A simple analytical model for electronic conductance in a one dimensional atomic chain across a defect

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Abstract. An analytical model is presented for the electronic conductance in a one dimensional atomic chain across an isolated defect. The model system consists of two semi infinite lead atomic chains with the defect atom making the junction between the two leads. The calculation is based on a linear combination of atomic orbitals in the tight-binding approximation, with a single atomic one s-like orbital chosen in the present case. The matching method is used to derive analytical expressions for the scattering cross sections for the reflection and transmission processes across the defect, in the Landauer-Buttiker representation. These analytical results verify the known limits for an infinite atomic chain with no defects. The model can be applied numerically for one dimensional atomic systems supported by appropriate templates. It is also of interest since it would help establish efficient procedures for ensemble averages over a field of impurity configurations in real physical systems.

1. Introduction

Impurities, whether chemical or structural, are common place inside physical devices, and exist at unpredictable points in the components material. Their presence affects physical quantities to the extent that the calculated predictions of any theory should be evaluated over the field of impurity configurations. The quantitative evaluation of the consequences of impurity effects is hence of crucial importance to nanoelectronics since device properties are strongly influenced by or even built on such effects [1]. Typical examples to cite are electron scattering by doping elements in semiconductor nanowires [2] and field effect transistors, the spin scattering by disorder in magnetic tunnel junctions [3], and transport of spinpolarized current in dilute magnetic semiconductors [4].

The main aim of the present work is to describe a simple theoretical model for the electronic transport in a one-dimensional atomic chain with a single defect [5]. This model is of interest insofar that if one could present a clear and transparent analytical model for electronic transport via a single defect, this should help establish efficient procedures for ensemble averages over the field of impurity configurations. A widely used technique for these averages is the coherent potential approximation (CPA) [6] as implemented in the Korringa-Kohn-Rostoker [7] and linear muffin-tin orbital (LMTO) [8] first principles methods. CPA has been applied to equilibrium electronic structure and transport calculations [9]. However, since most devices operate under nonequilibrium conditions it is also important to develop appropriate techniques for impurity averaging.

This paper is organized in the following manner. In section 2 we present our model, based on the tight-binding approximation [10-11], and on the matching method [12-13]. The transmission and reflection probabilities, in a Landauer-Buttiker representation [14-15], are calculated in section 3. Finally we present our conclusions in section 4.
2. Model
The system under study is presented in figure 1, along with the associated physical quantities. As can be clearly seen, the system consists of two semi-infinite chains of white atoms, namely the leads, connected by a single black atom, the defect, where lattice spacing is the same everywhere and is equal to $a$. The model assumption is that each atom has one s-like orbital.

![Figure 1. Schematic representation of a one-dimensional chain of atoms along with associated physical quantities.](image)

The defect has values for the potential energy of its electrons given by $U_n$, onsite matrix element for orbitals $\varepsilon'_s$ and associated overlap integrals $V'_{ss}$, different than those for the atoms on the lead chains. These latter are given by the same symbols without the apostrophe.

For the nano junction of Fig.1, the motion of electrons may be described by a Schrödinger equation discretized in real space, which is a common method used for solving one-dimensional quantum mechanics problems. Differences between this version and the continuous Schrödinger equation are generally viewed as a weakness of the discrete model from a purely mathematical point of view, where the discrete equation is often presented as the numerical approximation to the continuous one, exact only in the limit of infinitesimal lattice spacing [11].

The tight-binding (TB) or atomic orbital (AO) methods represent a more adequate approach which we adopt in what follows. Since the pioneer work of Slater and Koster [10], the TB method has been extensively applied to semiconductors. Several different tight-binding Hamiltonians have been proposed in the past [16] as many complicated problems can only be managed using this economic yet realistic approach. Consider that the matrix elements of the Hamiltonian that couple nearest neighbor orbitals, are given in this approach by

$$
\langle s; ja | H | s; j' a \rangle = (\varepsilon_s + U_j) \delta_{j,j'} + V_{ss} \left( \delta_{j,j+1} + \delta_{j,j-1} \right),
$$

(1)

$| s; na >$ signifies an s-orbital on the atom located at $na$, and the $\delta$'s are the Dirac deltas. In our case the assumed overlap integrals would be equal to zero unless the two neighbor atoms are close enough so that their orbitals overlap to an appreciable extent. Further, the electronic wave function may be written as

$$
| \psi > = \sum_{j} C_j | s; ja >.
$$

(2)

Using equation (1) and assuming that $j'$ is the $n$th site, such that $< s; j'a | = < s; na |$, our Schrödinger equation (1) appears as a tri-diagonal matrix eigenvalue equation with successive rows.
\[ s_n a \hat{H} - \hat{E} | \psi \rangle = V_{ss} C_{n-1} + (\epsilon_s + U_n - E) C_n + V_{ss} C_{n+1} = 0. \] (3)

Equation (3) is a key relation which is the basis for our discussion in the present work. The coefficients \( C_n \) can be viewed as the amplitudes of the wave function of the propagating electron on the \( n \)th site. In this respect, this equation is equivalent in its form to the equation of motion of a phonon on a 1D atomic chain \([12]\), and to the spin dynamics of a magnon on a magnetically ordered system \([13]\). Note, furthermore, that the present approach, streamlined here, is effectively comparable to the real-space finite-difference method for electronic conductance calculations \([17-18]\).

3. The scattering cross sections for transmission and reflection

In this section we derive the transmission and reflection coefficients for the system illustrated by Fig.1. To do so we specifically use the matching method; this allows one to effectively solve the infinite set of equations of motion \([12-13]\).

Applying equation (3), we may write the Schrödinger’s equations for every atom in our system. In this way we obtain an infinite number of coupled equations of motion, of which the first five are

\[ s(n+1) a \hat{H} - \hat{E} | \psi \rangle = V_{ss} C_{n-1} + (\epsilon_s + U_{n+1} - E) C_{n+1} + V_{ss} C_{n+2} = 0, \]

\[ s(n+2) a \hat{H} - \hat{E} | \psi \rangle = V_{ss} C_{n+1} + (\epsilon_s + U_{n+2} - E) C_{n+2} + V_{ss} C_{n+3} = 0, \]

\[ s(n+1) a \hat{H} - \hat{E} | \psi \rangle = V_{ss} C_{n+1} + (\epsilon_s + U_{n+1} - E) C_{n+1} + V_{ss} C_{n+2} = 0, \]

\[ s(n-2) a \hat{H} - \hat{E} | \psi \rangle = V_{ss} C_{n+2} + (\epsilon_s + U_{n-2} - E) C_{n+2} + V_{ss} C_{n+1} = 0. \] (4)

We make some parametric simplifications by introducing the new variables:

\[ U_s = U_{n+1} = U_{n+2} = U_{n-1} = U_{n-2}, \quad U_s' = U_n, \quad \Omega = (\epsilon_s + U_s - E) / V_{ss}, \quad \Omega' = (\epsilon_s' + U_s' - E) / V_{ss}, \]

\[ \rho = V_{ss} / V_{ss} \]. Based on these we can rewrite equations (4) in the simpler form

\[ \rho C_n + \Omega C_{n+1} + C_{n+2} = 0, \]

\[ C_{n+1} + \Omega C_{n+2} + C_{n+3} = 0, \]

\[ \rho C_n + \Omega C_{n-1} + C_{n-2} = 0, \]

\[ C_{n-1} + \Omega C_{n-2} + C_{n-3} = 0. \] (5)

As it was mentioned earlier the set of equations (5) cannot be solved in a classical manner, since the above five equations are coupled to an infinite set of equations on the semi-infinite lead chains. To overcome this problem we use the matching method. Let us write this set of equations in matrix form as

\[ A(5 \times 7) B(7) = 0, \] (6)

where

\[ A(5 \times 7) = \begin{pmatrix} \Omega' & \rho & \rho & 0 & 0 & 0 & 0 \\ \rho & \Omega & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \Omega & 1 & 0 & 0 \\ \rho & 0 & \Omega & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & \Omega & 1 \end{pmatrix}, \]

\[ B(7) = \begin{pmatrix} \Omega' & \rho & \rho & 0 & 0 & 0 & 0 \\ \rho & \Omega & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & \Omega & 1 & 0 & 0 \\ \rho & 0 & \Omega & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & \Omega & 1 \end{pmatrix}, \] (7)
and
\[
\begin{pmatrix}
C_n \\
C_{n+1} \\
C_{n-1}
\end{pmatrix}
\]
\[
\overline{B}(7)
\]
(8)

In the matching method we may write the vector \( B \) using a generalized phase factor \( z \) [12-13], which relates the phases on successive lattice site, and employ a Hilbert space spanned by two base vectors \( R \) and \( T \), for the present one dimensional case. It follows that the vector \( B \) may be expressed as
\[
\overline{B}(7) = C(7 \times 5) \overline{D}(5) + \overline{E}(7),
\]
(9)

where
\[
C(7 \times 5) =
\begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 \\
0 & 0 & 0 & 0 & 1
\end{pmatrix},
\]
\[
\overline{D}(5) =
\begin{pmatrix}
C_n \\
C_{n+1} \\
C_{n-1} \\
T \\
R
\end{pmatrix},
\]
and
\[
\overline{E}(7) =
\begin{pmatrix}
0 \\
0 \\
0 \\
z^{-2} \\
z^{-3}
\end{pmatrix}.
\]
(10)

Equation (9) may then be substituted into equation (6) to yield the scattering relation
\[
A(5 \times 7) \left[ C(7 \times 5) \overline{D}(5) + \overline{E}(7) \right] = A(5 \times 7) C(7 \times 5) \overline{D}(5) + A(5 \times 7) \overline{E}(7) = 0.
\]
(11)

To solve equation (11), use of the evanescent dynamics on the perfect lead chains is made so that it is recast in a square matrix form as
\[
F(5 \times 5) \overline{D}(5) = -\overline{G}(5).
\]
(12)

In equation (12), we have
\[
F(5 \times 5) =
\begin{pmatrix}
\Omega' & \rho & \rho & 0 & 0 \\
\rho & \Omega & 0 & z^2 & 0 \\
\rho & 0 & \Omega & 0 & z^2 \\
0 & 1 & 0 & -z & 0 \\
0 & 0 & 1 & 0 & -z
\end{pmatrix},
\]
\[
\overline{G}(5) =
\begin{pmatrix}
0(37) \\
0(38) \\
(z^{-2})^{(39)} \\
0(40) \\
-z^{-1}
\end{pmatrix}.
\]
(13)

Equations (12) and (13) yield analytically the transmission and reflection amplitudes, \( R \) and \( T \), as respectively
\[
R = -\frac{\rho^2 z + \rho^2 z^{-1} + \Omega'}{\Omega' + 2 \rho^2 z},
\]
(14)

and
\[ T = \frac{\rho^2 \left( \frac{1}{z} - \frac{1}{z'} \right)}{\Omega' + 2\rho^2 z}. \] (15)

To verify the validity of these results, the limits when \( \Omega' = \Omega \), and \( \rho \to 1 \), are analyzed. These known limits correspond indeed to the situation where the defect atom becomes identical to the atom of the lead chains. We have calculated \( R \) and \( T \) under these limits, and verified that they do go respectively to the obviously known limits of zero and unity, using equations (14) and (15).

Furthermore, using the analytical results of equations (14) and (15), we obtain in general the scattering cross-sections for the reflection and transmission processes on the one dimensional atomic chain with a single atomic one s-like orbital per site, as follows

\[ r = |R|^2, \]
\[ t = |T|^2. \] (16)

For the present case of a single mode of propagation, the electronic conductance across the defect is given by the basic Landauer-Buttiker relation

\[ G = \frac{2e^2}{h} \sum_i |T_i|^2 = \frac{2e^2}{h} |T|^2. \] (17)

Equation (17) may be applied numerically to calculate the ballistic electronic transport for the case of one-dimensional atomic chains with a single defect by adopting the appropriate physical quantities. The case of a silicon defect atom on a carbon atomic chain, for example, needs to generalize the presented approach to sites with a greater number of orbitals which is a straightforward procedure.

4. Conclusions
This work is a contribution to the study of electronic transport in nanostructures. It presents a model calculation in the tight-binding approximation with a single s-state electronic orbital, to calculate the ballistic transport in one-dimensional atomic chains across a single defect. This system is analyzed specifically to illustrate the validity of the approach, insofar that if one could present a clear and transparent analytical model for electronic transport via a single defect, this may eventually help establish efficient procedures for ensemble averages over a field of impurity configurations in physical devices.

Analytical relations are derived to express the transmission, \( T \), and reflection, \( R \), amplitudes. The corresponding cross sections for ballistic transmission and reflection processes across the defect are hence derived in the framework of the Landauer-Büttiker approach. The accuracy of these relations is verified in the appropriate limits of an infinite atomic chain with no defects.

The presented model can be applied numerically to calculate the electronic transport in one dimensional atomic systems supported by appropriate templates. It may be generalized to higher dimensions and to more complex systems, and is effectively a precursor model which would allow one to treat more complex nanostructures. The model is also of interest since it should help establish efficient procedures for ensemble averages over a field of impurity configurations in real physical systems, as has been done [19] for the propagation of magnons in two-dimensional disordered magnetic alloys using a modified CPA approach.

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Figures

Fig.1: Schematic representation of a one-dimensional chain of atoms along with associated physical quantities. The top row numbers the atoms in the chain. The first bottom row shows the overlap integrals $V_{ss}$ which describe the interactions between nearest neighbor atoms, the lattice spacing $a$, the potential energy of electrons $U_n$ and the wavefunction site coefficients $C_n$. The second bottom row shows onsite matrix elements for the electronic 1s orbitals $\epsilon_s$.