Embedding on to a one-dimensional crystal

J.E. Inglesfield

School of Physics and Astronomy, Cardiff University,
The Parade, Cardiff, CF24 3AA, United Kingdom
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Abstract

A simple expression is derived for the band structure of a one-dimensional periodic potential in terms of two solutions of the Schrödinger equation within the unit cell, one with a zero-derivative boundary condition on the left-hand end of the cell and the other with zero derivative on the right-hand end. From this starting point, a new expression is derived for the embedding potential – this can be added to the Hamiltonian for the surface region of a crystal to replace the semi-infinite substrate, in a one-dimensional approximation. The results are demonstrated in calculations of the band structure and embedding potential for Al in the [001] direction, and the surface electronic structure of the Al(001) surface.

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I. INTRODUCTION

Embedding provides a way of including the effects of the substrate in a calculation of electronic structure over a restricted region of space. For example, embedding allows us to find the electronic structure at a surface by solving the Schrödinger equation in the surface region, adding embedding potentials to the Hamiltonian to include the effects of the semi-infinite substrate and vacuum regions. The embedding potentials ensure that the wave-functions (or the Green function) in the surface region have the correct boundary corrections on the boundaries of the region, without matching wave-functions explicitly. The alternative to embedding is to solve the Schrödinger equation for a slab of material, or a periodic array of slabs. However, slab calculations do not give the energy continuum of bulk states, and unless the slab is very thick, the localised surface states interact across the slab. Embedding calculations have neither of these drawbacks. Several methods have been developed over the years for finding the embedding potential for a semi-infinite substrate, with the full crystal potential, for solving the energy-dependent Schrödinger equation in full-potential calculations of surface electronic structure. In this paper we develop a very fast method for calculating the embedding potential to replace a semi-infinite one-dimensional periodic potential.

Going from the full three-dimensional crystal potential to a one-dimensional potential may seem a retrograde step, but Chulkov et al. have recently developed one-dimensional models of the bulk and surface potential (figure 1), which give an accurate description of electronic states at the surface. This has proved particularly useful in many-body and lifetime studies of Shockley and image potential-induced surface states. This one-dimensional potential is of course felt by electrons moving in three dimensions, with a wave-function of the form

$$\Psi(r) = \exp(iK \cdot R)\psi(z),$$  \hspace{1cm} (1)

where $K$ is the free-electron wave-vector parallel to the surface, which lies in the $R$ plane. Our own interest lies in using these model surface potentials in the time-dependent Schrödinger equation, which we solve by a new embedding technique. The crystal substrate is replaced by a time-dependent embedding potential, essentially the Fourier transform of the energy-dependent embedding potential. This must be evaluated at a very fine energy grid over a very wide energy range – hence we need a method for finding the energy-dependent embedding potential as efficiently as possible.
FIG. 1. One-dimensional potential for modelling the Al(001) surface. At \( z_v \) the surface region is embedded on to the vacuum Coulomb tail, and at \( z_c \) it is embedded on to the semi-infinite crystal potential.

The general idea of embedding is that we partition space into two (or more) regions, solving the Schrödinger equation explicitly in what we call region I, with the rest of space, region II, replaced by an embedding potential added to the Hamiltonian of region I. The embedding potential is defined over the interface \( S \) between regions I and II. Using a variational method, it can be shown that the wave-function for the system, \( \psi(\mathbf{r}) \), satisfies the following Schrödinger equation in region I,

\[
\left( -\frac{1}{2} \nabla^2 + V(\mathbf{r}) \right) \psi(\mathbf{r}) + \delta(\mathbf{r} - \mathbf{r}_S) \left[ \frac{1}{2} \frac{\partial \psi}{\partial n_S} \right] + \int_S d\mathbf{r}'_S \left( \Sigma(\mathbf{r}_S, \mathbf{r}'_S; \epsilon) + (E - \epsilon) \frac{\partial \Sigma}{\partial \epsilon} \right) \psi(\mathbf{r}'_S) = E\psi(\mathbf{r}),
\]

where the integral is over \( S \). The embedding potential \( \Sigma \) is a function of two interface coordinates and is evaluated at trial energy \( \epsilon \); the energy derivative term gives \( \Sigma \) at the required energy \( E \), to first order in \((E - \epsilon)\). The embedding potential gives the generalised logarithmic derivative over \( S \) of the wave-function in region II,

\[
\frac{\partial \psi(\mathbf{r}_S)}{\partial n_S} = -2 \int_S d\mathbf{r}'_S \Sigma(\mathbf{r}_S, \mathbf{r}'_S; E)\psi(\mathbf{r}'_S),
\]
and this ensures that $\psi$ in region I matches correctly in amplitude and derivative on to the solution in II. In three-dimensional applications, we find $\Sigma$ from the Green function for region II satisfying the zero-derivative boundary condition on $S$. However, in the one-dimensional application described in this paper, we use Eq. 3 to find the embedding potential — in one-dimension, this becomes a relation between amplitude and derivative at the point between regions I and II.

As the use of $\Sigma$ suggests, the embedding potential is a form of self-energy, an energy-dependent, possibly complex potential added on to the Hamiltonian to replace a region of phase space or Hilbert space. In fact the embedding potential in the linear combination of atomic orbitals formalism is usually called the self-energy, often in connection with conduction through linear molecules attached at each end to metallic contacts. The contacts and associated electron reservoirs are replaced in the tight-binding Hamiltonian of the system by self-energies (embedding potentials in tight-binding guise). In our embedding method, in which space is partitioned, we can use any convenient basis set for expanding the wave-function or Green function in region I.

We now briefly describe the structure of this paper. In section II we shall use solutions of the Schrödinger equation in one unit cell to calculate the complex band structure, which describes the allowed solutions for the semi-infinite crystal at energy $E$, and the logarithmic derivative of these solutions, hence the embedding potential $\Sigma(E)$. Related results have been derived by Butti, using a different method, and his expression for the one-dimensional embedding potential was used in a recent analysis of electron spectroscopies from adsorbates. The result for the band structure has previously been derived by Kohn and with particular reference to the sinusoidal potential (the Mathieu problem), by McLachlan. The expressions are remarkably simple, and the band structure formula in particular may be useful in teaching, where one-dimensional potentials such as the Kronig-Penney model frequently serve as an introduction to band theory. In section III we shall illustrate the use of the embedding potential in a calculation of the density of states at the Al(001) surface using the one-dimensional model potential of Chulkov et al. The expression for the embedding potential of a one-dimensional crystal is useful not only in the energy domain, but we are also using it in Fourier transform (with an extra factor of $1/E$) to study time-dependent processes at surfaces, such as electron emission.

Atomic units are used in this paper, with $e^2 = \hbar = m_e = 1$. 
Our starting point for finding the band structure and embedding potential is the Green function formula for the wave-function $\psi(z)$ in some interval in terms of the derivatives at the ends of the range,

$$
\psi(z) = \frac{1}{2} [G(z, a)\psi'(a) - G(z, 0)\psi'(0)], \quad 0 \leq z \leq a,
$$

where we take the range to be the unit cell between $z = 0$ and $z = a$ of the infinite one-dimensional crystal; $G$ is the Green function with zero-derivative boundary conditions at the ends of the unit cell. This formula is analogous to the equation in electrostatics giving the potential inside some region of space in terms of the boundary values of the electric field, and can be derived in exactly the same way.

This equation satisfied by the wave-function within the unit cell does not depend on $\psi(z)$ in the rest of the crystal, but we now impose the Bloch form of wave-function. Evaluating $\psi$ at $z = 0$, Eq. 4 becomes

$$
\psi(0) = \frac{1}{2} \psi'(0)[G(0, a)\exp(ika) - G(0, 0)],
$$

where $k$ is the Bloch wave-vector. But we can also evaluate Eq. 4 at $z = a$, giving

$$
\psi(a) = \frac{1}{2} \psi'(a)[G(a, a) - G(a, 0)\exp(-ika)].
$$

Now the logarithmic derivative $\psi'/\psi$ is invariant to a lattice displacement, so comparing these two equations we obtain

$$
G(0, a)\exp(ika) - G(0, 0) = G(a, a) - G(a, 0)\exp(-ika).
$$

The Green function is symmetric in its spatial variables, so $G(0, a) = G(a, 0)$, and Eq. 7 simplifies to

$$
\cos(ka) = \frac{G(0, 0) + G(a, a)}{2G(0, a)}.
$$

This can be simplified further by using the expression for the Green function in terms of wave-functions $\phi_1(z)$ and $\phi_2(z)$, which satisfy the boundary conditions of the Green function at each end of the unit cell: $\phi_1$ satisfies the Schrödinger equation with $\phi_1'(0) = 0$, and at the other end of the unit cell $\phi_2'(a) = 0$,

$$
G(z, z') = -\frac{2\phi_1(z_<)\phi_2(z_>)}{W(\phi_1, \phi_2)},
$$

where $z_<$ and $z_>$ denote the left and right limits of $z$, respectively, and $W(\phi_1, \phi_2)$ is the Wronskian of $\phi_1$ and $\phi_2$.
where $W$ is the Wronskian. Furthermore, we take $\phi_1(0) = 1$, $\phi_2(a) = 1$. Then substituting Eq. 9 into Eq. 8 gives the remarkably simple expression for the wave-vector,

$$\cos(ka) = \frac{\phi_1(a) + \phi_2(0)}{2}. \quad (10)$$

So we can find the Bloch wave-vector corresponding to a particular energy by two integrations through the unit cell, one in each direction, to find $\phi_1$ and $\phi_2$. If the potential is symmetric with respect to the origin, $\phi_1(a) = \phi_2(0)$, and the result simplifies to

$$\cos(ka) = \phi_1(a), \quad (11)$$

Using wave-function matching, Kohn gives a result related to Eq. (10), though instead of using $\phi_2$, his second wave-function has zero amplitude at $z = 0$ and unit derivative. Abramowitz and Stegun quote Eq. (11) in section 20.3.10 in the chapter on Mathieu functions, and this is proved by McLachlan using a Fourier expansion of the wave-function. An alternative approach is given by Butti: he uses the same starting wave-functions as Kohn to find the transfer matrix; this relates solutions of the Schrödinger equation at each end of the unit cell, and its eigenvalues give the Bloch phase factors.

If the solutions $\phi_1$ and $\phi_2$ at real energy $E$ satisfy $|\phi_1(a) + \phi_2(0)|/2 > 1$, then $E$ lies in a bulk band-gap, and the wave-vector $k$ satisfying Eq. (10) is complex (either pure imaginary, or complex with a real part at the Brillouin zone boundary). This corresponds to a Bloch solution forbidden in the infinite bulk crystal, but allowed in the semi-infinite crystal, for example in the case of a crystal with a surface. More generally we can find the band-structure at complex $E$ – we shall need this in section III. In this case, $k$ satisfying Eq. (10) is always complex, and the two solutions correspond to two different physical cases. One solution corresponds to waves travelling to the right and decaying in this direction, with $\text{Im} \, k > 0$; the other solution, with $\text{Im} \, k < 0$ is travelling and decaying to the left. Which solution we take depends on the particular problem – in our case, with the semi-infinite bulk crystal lying in the positive $z$-direction (figure 1) the physical solution corresponds to $\text{Im} \, k > 0$.

To illustrate the method, we evaluate the complex band structure of a one-dimensional pseudopotential corresponding to Al in the [001] direction,

$$V(z) = A \cos(2\pi z/a), \quad (12)$$
FIG. 2. Complex band structure for Al in the [001] direction with the one-dimensional potential. Re $E$ is plotted along the $y$-axis, and Im $E$ is kept fixed at 0.002 a.u. Solid line, Re $k$; dashed line, Im $k$.

where the amplitude is given by $A = 0.0618$ a.u. and the lattice constant $a$ is 3.8 a.u. – the bulk potential of figure 1. This is the Mathieu problem, but our method holds for arbitrary potential and arbitrary origin. We calculate the band structure at complex energy, keeping the imaginary part of the energy fixed at 0.002 a.u. At each energy we find $\phi_1$ and $\phi_2$ by integrating the Schrödinger equation through the unit cell using Numerov’s method \cite{Quiroz26} with a spatial interval of 0.002 a.u., starting off the integrations using the method described by Quiroz Gonzáles and Thompson \cite{Quiroz26}. The resulting band structure, smoothed by working with the small imaginary energy, is shown in figure 2. Re $k$ is plotted in the extended zone scheme to give a continuous curve, weaving its way from band to band around the bulk band gaps; as we expect, Im $k$ is non-zero below the bottom of the band, and in the band gaps. Our analysis of the complex band structure is important now that we turn to the embedding potential.

We need the embedding potential $\Sigma_c$ to replace the semi-infinite bulk crystal, which we assume lies to the right of $z_c$ (figure 1), where we now put the origin of the unit cell. In the
one-dimensional case, Eq. 3 simplifies to the logarithmic derivative,

$$\Sigma_c = -\frac{1}{2} \frac{\psi'(0)}{\psi(0)},$$

(13)

where $\psi$ is the solution of the Schrödinger equation for the semi-infinite crystal travelling or decaying as $z \to \infty$. We can find this logarithmic derivative directly from Eq. 5, and substituting the Wronskian expression for the Green function, Eq. 9 we obtain the following result for the embedding potential,

$$\Sigma_c = \frac{W(\phi_1, \phi_2)}{2[\exp(ika) - \phi_2(0)]}. $$

(14)

The wave-vector $k$ in this expression corresponds to the wave travelling or decaying to the right – this is precisely the value of $k$ which was discussed above in the band structure calculation (figure 2). This result is different in form from the expression derived by Butti, but the two must be identical.

![Graph of embedding potential](image)

**FIG. 3.** Embedding potential for a bulk Al substrate with the one-dimensional potential, evaluated at $z_c = 10$ a.u., as a function of Re $E$. Im $E$ is kept fixed at 0.0002 a.u. Solid line, Re $\Sigma_c$; dashed line, Im $\Sigma_c$.

We now calculate the embedding potential for the Al substrate at $z_c = 10$ a.u., at a complex energy with an imaginary part equal to 0.0002 a.u. The only additional feature
compared with the band structure calculation is that the expression for the embedding potential involves the Wronskian, in which we evaluate the derivatives by finite differences. The results are shown in figure 3, and we note that Im Σ is negative, as we require from causality.

III. SURFACE DENSITY OF STATES

The Al(001) surface is suitable for demonstrating this embedding potential – the one-dimensional crystal potential of Chulkov et al.\textsuperscript{6} should work well in this s-p bonded metal, and the (001) surface shows a Shockley surface state,\textsuperscript{28} as well as structure induced by the image potential.\textsuperscript{29}

We shall calculate the local density of states $\sigma(z, \varepsilon)$ in the surface region, the charge density of states with energy $\varepsilon$. This is given by the sum over states

$$\sigma(z, \varepsilon) = \sum_i |\psi_i(z)|^2 \delta(\varepsilon - \varepsilon_i), \quad (15)$$

where $\psi_i(z)$ is a wave-function of the system with energy $\varepsilon_i$, and it can be written in terms of the Green function evaluated at an energy with a small imaginary part,

$$\sigma(z, \varepsilon) = \frac{1}{\pi} \text{Im} G(z, z; \varepsilon + i\eta). \quad (16)$$

(Note that we use $\varepsilon$ to denote a real energy, and $E$ to denote an energy which may be complex – here, $E = \varepsilon + i\eta$.)

Let us take the surface region, where we calculate $G$, between $z_v$ on the vacuum side and $z_c$ on the crystal side (figure 1), and then in this region $G$ satisfies the Schrödinger equation embedded on both sides,

$$-\frac{1}{2} \frac{\partial^2 G}{\partial z^2} + (V - E)G(z, z'; E) + \delta(z - z_c) \left[ \frac{1}{2} \frac{\partial G}{\partial z} + \Sigma_c(E)G(z_c, z'; E) \right]$$

$$+ \delta(z - z_v) \left[ -\frac{1}{2} \frac{\partial G}{\partial z} + \Sigma_v(E)G(z_v, z'; E) \right] = \delta(z - z'). \quad (17)$$

The surface region is embedded at $z_c$ on to the crystal, with the crystal embedding potential $\Sigma_c$, and at $z_v$ on to the vacuum region, which is replaced by $\Sigma_v$. Unlike Eq. 2, the embedded Schrödinger equation for the Green function does not contain the energy derivative of the embedding potentials; this is because we know the energy at which they should be evaluated – the energy $E$ of the Green function.
FIG. 4. Embedding potential for the vacuum region, evaluated at $z_v = -10$ a.u. with the image plane at $z_0 = -3.44$ a.u., as a function of $\text{Re} \ E$. $\text{Im} \ E$ is kept fixed at 0.0002 a.u. Solid line, $\text{Re} \ \Sigma_v$; dashed line, $\text{Im} \ \Sigma_v$.

Although it is not the main topic of this paper, we shall say a few words about the embedding potential $\Sigma_v$, which replaces the vacuum region outside the crystal. Here the electron feels the Coulomb tail of the image potential,

$$ V(z) = V_0 - \frac{1}{4|z_0 - z|}, \quad (18) $$

where $V_0$ is the vacuum zero (we take the average potential in the bulk crystal as the zero of energy), and $z_0$ is the position of the image plane. Again we calculate the embedding potential from the logarithmic derivative of the outgoing or decaying solution of the Schrödinger equation – this is a combination of the regular and irregular Coulomb functions $F_0$ and $G_0$ (in the notation of Abramowitz and Stegun23), with angular momentum $L = 0$

$$ \psi(z) = H_0^-(\eta, \rho) = G_0(\eta, \rho) - iF_0(\eta, \rho) \quad (19) $$
with arguments given by
\[ \rho = \sqrt{2(E - V_0)(z - z_0)} \]
\[ \eta = \frac{1}{4\sqrt{2(E - V_0)}}. \]  
(20)

Thompson and Barnett\(^{31}\) give a rapidly converging continued fraction expression for \(H_0^{-1}/H_0^{-1}\), from which we can immediately find the vacuum region embedding potential \(\Sigma_v\). Figure 4 shows \(\Sigma_v\), at \(z_v = -10\) a.u. with the image plane at \(z_0 = -3.44\) a.u. as a function of energy, taking \(\text{Im} E = 0.0002\) a.u. The structure just below the vacuum zero at \(E = 0.577\) a.u. comes from bound states of the Coulomb potential.

We are now in a position to solve the embedded Schrödinger equation in region I, the near-surface region, using a basis set expansion for \(G\),

\[ G(z, z'; E) = \sum_{i,j} G_{ij}(E) \chi_i(z) \chi_j(z'). \]  
(21)

The Schrödinger equation Eq. 17 then reduces to a matrix equation,

\[ \sum_j (H_{ij} + \Sigma_{ij}(E) - ES_{ij}) G_{jk} = \delta_{ik}, \]  
(22)

where the Hamiltonian matrix is given by

\[ H_{ij} = \frac{1}{2} \int_{z_v}^{z_c} d\zeta d\chi_i d\chi_j + \int_{z_v}^{z_c} d\zeta \chi_i(z) V(z) \chi_j(z), \]  
(23)

the embedding matrix by

\[ \Sigma_{ij}(E) = \Sigma_c(E) \chi_i(z_c) \chi_j(z_c) + \Sigma_v(E) \chi_i(z_v) \chi_j(z_v), \]  
(24)

and \(S\) is the overlap matrix,

\[ S_{ij} = \int_{z_v}^{z_c} d\zeta \chi_i(z) \chi_j(z). \]  
(25)

We usually use trigonometric basis functions,

\[ \chi_m(z) = \begin{cases} \cos \frac{m\pi \zeta}{2D}, & m \text{ even} \\ \sin \frac{m\pi \zeta}{2D}, & m \text{ odd} \end{cases}, \]  
(26)

where \(\zeta\) is measured from the mid-point of region I,

\[ \zeta = z - \frac{z_v + z_c}{2}. \]  
(27)
FIG. 5. Surface density of states of Al(001), the local density of states integrated through region I, taken between $z_v = -10$ a.u. and $z_c = +10$ a.u.

and a value of $D > (z_c - z_v)/2$ gives a range of logarithmic derivatives at $z_v$ and $z_c$ for matching on to the embedding potentials. Solving Eq. 22 then gives us $G$, and via Eq. 15 the local density of states.

Integrating the local density of states over the surface region, we obtain the surface density of states for Al(001), shown in figure 5. Here we take region I between $z_v = -10$ a.u. and $z_c = +10$ a.u., and 20 basis functions are used, defined with $D = 13$ a.u. These results, which correspond to $K = 0$ in three dimensions, show the Shockley surface state near the bottom of the band gap, broadened by the imaginary part of the energy at which the the Green function and embedding potentials are evaluated, here taken to be 0.0002 a.u. Less familiar is the structure just below the vacuum edge, at $E = 0.577$ a.u., which comes from surface resonances induced by the image potential. These are the image potential surface states, broadened into resonances by interacting with the continuum of bulk states. All the features in the surface electronic structure – the continuum of bulk states, the Shockley and image surface states – depend on a correct treatment of the substrate and vacuum regions,
via the embedding potentials.

IV. CONCLUDING REMARKS

The motivation for this work was to derive the embedding potential for a one-dimensional model of a crystal as efficiently as possible, for subsequent use in energy-dependent or time-dependent surface calculations. We have shown how the band structure and embedding potential can be found by integrating through the unit cell at a chosen energy, starting at each end of the cell with a zero-derivative boundary condition. Using these results, we have calculated the band structure and embedding potential for Al in the [001] direction as a function of complex energy, and applied this to calculating the surface density of states at the Al(001) surface.

We are now using these results in studies of time-dependent excitation processes at surfaces, taking the Fourier transform of the embedding potential to find the time-dependent embedding potential. But one-dimensional periodic potentials occur in a variety of contexts – not least in teaching – and we hope that the results and their derivations will be of wider interest.

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