An embedding potential definition of channel functions

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Abstract
We show that the imaginary part of the embedding potential, a generalised logarithmic derivative, defined over the interface between an electrical lead and some conductor, has orthogonal eigenfunctions which define conduction channels into and out of the lead. In the case of an infinitely extended interface we establish the relationship between these eigenfunctions and the Bloch states evaluated over the interface. Using the new channel functions, a well-known result for the total transmission through the conductor system is simply derived.

1 Introduction
In scattering theory, and consequently in the theory of electrical conductance \[1\], the concept of channels is fundamental – channels are the asymptotic states at a particular energy, identified by some quantum numbers, between which the electrons are scattered. In conductance studies, which is our main concern, the current enters a nanostructure (for example) through open channels in the leads on one side, and is transmitted into the open channels on the other side \[2\]. The theoretical problem in finding the conductance then
becomes one of calculating the transmission probability between the channels \[3\]. In this paper we show that channels can be usefully defined in terms of the embedding potentials which embed the nanostructure on to the leads \[4, 5\]. Moreover, this gives a simple derivation of the well-known result \[6, 7, 8\] that the total transmission through the nanostructure between the left- and right-hand leads at energy \(E\) is given by

\[
T_{lr}(E) = 4\text{Tr}[G_{lr}(E)\Im\Sigma_r(E)G^*_{rl}(E)\Im\Sigma_l(E)].
\]

Here \(G_{lr}\) is the Green function connecting the left- and right-hand surfaces of the nanostructure, and \(\Sigma_{l/r}\) is a self-energy, or embedding potential, which couples each surface to the left- or right-hand contact respectively. The trace is over the quantum numbers of the channels in each contact. It was Wortmann et al. \[8\] who realised that \(\Im\Sigma_{l/r}\) in (1) is the same as Inglesfield’s embedding potential \[4\], and derived (1) in the embedding context. They have used this result with embedding to study the transmission of metallic interfaces \[8\], and recently field emission has been calculated using the same formalism \[9\].

The embedding potential in (1) has been widely used in surface, interface, and transport calculations \[3, 10, 11\]. In surface calculations, for example, the surface region is joined on to a semi-infinite substrate, which can be replaced by an embedding potential. The embedding potential, added on to the Hamiltonian for the surface region, ensures that the surface wave-functions match onto the substrate wave-functions. This means that the whole problem can be treated by solving the Schrödinger equation for one or two layers of atoms at the surface rather than the whole semi-infinite substrate.

In this paper we shall show how the embedding potential over a surface can be used to define channels crossing the surface. We shall relate these channels for the case of an infinitely extended two-dimensional surface of a semi-infinite solid to the Bloch states in the solid. Our results enable us to derive some interesting formulae in scattering theory, and in particular allow us to derive (1) rather easily.

We use atomic units (a.u.), in which \(e^2 = \hbar = m_e = 1\), and also eV for energy (27.2 eV = 1 a.u.).
2 The embedding potential and flux

The embedding potential Σ, which is the basis of this paper, is a generalised logarithmic derivative for the substrate region which it replaces \[4\], satisfying

\[
\frac{\partial \psi}{\partial n}(r_S) = -2 \int_S d^2r_S \Sigma(r_S, r'_S) \psi(r'_S).
\]

(2)

Here the integral is over the boundary \(S\) between the surface and substrate, and in the partial derivative \(n\) is the normal to \(S\), taken into the substrate; \(\psi(r)\) is the solution of the Schrödinger equation in the substrate, integrated from some boundary value \(\psi(r_S)\) on \(S\) with outgoing boundary conditions into the substrate. Σ is the same as the mathematicians’ Dirichlet to Neumann map \[12\].

The embedding potential can be found from \(G_0\), the substrate Green function satisfying a zero-derivative boundary condition on \(S\) \[4\],

\[
\Sigma(r_S, r'_S) = G_0^{-1}(r_S, r'_S),
\]

(3)

where \(G_0^{-1}\) is the inverse of \(G_0\) over \(S\). The surface inverse can be avoided by writing Σ in an alternative form, in terms of a double normal derivative of the Green function \(\hat{G}\) satisfying the zero amplitude boundary condition \[13\],

\[
\Sigma(r_S, r'_S) = -\frac{1}{4} \frac{\partial \hat{G}}{\partial n_S \partial n'_S}(r_S, r'_S).
\]

(4)

In this paper we shall be considering the embedding potential as a surface operator in the real-space representation of the Hamiltonian, but it can also be found in tight-binding form \[5\ \[14\], where it is usually called a self-energy.

The current can be written in terms of \(\Im \Sigma\), which is ultimately why this term appears in the transmission expression \[1\]. To show this, we start from the expression for the current density

\[
J = \frac{1}{2i} \{\psi^* \nabla \psi - \psi \nabla \psi^*\}.
\]

(5)

We now consider an embedding surface \(S\), the interface, say, between the nanostructure and one of the leads (figure 1). Substituting (2) into (5), the flux across \(S\) is given by

\[
I = i \int_S d^2r_S \int_S d^2r'_S [\psi^*(r_S)\Sigma(r_S, r'_S)\psi(r'_S) - \psi(r_S)\Sigma^*(r_S, r'_S)\psi^*(r'_S)].
\]

(6)

Note that because of the convention for the sign of the normal derivative in (2), this is the flux from the nanostructure into the lead. As the embedding potential has the symmetry property of Green functions, namely

\[
\Sigma(r_S, r'_S) = \Sigma(r'_S, r_S),
\]

(7)
Figure 1: Nanostructure joined on to metallic leads, represented by shaded areas. Region I, consisting of the nanostructure + right-hand lead is embedded over $S$ onto the left-hand lead, region II. Subsequently it is convenient to label the left- and right-hand interfaces by $S_L$ and $S_R$.

equation (6) simplifies to

$$I = -2 \int_S d^2r_S \int_S d^2r'_S \psi^*(r_S) \Im \Sigma(r_S, r'_S) \psi(r'_S).$$  \hspace{1cm} (8)

The fact that (8) gives the flux into the lead is associated with our convention that $\Sigma$ corresponds to outgoing waves. This is because $G_0$, whose surface inverse gives the embedding potential (3), is evaluated at energy $E + i\epsilon$, where $\epsilon$ is a positive infinitesimal.

At this stage we introduce the eigenfunctions of $\Im \Sigma$ at each energy as a natural choice of channel functions, given by the equation

$$\int_S d^2r'_S \Im \Sigma(r_S, r'_S) \psi_i(r'_S) = \lambda_i \psi_i(r_S).$$  \hspace{1cm} (9)

Although (9) only gives the channel function $\psi_i(r_S)$ over $S$, this uniquely defines the corresponding outgoing wave-function throughout the substrate. Because $\Im \Sigma(r_S, r'_S)$ is real, and symmetric in $r_S$ and $r'_S$, the eigenvalues are all real. The eigenfunctions can be taken to be real and orthogonal. If the eigenfunctions are normalised to unity over $S$,

$$\int_S d^2r_S \psi_i(r_S)^2 = 1,$$  \hspace{1cm} (10)
we see by substituting into (8) that the flux associated with \( \psi_i \) is \(-2\lambda_i\). This must be positive or zero, because of the outgoing boundary conditions implicit in the embedding potential, so we conclude that \( \Im \Sigma \) is negative semi-definite, with eigenvalues negative or zero. The eigenfunctions with non-zero eigenvalue correspond to flux-carrying, open channels; there is an infinite number of closed channel eigenfunctions satisfying (9) with zero eigenvalue.

\( \Im \Sigma \) can be expanded in the usual way, as a sum over its eigenfunctions, and with the normalisation given by (10) we have

\[
\Im \Sigma(r_S, r'_S) = \sum_i \lambda_i \psi_i(r_S) \psi_i(r'_S). \tag{11}
\]

This reduces to a sum over the open channel functions,

\[
\Im \Sigma(r_S, r'_S) = \sum_{\text{open} \ i} \lambda_i \psi_i(r_S) \psi_i(r'_S), \tag{12}
\]

a result which we shall find useful later on.

In conductance, it is only the open channels which are important, those with non-zero eigenvalue. The same open channel functions can be used for flux \emph{out} of the lead into the nanostructure; this corresponds to using the \( \Sigma \) appropriate to incoming waves, which just involves a change in the sign of \( \Im \Sigma \). These channels have the advantage of being defined via (9) over the interface between the lead and the nanostructure, precisely where they are needed. They do in fact correspond to the usual channels in at least one case, the case of waveguides. With a waveguide lead, the separability of the Schrödinger equation for motion along the waveguide and across the guide leads to different waveguide modes, and an embedding potential which is diagonal in a mode representation \( \Sigma \). As a result, each embedding potential channel function \( \psi_i(r_S) \) corresponds to a waveguide mode.

### 3 Bloch states and channel functions

In the case of an infinitely extended interface, it is interesting to study the relationship between our channel functions and the substrate Bloch states evaluated over this interface. With an extended interface, the “lead” on one side consists of a semi-infinite metal in which all wave-functions can be labelled by the Bloch wave-vector parallel to the interface, \( K \). The embedding potential can be expanded as

\[
\Sigma(r_S, r'_S) = \sum_K \sum_{n,m} \Sigma_{K,nm} \chi_K^n(r_S) \chi_K^m(r'_S) \tag{13}
\]
using a set of orthonormal surface functions \( \chi_{K,n}(r_S) \), in general complex, that satisfy Bloch’s theorem with wave-vector \( K \). Using (7) it follows that

\[
\Im m \Sigma(r_S, r'_S) = \sum_K \tilde{\Sigma}_K(r_S, r'_S) \tag{14}
\]

with \( \tilde{\Sigma}_K \) expanded as

\[
\tilde{\Sigma}_K(r_S, r'_S) = \sum_{n,m} \tilde{\Sigma}_{K,nm} \chi_{K,n}(r_S) \chi^*_{K,m}(r'_S) \tag{15}
\]

where

\[
\tilde{\Sigma}_{K,nm} = \frac{1}{2i} \left[ \Sigma_{K,nm} - \Sigma^*_{K,mn} \right]. \tag{16}
\]

\( \tilde{\Sigma}_K \) is Hermitian and so has real eigenvalues, and its eigenfunctions are the channel functions since the flux across the surface \( S \) of an outgoing state with Bloch wave-vector \( \psi(r_S) = \sum_n c_{K,n} \chi_{K,n}(r_S) \), (17)
is given by

\[
I = -2 \sum_{n,m} c^*_{K,n} \tilde{\Sigma}_{K,nm} c_{K,m}. \tag{18}
\]

At each \( K \) and energy \( E \) there are Bloch states travelling towards and away from the interface, as well as solutions decaying exponentially into the bulk [15]. These Bloch states and evanescent states can be considered as open and closed channels respectively, and channels defined in this way have been used in transport studies across interfaces [8, 16]. In line with our convention, let us take the open Bloch channels to be the states propagating away from the interface, into the bulk; the states travelling in the opposite direction simply involve the perpendicular component of the wave-vector changing sign. We shall denote these Bloch states and the exponentially decaying states by \( \phi_{K,i}(r) \), with \( i \) labelling the states at fixed \( K \) and \( E \).

These Bloch states, evaluated over the interface, also diagonalize \( \tilde{\Sigma}_K \) (hence \( \Im m \Sigma \)), but we shall see that they are not the same as our channel functions \( \psi_{K,i} \). As before, the flux associated with \( \phi_{K,i} \) is given by

\[
I_i = -2 \int_S d^2 r_S \int_S d^2 r'_S \phi^*_{K,i}(r_S) \tilde{\Sigma}_K(r_S, r'_S) \phi_{K,i}(r'_S). \tag{19}
\]

There is also a well-known result [8], which follows from Green’s theorem and the Bloch property of the wave-functions, that for \( i \neq j \)

\[
\int_S d^2 r_S \left[ \phi^*_{K,i}(r_S) \frac{\partial \phi_{K,j}}{\partial n_S}(r_S) - \phi_{K,j}(r_S) \frac{\partial \phi^*_{K,i}}{\partial n_S}(r_S) \right] = 0, \tag{20}
\]
\[
\int_S d^2 r_S \int_S d^2 r'_S \phi^*_K, i(r_S) \tilde{\Sigma}_K(r_S, r'_S) \phi_K, j(r'_S) = 0, \quad i \neq j. \tag{21}
\]

Unfortunately, equations (19) and (21) do not imply that the \( \phi_K, i \)'s are eigenfunctions of \( \tilde{\Sigma}_K \) or \( \Im m \Sigma \). Although these functions are orthogonal over the three-dimensional unit cell, it is known that the \( \phi_K, i \)'s are not orthogonal when integrated over the surface,

\[
\int_S d^2 r_S \phi^*_K, i(r_S) \phi_K, j(r_S) = 0, \quad i \neq j. \tag{22}
\]

However, the \( \phi_K, i \)'s are linearly independent – this makes it possible to use them in surface and interface matching procedures. In order for the function space spanned by the open \( \phi_K, i(r_S) \) and \( \psi_K, i(r_S) \) to be the same, there must be the same number of Bloch functions as our channel functions carrying finite flux.

The transformation matrix, which relates the flux-carrying Bloch states with the open channel functions, has the very useful property of being unitary. Let us normalise the open \( \phi_K, i(r_S) \) and \( \psi_K, i(r_S) \) to carry unit flux per two-dimensional unit cell, away from the interface, so that

\[
\int d^2 r_S \int d^2 r'_S \phi^*_K, i(r_S) \tilde{\Sigma}_K \phi_K, j(r'_S) = -\frac{\delta_{ij}}{2}, \quad \int d^2 r_S \int d^2 r'_S \psi^*_K, i(r_S) \tilde{\Sigma}_K \psi_K, j(r'_S) = -\frac{\delta_{ij}}{2}. \tag{23}
\]

We now expand the flux-carrying Bloch functions \( \phi_K, i, \phi_K, j \) in terms of the open and closed channel functions (the closed channel functions can be normalised to unity using (10)),

\[
\phi_K, i(r_S) = \sum_{\text{open + closed}} a_{im} \psi_K, m(r_S), \quad \phi_K, j(r_S) = \sum_{\text{open + closed}} a_{jn} \psi_K, n(r_S). \tag{24}
\]

Then from (23) we obtain

\[
\int d^2 r_S \int d^2 r'_S \phi^*_K, i(r_S) \tilde{\Sigma}_K \phi_K, j(r'_S) = -\frac{\delta_{ij}}{2} \quad = \sum_{\text{open + closed}} a^*_{im} a_{jn} \int d^2 r_S \int d^2 r'_S \psi^*_K, m(r_S) \tilde{\Sigma}_K \psi_K, n(r'_S). \tag{25}
\]

But the integral on the right of (25) vanishes when \( m \) or \( n \) is a closed channel, and when \( m, n \) are both open the integral is given by the second equation in (23). Substituting, this gives

\[
\sum_{\text{open}} a^*_{im} a_{jm} = \delta_{ij}, \tag{26}
\]
Figure 2: Au(001) interface at $\mathbf{K} = 0$: (a) band-structure in the $\Gamma X$ direction; (b) eigenvalues of $\tilde{\Sigma}_{\mathbf{K}=0}$ on an embedding plane midway between atomic planes. The calculation uses a finite imaginary energy of 0.1 meV; (c) eigenvalues of $\tilde{\Sigma}_{\mathbf{K}=0}$ on an embedding plane not midway between atomic planes. The numbers label the symmetry of the corresponding eigenfunctions.

showing that the matrix $a_{im}$ in the space of open functions is unitary.

As an example, we consider the case of embedding onto semi-infinite Au(001), taking $\mathbf{K} = 0$, zero wave-vector parallel to the interface. The band-structure as a function of $k_\perp$, the perpendicular component of the wave-vector, is shown in figure 2a, corresponding to the $\Gamma X$ direction in the bulk Brillouin zone. For comparison, the figure also shows the eigenvalues of $\tilde{\Sigma}_{\mathbf{K}}$ for $\mathbf{K} = 0$ as a function of energy, in figure 2b where the embedding surface $S$ is midway between atomic planes, and in figure 2c where the embedding potential has been transferred to a plane that does not intersect muffin-tin regions of the Au potential \cite{17, 10}. We see that the number of bands is indeed the same as the number of non-zero eigenvalues, except at isolated energies where there are $\delta$-function peaks. The $\delta$-function peaks will be discussed later, but other features in the eigenvalue spectrum can be understood in terms of a one-dimensional nearly-free electron model. In this model the embedding potential near a band edge $E_0$ behaves like \cite{18}

$$\Im m \Sigma \propto -\sqrt{|E - E_0|}$$

if the amplitude of the wave-function at $E_0$ is finite on the interface. On the
other hand, if the wave-function at \( E_0 \) is zero on the interface, the embedding potential blows up at the band edge like

\[
\Im m \Sigma \propto \frac{1}{\sqrt{|E - E_0|}}. \tag{28}
\]

Even though this one-dimensional model cannot be directly applied to the complicated bands of an fcc transition metal, our eigenvalues behave like (27) or (28) at band extrema, exhibiting the square root singularity on the embedding surface midway between atomic planes (figure 2b) where symmetry permits the band edge wavefunction to vanish.

The interplay between the eigenvalues and the band-structure can be quite complicated. The tiny semi-circle in the eigenvalue figures, centred on \(-6.8\) eV, varies in energy between the lowest \( X_1 \) state and the maximum of the first \( \Delta_1 \) band. For each energy in this range there are two non-zero eigenvalues, corresponding to the two \( \Delta_1 \) Bloch states in the band structure. Similarly, there is a small eigenvalue semi-ellipse with energies between the minimum of the second \( \Delta_1 \) band at \( E = -3.7 \) eV and its maximum at \( \Gamma_{12} \). It overlaps in energy with an outer eigenvalue starting and finishing at \( \lambda = 0 \), in the range of energies for which there are again two \( \Delta_1 \) Bloch states. This topology shows that when there is more than one \( \phi_{K,i} \) at a particular energy with the same symmetry, there is not a one-to-one relationship with the \( \psi_{K,i} \) channel functions. In the cases we have just described, the two \( \Delta_1 \) Bloch states are associated with one continuous band. This cannot have a one-to-one relationship with the two eigenvalues having the topology shown in figure 2. Rather, each Bloch state is a linear combination of all the channel functions at that energy, as given by (24). Of course, in the case of a symmetry point like \( K = 0 \), the different bands at the same energy frequently have different symmetry, and then we can identify each band with one eigenvalue of \( \tilde{\Sigma}_K \).

The \( \delta \)-function peaks are associated with discrete energies in a symmetry gap, at \( E = -6.0 \) eV (\( \Delta_1 \) symmetry) and \(-0.5 \) eV (\( \Delta_5 \) symmetry). At these energies, the embedding potential has a singularity and its inverse \( \Sigma^{-1} \) has a zero eigenvalue, which from (2) means that there is a normal derivative satisfying

\[
\int_S d^2 r'_S \Sigma^{-1}(r_S, r'_S) \frac{\partial \psi(r'_S)}{\partial n_S} = 0. \tag{29}
\]

In other words, there is a wave-function in the system, with an exponentially decaying envelope, with zero amplitude over the interface, and consequently infinite logarithmic derivative. This gives the \( \delta \)-function peak in the eigenvalue of \( \tilde{\Sigma}_K \). This singularity only appears at an isolated energy in the limit
of $\Sigma_K$ being evaluated at a real energy with an infinitesimal positive imaginary part, and as the associated eigenvector $\psi_i(r_S) = 0$ there is no flux associated with it.

4 Channel functions and scattering

We now use our channel states to provide a simple proof of (1), starting off by deriving a general scattering result containing $\Im m \Sigma$. Let us consider the geometry shown in figure 1 – we wish to find the full wave-function $\chi(r)$ in region I, given an incoming incident wave $\psi(r)$ in the substrate region II. This can be done in several ways starting from Green’s theorem [8, 11, 19], and it follows straightforwardly that $\chi$ in region I is given by

$$\chi(r) = \frac{1}{2} \int_S d^2 r_S \left[ G(r, r_S) \frac{\partial \psi}{\partial n_S}(r_S) - \frac{\partial G}{\partial n_S}(r, r_S) \psi(r_S) \right], \quad (30)$$

where $G$ is the Green function for the combined system of I and II; the surface normal in (30) is taken to be outwards from region I. Now because $G$ in (30) is the outgoing Green function, we can use (2) to substitute for $\partial G/\partial n_S$ as follows

$$\frac{\partial G}{\partial n_S}(r, r_S) = -2 \int_S d^2 r_S' G(r, r_S') \Sigma(r_S', r_S). \quad (31)$$

The incident wave-function, on the other hand, satisfies

$$\frac{\partial \psi}{\partial n_S}(r_S) = -2 \int_S d^2 r_S' \Sigma^*(r_S, r_S') \psi(r_S'), \quad (32)$$

the complex conjugation arising because this is an incoming wave. Substituting (31) and (32) into (30) gives the pleasing result

$$\chi(r) = 2i \int_S d^2 r_S \int_S d^2 r_S' G(r, r_S) \Im m \Sigma(r_S, r_S') \psi(r_S'), \quad \text{r in I.} \quad (33)$$

At this stage we must be clear about the incident wave $\psi$ in (33). This can be any wave in region II in the energy continuum (otherwise $\Im m \Sigma$ in (33) vanishes), satisfying incoming boundary conditions. If region II is a semi-infinite bulk crystal, for example, $\psi$ is an arbitrary combination of the Bloch states approaching $S$, at fixed energy, together with exponentially decaying states. The incident wave is defined entirely by its value over $S$, $\psi(r_S)$, which can take an arbitrary form, provided that it has some projection onto the flux-carrying states.

We now apply (33) to a nanostructure connected to contacts over interfaces $S_l$ and $S_r$ (figure 1). In dividing the system in this way, the nanostructure region also contains the atoms of the contacts which are perturbed.
by the nanostructure. Region I consists of the whole structure to the right of $S_l$, that is, the nanostructure plus the right-hand contact and lead. If $\psi(r)$ is the wave in the left-hand lead incident on the nanostructure, the full wave-function everywhere to the right is given by (33), with the double integral evaluated over $S_l$. We take the incident wave to correspond to the open channel function $\psi_l^i$ defined over the left-hand interface, normalised to unit flux over this interface. Then the wave-function over the right-hand interface is given by

$$\chi_i(r_r) = 2i\lambda^l_i \int_{S_l} d^2 r_l G(r_r, r_l) \psi_l^i(r_l), \quad (34)$$

where $\lambda^l_i$ is the non-zero channel eigenvalue (9). We now expand $\chi_i(r_r)$ in terms of the complete set of channel functions $\psi^r_j(r_r)$ for the right-hand interface,

$$\chi_i(r_r) = \sum_j t_{ij} \psi^r_j(r_r), \quad (35)$$

and normalising the right-hand open channel functions to unit flux we find, for open channels,

$$t_{ij} = 4i\lambda^l_i \lambda^r_j \int_{S_l} d^2 r_l \int_{S_r} d^2 r_r \psi^r_j(r_r) G(r_r, r_l) \psi_l^i(r_l). \quad (36)$$

The transmission coefficient $T_{ij}$ is the transmitted flux in the $j$th channel corresponding to unit incident flux in the $i$th channel, and with our normalisation this is given by

$$T_{ij} = |t_{ij}|^2 = 16(\lambda^l_i \lambda^r_j)^2 \left| \int_{S_l} d^2 r_l \int_{S_r} d^2 r_r \psi^r_j(r_r) G(r_r, r_l) \psi_l^i(r_l) \right|^2. \quad (37)$$

This expression for the transmission coefficient is very simple, with the clear interpretation of $G$ as a propagator from one channel to the other.

Let us now sum $T_{ij}$ over all the open exit channels, to give the total transmitted flux for unit incident flux in channel $i$. Changing and simplifying the notation for spatial coordinates, this is given by

$$\sum_{\text{open}} T_{ij} = 16(\lambda^l_i \lambda^r_j)^2 \int_{S_l} d^2 r_l \int_{S_r} d^2 r_r \psi^r_j(r_r) G(r_r, r_l) \psi_l^i(r_l). \quad (38)$$

Now we have seen that $\Im \Sigma$ can be expanded in terms of the open channel eigenfunctions alone, and with unit flux normalisation (12) becomes

$$\Im \Sigma(r_S, r'_S) = -2 \sum_{\text{open } i} \lambda^2_i \psi_i(r_S) \psi_i^*(r'_S). \quad (39)$$
Hence (38) simplifies to

\[
\sum_{\text{open}} T_{ij} = -8(\lambda_i^j)^2 \int d1_r \int d2_i \int d3_r \int d4_l G(2_l, 1_r) \Im \Sigma_r(1_r, 3_r) \\
\times G^*(3_r, 4_l) \psi_i^l(4_l) \psi_j^l(2_l).
\] (40)

Now we sum over all incident channels, to give

\[
\sum_{\text{open}} T_{ij} = -8 \int d1_r \int d2_i \int d3_r \int d4_l G(2_l, 1_r) \Im \Sigma_r(1_r, 3_r) \\
\times G^*(3_r, 4_l) \left( \sum_{\text{open}} (\lambda_i^j)^2 \psi_i^l(4_l) \psi_j^l(2_l) \right),
\] (41)

and making use of (39) once again, we obtain the result

\[
\sum_{\text{open}} T_{ij} = 4 \int d1_r \int d2_i \int d3_r \int d4_l G(2_l, 1_r) \Im \Sigma_r(1_r, 3_r) \\
\times G^*(3_r, 4_l) \Im \Sigma_r(1_r, 3_r) G^*(4_l, 2_l).
\] (42)

This gives the total transmission for unit flux in each of the incident channels.

This result for total transmission is only useful if there is the same flux in each open incident channel. To understand this let us consider the case of semi-infinite interfaces, with unit flux in each of the incident Bloch functions at fixed \( K \). Then the flux in the \( m' \)th channel function due to the flux in the \( i' \)th Bloch function is given in terms of the coefficients \( a_{im} \) (24) by \( a^*_im \). So the total flux in the \( m' \)th channel due to all the open Bloch channels, each carrying unit flux, is given by \( \sum_i a^*_im \). But because \( a_{im} \) is a unitary matrix, we have \( \sum_i a^*_im = 1 \), and unit flux in each Bloch function implies unit flux in each channel function. This is the result we require: with energy normalisation, the Bloch functions – hence the channel functions – all carry the same flux. We can then write the total transmission between left and right as

\[
T_{lr} = 4 \int d1_r \int d2_l \int d3_r \int d4_l G(2_l, 1_r) \Im \Sigma_r(1_r, 3_r) G^*(3_r, 4_l) \Im \Sigma_l(4_l, 2_l)
\]

\[
= 4 \Tr[G_{lr} \Im \Sigma_r G^*_{rl} \Im \Sigma_l],
\] (43)

recovering (1). This result is manifestly independent of choice of channel functions.

To summarise, we have shown how the eigenfunctions of the embedding potential, a generalised logarithmic derivative, may be used to define conduction channels across a surface. These new channel functions are orthogonal,
which could instil distinct advantages in applications compared to Bloch states as conduction channels. Using the new channel functions we have provided a simple derivation of a well-known result for the total transmission through a conductor system.

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