 + |t|^2 < 1$ and Eq. (50) becomes useful.

To generalize to multiple bands, all transmission and reflection coefficients become matrices. The algebra is easily carried through, with the only complication that at the end, instead of Eq. (46), we find an eigenvalue equation for the left-going waves,

$$t^{\dagger}C = e^{i(k_n a - k_0 a_0)}C, \tag{51}$$

where t is now a matrix, C is a vector, and n=1, ..., N is the band label. The equation for the right-going waves is similar. The total transmission probability is

$$T = \operatorname{Tr}(t^{\dagger}t) = \sum_{n=1}^{N} e^{-2|\operatorname{Im} k_n a - \operatorname{Im} k_0 a_0|}.$$
 (52)

The exponential terms decay at different rates. For sufficiently large thickness, only the term with the smallest Im k_n survives. At the end,

$$T = e^{-2\lambda},\tag{53}$$

where

$$\lambda = \left| \operatorname{Im} k_n a - \operatorname{Im} k_0 a_0 \right| \tag{54}$$

and k_n is the complex wave vector with the smallest imaginary part.

V. TESTS IN MODEL PROBLEMS

We first test our method on an exactly soluble problem of transmission through a square potential barrier. Several values for the potential height and width are used for this test. For all values, we found minimal difference between the numerical result from Eq. (54) and the exact result. In Fig. 4, we present the result for one of the calculations. Here, the height of the potential barrier is 1 hartree and the width is 10 bohrs. The total period of the one-dimensional system is 20 bohrs. Equation (30) is used for the imaginary potential in the absorbing layers, with c=2.62 and d=20 (in a.u.). We see that for the entire energy range, even for energies well above the barrier, the numerical solution from Eq. (54) is essentially exact. Note also the complete absence of the quantum well oscillations that would arise if one used real periodic boundary conditions.

Next, we demonstrate the flexibility of the method by solving the scattering of a phonon in an inhomogeneous twodimensional nanowire with a width d. We consider the horizontally polarized shear wave for which the wave equation in the frequency domain is



FIG. 4. Transmission probability as a function of electron energy through a one-dimensional square barrier. Two curves (calculated and exact) are indistinguishable in the figure.

$$v^2 \nabla^2 \psi(x, y) + \omega^2 \psi(x, y) = 0, \qquad (55)$$

where ω is the frequency and v is the phase velocity which may vary with position along the direction of the wire (*x* direction) due to the inhomogeneity. Assuming that there is no inhomogeneity across the width of the nanowire (*y* direction), the transverse modes are $\cos(n\pi y/d)$ for free edges, where 0 < y < d, and *n* is an integer. The total solution is a summation over all transverse modes,

$$\psi(x,y) = \sum_{n} A_{n} \psi_{n}(x) \cos\left(\frac{n \pi y}{d}\right), \tag{56}$$

where $\psi_n(x)$ satisfy the one-dimensional wave equation,

$$v^{2}(x)\frac{\partial^{2}}{\partial x^{2}}\psi_{n}(x) + \left[\omega^{2} - v^{2}(x)\left(\frac{n\pi}{d}\right)^{2}\right]\psi_{n}(x) = 0.$$
 (57)

The inhomogeneity of the nanowire is represented by the x dependence of the velocity v(x). For our example, we use $v(x) = v_0 + \cos^2(x) \pm \exp(-2x^2)$. The oscillatory second term mimics a superlattice. Semiconductor superlattices in three dimensions have been studied for folded phonon modes.^{21,22} The last term represents the effect of localized stress, for example, due to a local defect or bending of the nanowire. It can be either positive (faster) or negative (slower). In Fig. 5, we show the transmission of the first three transverse modes, n=0, 1, and 2, as a function of frequency for both cases.Without the defect, the periodic inhomogeneity does not produce scattering and the transmission should be unity at all frequencies. The defect suppresses the transmission of the n=0 mode at intermediate frequencies and nearly completely blocks low frequency phonons for modes n > 0. There are no n > 0 propagating modes for frequencies below $\omega = (v_0 + 1)$ $\times (n\pi/d)$, as indicated by the low frequency gaps in the transmission for n=1 and 2.

VI. CALCULATION OF RESISTANCE OF A TWIN BOUNDARY

In this section, we apply the theory to the interesting problem of the resistance of a twin boundary in crystalline



FIG. 5. Transmission of a phonon through a nanowire with a localized defect as a function of frequency. The transverse modes are n=0, 1, and 2. The impurity potential is positive (negative) for the top (bottom) panel.

copper. Recent work²³ on nanocrystalline copper shows that high strength and low resistivity can be achieved by introducing a large number of twin boundaries in the crystal. Twin boundaries have much lower resistance than other types of grain boundaries. Reference 23 puts the resistance of a coherent twin boundary at about $1.7 \times 10^{-17} \Omega m^2$. Here, we use our complex band approach to calculate this resistance from first principles. The complex band structures are computed for both the reference system and one containing a twin boundary. In this case, we used a constant imaginary potential of 0.01 hartree in the absorbing layers, which was sufficient to damp out the interference effects between two neighboring twin boundaries. The decaying wave numbers are found for 4481 k points within a symmetry-reduced, 1/3 of the two-dimensional Brillouin zone. The first-principles code using the layer KKR method is used in this calculation.10 Transmission probabilities through the twin boundary for all **k** points are integrated to obtain a total conductance. This is then subtracted from the integral obtained over the same number of k points but with perfect transmission to calculate the resistance due to the twin boundary. We obtain the resistance of $1.48 \times 10^{-17} \ \Omega \ m^2$ for a clean twin boundary, which is slightly below the experimental value.

A possible source of error in this calculation is the interfacial resistance between the electrode and the absorbing layer. This is a very small resistance in proportion to the second order of the imaginary part of the energy. In addition, the interfacial resistance of the absorbing layer should be approximately the same between the full system and the reference system, and thus approximately canceled in Eq. (54). However, due to the very small twin boundary resistance in



FIG. 6. Resistance of a twin boundary in copper as a function of impurity concentration on the interface layer. The two solid lines are vacancies and Pb impurities. The dashed line is vacancies without vertex corrections (VC).

copper, we estimate that the error bar in the calculated twin boundary resistance is roughly 30% when using the imaginary energy of 0.01 hartree.

We also calculate the twin boundary resistance when impurities are segregated at the interface using the coherent potential approximation (CPA).²⁴ Two types of impurities are considered, vacancies and Pb atoms. The results are shown in Fig. 6. A vacancy concentration of 0.6% or a minute amount of Pb atoms on the interface can increase the interface resistance to the experimental value of 1.7 $\times 10^{-17} \Omega$ m².

Direct application of the CPA without vertex corrections (the scatter-in terms) would yield a resistance that is too large, shown also in Fig. 6 for vacancies. This error arises because the CPA does not conserve flux. The vertex corrections are calculated approximately with a simple two-step procedure. First, we find an imaginary constant potential Im V on the interface layer such that the CPA scattering matrix t_{CPA} computed at the Fermi energy E_F conserves the total flux. The mathematical expression for this condition is

det $|2t_{CPA}+I|=1$, where *I* is the unit matrix. An interface resistance is computed with these flux conserving CPA scattering matrices, which remove all diffusive effects to the resistance. The diffusive contribution is then computed using a lifetime approximation over the thickness of a single atomic layer with the lifetime $\tau=2\hbar/\text{Im }V$, where the factor of 2 accounts for the difference between the electron density and the wave function. Note that this procedure becomes exact for the model of free electrons with random point scatterers.²⁵

VII. CONCLUSION

We have shown that the Bloch theorem can be generalized in a way that is suitable for transport problems. The exact agreement between the approach here and the exact solution in the model test case highlights the accuracy and robustness of the method.

We note that in all three numerical examples, even when the original unaltered scattering problems do not contain evanescent solutions, the transmission amplitudes obtained from the evanescent solutions with the absorbing boundary conditions are still highly accurate. The accuracy is clearly evident from the high degree of agreement between the calculated and the exact solutions in the first example. This result significantly broadens the usefulness of complex bands beyond the description of evanescent waves in a tunneling barrier. In the form of Eq. (54), it can be used to describe a broad range of single-particle scattering problems.

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