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A real-space rescaling treatment of the spectral properties of an adatom-contaminated crystal system

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Abstract. An exact real-space rescaling transformation is used to calculate the local Green's functions and the densities of states for a semi-infinite nearest-neighbour tight-binding system with an adatom and an impurity atom located at an arbitrary distance from the surface. The influence of both the surface and impurity atom characteristics on the adatom density of states can be determined in a simple manner.

1. Introduction

Recent work (Southern *et al* 1983a, b, Langlois *et al* 1983, Tremblay *et al* 1983) has demonstrated the effectiveness of the real-space rescaling approach for the study of tight-binding systems. The method can be applied to a wide range of problems and provides a direct method of calculating local Green's functions. The basic idea of the method is to take equations which describe the system with N degrees of freedom and to perform a transformation in which the number of degrees of freedom is reduced. One formulation of the method (Southern *et al* 1983a, b) yields difference equations for the Green's functions and the transformation is constructed in such a way that it leaves the form of these equations invariant when expressed in terms of a set of modified (renormalised) parameters. An equivalent formulation can be constructed in terms of a generating function (Langlois *et al* 1983, Tremblay and Southern 1983) which under the transformation remains invariant apart from an additive term. This latter approach has the advantage of exposing rather clearly the close similarity between the method used here to calculate the Green's functions and the real-space renormalisation approach to the investigation of critical phenomena (Niemeijer and van Leeuwen 1976). Whichever formulation is adopted a set of relationships or recurrence equations are obtained between the renormalised energy parameters and the original set. Iteration of these equations leads to an effective diagonalisation of the Green's function matrix and the local diagonal Green's functions are obtained from the limiting values of the renormalised parameters. If the diagonal Green's functions are analytically continued into the complex z-plane, where $z = E + i\theta$ and E is the energy, the localised states will appear as isolated singularities on the real axis and extended states will appear as branch cuts

on the real axis (Economou 1983). The transformation is exact and these non-regular regions are invariant subspaces.

This method has been used to study the properties of a translationally invariant tight-binding system on a one-dimensional lattice with arbitrary range of interaction (Southern *et al* 1983b), disordered binary harmonic chains (Langlois *et al* 1983), chains with impurities (Southern *et al* 1983a) and fractal systems (Tremblay and Southern 1983). In this paper we apply the technique to a semi-infinite linear chain with an adatom at the surface and an impurity atom situated at some arbitrary site in the bulk. This problem has been considered previously by Ueba (1980) for special values of the interactions between the surface atom and the bulk, and between the impurity atom and the bulk. Using the conventional methods, he calculated the surface and adatom Green's functions and derived the density of states. Our method yields computational procedures which are so simple that we are able to consider the model with no special restrictions on the interactions. We are able to obtain Green's functions and local densities of states at the adatom and at any site of the lattice. In comparing the results of our calculations with those of Ueba (1980) we uncovered errors in his paper which are discussed further in § 5. The outline of the paper is as follows. In § 2 the general approach is described and in § 3 it is applied to the homogeneous chain. Section 4 treats the semi-infinite system with an adatom and impurity. In § 5 we present some sample results and in § 6 we state our conclusions.

2. The general nearest-neighbour transformation

We consider the nearest-neighbour tight-binding Hamiltonian

$$H = \sum_j \left(|j\rangle \varepsilon(j) \langle j| + |j\rangle V(j, j+1) \langle j+1| + |j+1\rangle V(j, j+1) \langle j| \right) \quad (1)$$

where the state $|j\rangle$ is an atomic-like orbital centred at site j and the sites form a regular one-dimensional lattice of N sites with periodic boundary conditions. The parameters $\varepsilon(j)$ and $V(j, j+1) = V(j+1, j)$ represent the diagonal and off-diagonal elements of the Hamiltonian in this basis. The spectral properties of the atom at site j can be obtained from the diagonal element $\langle j|G(N, H; z)|j\rangle$ of the lattice Green's function operator $G(N, H; z) = (zI - H)^{-1}$ where I is the identity operator and $z = E + i\theta$, E being the energy.

Let

$$|u\rangle = \sum_j u(j)|j\rangle \quad (2)$$

where the coefficients $u(j)$ are all real. Then it is not difficult to show (Langlois *et al* 1983) that

$$G(N, H; z) = -\frac{\tau(z) i \int \mathcal{D}u |u\rangle \langle u| \exp[\frac{1}{2} i \tau(z) \langle u|(zI - H)|u\rangle]}{\int \mathcal{D}u \exp[\frac{1}{2} i \tau(z) \langle u|(zI - H)|u\rangle]} \quad (3)$$

where

$$\int \mathcal{D}u = \prod_j \int_{-\infty}^{\infty} du(j) \quad (4)$$

and $\tau(z) = \mathrm{sgn}(\mathrm{Im}(z)) = \mathrm{sgn}\,\theta$ to ensure convergence of the integrals.

We define the generating function by

$$F(N, H; z) = -\ln \Xi(N, H; z) \tag{5}$$

where

$$\Xi(N, H; z) = \int \mathcal{D}u \, \exp[\tfrac{1}{2}i\tau(z) \langle u|(zI - H)|u\rangle] \tag{6}$$

is the analogue of the partition function in statistical mechanics. From equations (3) to (6)

$$G(N, H; z; j) \equiv \langle j|G(N, H; z)|j\rangle = -2\,\partial F/\partial \varepsilon(j) \tag{7a}$$

and the site average diagonal Green's function is

$$g(H; z) = \frac{1}{N} \sum_j G(N, H; z; j) = \frac{2}{N} \frac{\partial F}{\partial z}. \tag{7b}$$

The function

$$\rho(z; j) = -(\tau(z)/\pi) \, \mathrm{Im} \, G(N, H; z; j) \tag{8}$$

is the analytic continuation into the complex z-plane of the local density of states (LDOS) at site j. It follows from (7) and (8) that

$$\rho(z; j) = (2\tau(z)/\pi) \, \mathrm{Im} \, \partial F/\partial \varepsilon(j). \tag{9}$$

The calculation of the generating function F involves integrating over the N degrees of freedom $u(j)$, $j = 1, 2, \ldots, N$. In the real-space rescaling approach, F is calculated by performing a partial sum over a fraction of these degrees of freedom. The method proceeds as follows. We divide the lattice into two sublattices indexed (1) and (2) consisting of even- and odd-numbers sites respectively. The Hamiltonian is decomposed into

$$H = H_{11} + H_{12} + H_{21} + H_{22} \tag{10}$$

where

$$H_{11} = \sum_j |2j\rangle \varepsilon(2j) \langle 2j| \tag{11a}$$

$$H_{12} = \sum_j \left(|2j\rangle V(2j, 2j + 1) \langle 2j + 1| + |2j\rangle V(2j, 2j - 1) \langle 2j - 1| \right) \tag{11b}$$

$$H_{21} = \sum_j \left(|2j + 1\rangle V(2j + 1, 2j) \langle 2j| + |2j - 1\rangle V(2j - 1, 2j) \langle 2j| \right) \tag{11c}$$

$$H_{22} = \sum_j |2j + 1\rangle \varepsilon(2j + 1) \langle 2j + 1|. \tag{11d}$$

Writing

$$|u\rangle = |u: 1\rangle + |u: 2\rangle \tag{12}$$

where

$$|u: 1\rangle = \sum_j u(2j) |2j\rangle \tag{13a}$$

$$|u: 2\rangle = \sum_j u(2j + 1) |2j + 1\rangle \tag{13b}$$

we have

$$\langle u | (zI - H) | u \rangle = \langle u: 1 | (zI - H_{11}) | u: 1 \rangle - \langle u: 1 | H_{12} | u: 2 \rangle - \langle u: 2 | H_{21} | u: 1 \rangle$$
$$+ \langle u: 2 | (zI - H_{22}) | u: 2 \rangle. \tag{14}$$

Equation (14) can be rearranged into the form:

$$\langle u | (zI - H) | u \rangle = \langle w | (zI - H_{22}) | w \rangle + \langle u' | (zI - H') | u' \rangle \tag{15}$$

where

$$|w\rangle = |u: 2\rangle - (zI - H_{22})^{-1} H_{21} |u: 1\rangle = \sum_j w(j) |2j + 1\rangle \tag{16a}$$

with

$$w(j) = u(2j + 1) - \frac{V(2j + 1, 2j) u(2j)}{z - \varepsilon(2j + 1)} - \frac{V(2j + 1, 2j + 2) u(2j + 2)}{z - \varepsilon(2j + 1)} \tag{16b}$$

$$|u'\rangle = |u: 1\rangle = \sum_j u'(j) |2j\rangle \tag{17a}$$

with

$$u'(j) = u(2j) \tag{17b}$$

and

$$H' = H_{11} + H_{12}(zI - H_{22})^{-1} H_{21}. \tag{18}$$

We now transform the variables in the integral formula (6) from $\{u(j)\}$ to $\{u'(j), w(j)\}$. From (16b) and (17b) the Jacobian of the transformation is unity. Performing the gaussian integrations for the variables $\{w(j)\}$ and substituting into (5) we have

$$F(N, H; z) = \tfrac{1}{2} \sum_j \ln\left(\frac{\tau(z)[z - \varepsilon(2j + 1)]}{2\pi i}\right) + F(\tfrac{1}{2}N, H'; z) \tag{19}$$

where

$$H' = \sum_j \{|2j\rangle \varepsilon'(j)\langle 2j| + |2j\rangle V'(j, j + 1)\langle 2j + 2| + |2j + 2\rangle V'(j, j + 1)\langle 2j|\} \tag{20}$$

and from (18)

$$z - \varepsilon'(j) = z - \varepsilon(2j) - \frac{(V(2j, 2j + 1))^2}{z - \varepsilon(2j + 1)} - \frac{(V(2j, 2j - 1))^2}{z - \varepsilon(2j - 1)} \tag{21a}$$

$$V'(j, j + 1) = V(2j, 2j + 1) V(2j + 1, 2j + 2)/(z - \varepsilon(2j + 1)). \tag{21b}$$

Under the transformation represented by equations (19) to (21) there is an effective decoupling between the even- and odd-numbered sites of the lattice. The mapping is to an equivalent lattice problem with Hamiltonian H' which has renormalised couplings between the even-numbered sites. Beginning with the couplings $\varepsilon^{(0)}(j) = \varepsilon(j)$, $V^{(0)}(j, j + 1) = V(j, j + 1)$ and the Hamiltonian $H^{(0)} = H$ the equations (18) to (21) can be iterated to produce a sequence of couplings $\varepsilon^{(n)}(j)$, $V^{(n)}(j, j + 1)$ and Hamiltonians $H^{(n)}$, for $n = 0, 1, 2, \ldots$, where

$$H^{(n)} = \sum_j (|2^n j\rangle \varepsilon^{(n)}(j)\langle 2^n j| + |2^n j\rangle V^{(n)}(j, j + 1)\langle 2^n(j + 1)|$$
$$+ |2^n(j + 1)\rangle V^{(n)}(j, j + 1)\langle 2^n j|). \tag{22}$$

The dependence of the generating functions $F(2^{-n}N, H^{(n)}; z)$ on the initial couplings become increasingly complicated as n is increased and more sites of the lattice are subject to integration. The only exception to this is the site $j = 0$ for which

$$\partial \varepsilon^{(n)}(j)/\partial \varepsilon(0) = \delta_{j,0} \tag{23a}$$

$$\partial V^{(n)}(j, j + 1)/\partial \varepsilon(0) = 0 \tag{23b}$$

for $n = 1, 2, \ldots$ and we have from $(7a)$†

$$G(2^{-n}N, H^{(n)}; z; 0) = G(N, H; z; 0) \tag{24}$$

The diagonal Green s function is invariant, under the transformation at site $j = 0$, but not at any other site. The strategy adopted in these calculations, given that we wish to calculate the diagonal Green's function and LDOS at a particular lattice site, is to label the sites in such a way that the site of interest has index $j = 0$. It follows from equation (24) that the local Green's function for our chosen site is invariant under the transformation. This means that singular regions, either branch cuts corresponding to extended states, or isolated singularities corresponding to localised states are invariant under the transformation. That the localised states are invariant can also be seen from the fact that they are roots of

$$\det(zI - H) = 0. \tag{25}$$

Since the Jacobian of the transformation of variables given by (16b) and (17b) is unity these roots are invariant under the transformation.

A necessary condition for the iterative procedure to work is that $|V^{(n)}(j, j + 1)| \to 0$ as $n \to \infty$ uniformly on j. Whether this condition is satisfied can be determined during the numerical calculations. Given that it is, then for all $\delta > 0$, there exists an $n_0 > 0$ such that, for all $n > n_0$, $|V^{(n)}(j, j + 1)| < \delta$ for all j. It is now easy to show that

$$F(N, H; z) = \tfrac{1}{2} \sum_{s=0}^{n-1} \left[\sum_j \ln \left(\frac{\tau(z)(z - \varepsilon^{(s)}(2j + 1))}{2\pi i} \right) \right]$$

$$+ \tfrac{1}{2} \sum_j \ln \left(\frac{\tau(z)(z - \varepsilon^{(n)}(j))}{2\pi i} \right) + O \left(\frac{\delta^2 N}{2^n} \right) \tag{26}$$

for $n > n_0$. Thus from $(7a)$ and (26):

$$G(N, H; z; 0) = \lim_{n \to \infty} (z - \varepsilon^{(n)}(0))^{-1}. \tag{27}$$

The diagonal Green's function and DOS at $j = 0$ can be obtained from the limiting value of $\varepsilon^{(n)}(0)$.

3. The homogeneous case

In the case of a uniform chain we have $\varepsilon(j) = \varepsilon$ and $V(j, j + 1) = V$, for all j, and the equations (21) can be written in the form

$$\zeta' = 2\zeta^2 - 1 \tag{28a}$$

$$V' = V/2\zeta \tag{28b}$$

† Equations (23) and (24) are satisfied for nearest-neighbour interactions only. If the interaction range extends beyond nearest neighbours, then a more complicated chain rule applies. Alternatively the procedure outlined by Southern *et al* (1983a, b) can be adopted.

where

$$\zeta = (2 - \varepsilon)/2V. \tag{29}$$

The mapping

$$\zeta = (1 + t^2)/2t \tag{30}$$

from the complex ζ-plane to the complex t-plane, has two branches separated by the circle $|t| = 1$ which is the image of the branch cut $\zeta \in [-1, 1]$. The inverse mapping

$$t = \zeta[1 - (1 - \zeta^{-2})^{1/2}] \tag{31}$$

takes the ζ-plane into the closed region bounded by $|t| = 1$. Using (30) the recurrence relations (28) can be expressed in the form

$$t' = t^2 \tag{32a}$$

$$V' = Vt/(1 + t^2). \tag{32b}$$

Beginning with the values $t^{(0)} = t$, $V^{(0)} = V$ and iterating equations (32) we have $|t^{(n)}| \to 0$, $|V^{(n)}| \to 0$ whenever $|t^{(0)}| < 1$.

If $|t^{(0)}| = 1$ then $|t^{(n)}| = 1$ for all n. The image of the branch cut is an invariant subspace of the transformation. This is the band of extended states $-1 \leqslant \zeta \leqslant +1$. The band edges $\zeta = +1$ and $\zeta = -1$ correspond to $t = +1$ and $t = -1$, respectively. The former is a fixed point of (32a). The latter maps into that fixed point in one iteration. From (32)

$$t^{(n)} = t^{2^n} \tag{33a}$$

$$V^{(n)} = V \prod_{s=0}^{n-1} \frac{t^{2^s}}{1 + t^{2^{(s+1)}}}. \tag{33b}$$

Equation (33b) can be written in the form

$$V^{(n)} = \frac{V(1 - t^2)t^{(2^n - 1)}}{1 - t^{2^{(n-1)}}} \tag{33c}$$

and from (29)

$$z - \varepsilon^{(n)} = 2V^{(n)}\zeta^{(n)} = \frac{V^{(n)}(1 + t^{2^{(n-1)}})}{t^{2^n}} = \frac{V(1 - t^2)}{t}\left(\frac{1 + t^{2^{(n-1)}}}{1 - t^{2^{(n-1)}}}\right). \tag{34}$$

In the above expressions, each iteration of the transformation eliminates half the sites and corresponds to a scale factor of two. Iteration of the transformation n times leaves $1/2^n$ of the original sites to be integrated. This is equivalent to a scale factor $b = 2^n$. For a general scaling factor b the equations (33) and (34) become

$$t' = t^b \tag{35a}$$

$$V' = \frac{V(1 - t^2)t^{b-1}}{1 - t^{2b}} \tag{35b}$$

$$z - \varepsilon' = \frac{V(1 - t^2)}{t}\left(\frac{1 + t^{2b}}{1 - t^{2b}}\right). \tag{35c}$$

In the limit $n \to \infty$ or $b \to \infty$, when $|t| < 1$, we have from (27),

$$G(N, H; z; 0) = t/V(1 - t^2) = [(z - \varepsilon)^2 - 4V^2]^{-1/2} \tag{36}$$

which is a well-known result (Economou 1983). Using (32) we see that (36) satisfies the invariance conditions (24). An interesting alternative derivation of (36) can be obtained from (26) which, for the homogeneous system, takes the form:

$$F(N, H; z) = \tfrac{1}{4} N \sum_{n=0}^{\infty} (\tfrac{1}{2})^n \ln(z - \varepsilon^{(n)}) + \tfrac{1}{2} N \ln\left(\frac{\tau(z)}{2\pi i}\right). \tag{37}$$

Substituting in (37) from (34) and utilising the identity

$$\tfrac{1}{2} \ln(1 - t^2) = -\sum_{n=1}^{\infty} \ln\left[\left(\frac{1 + t^{2^n}}{1 - t^{2^n}}\right)^{1/2^{n-1}}\right] \tag{38}$$

which is used in a similar way in the computation of the free energy of the one-dimensional Ising model (Nauenberg 1975), we have

$$F(N, H; z) = \frac{N}{2} \ln\left(\frac{V\tau(z)}{2\pi i t}\right). \tag{39}$$

From (29) and (30)

$$dt/dz = t^2/V(t^2 - 1) \tag{40}$$
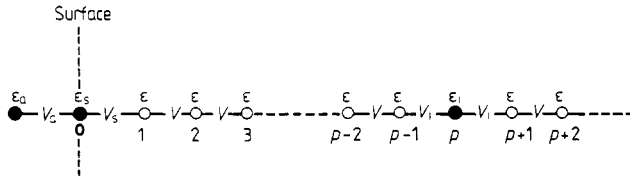
and using (7b) we recover (36).

Figure 1. A semi-infinite chain with an adatom and an impurity p sites from the surface.

4. Semi-infinite chain with adatom and impurity

A semi-infinite chain with an adatom and an impurity, p sites from the surface, is shown in figure 1. From the computational point of view, the simplest way to treat the system is to embed it in an infinite system with Hamiltonian given by (1). The adatom now occupies the site immediately to the left of the surface atom and the interaction between the adatom and the atom on its left is set at zero. If we wish to obtain the spectral properties at m lattice spacings from the surface then, according to the method described in § 2, that site must be assigned the label $j = 0$. Hence the adatom is at $j = -m - 1$, the surface at $j = -m$ and the impurity at $j = p - m$. The parameters in (1) have the values $\varepsilon(j) = \varepsilon$ and $V(j, j + 1) = V$ for all j except for:

$$\varepsilon(-1 - m) = \varepsilon_a \qquad \varepsilon(-m) = \varepsilon_s \qquad \varepsilon(p - m) = \varepsilon_i. \tag{41a}$$

Here ε_a, ε_s and ε_i are the self-energies of the adatom, surface and impurity atoms respectively, and

$$V(-2 - m, -1 - m) = 0 \qquad V(-1 - m, -m) = V_a \qquad V(-m, -m + 1) = V_s$$

$$V(p - m - 1, p - m) = V_i \qquad p > 1$$

$$V(p - m, p - m + 1) = V_i \qquad p > 0 \tag{41b}$$

where the first equation effectively terminates the chain at the adatom and V_a, V_s and V_i are the adatom–surface, surface–bulk and impurity–bulk interactions respectively. The inhomogeneity is thus confined to the strip of sites $\kappa = \{j: -1 - N_0 \leq j \leq N_0\}$ where $N_0 = \max(|1 + m|, |p - m|)$. Our procedure for evaluating $G(N, H; z; 0)$ is as follows:

(a) Choose the zero of energy such that the host self-energy $\varepsilon = 0$ and the energy scale such that $V = 0.5$. The homogeneous chain then has a continuum of states in the range $-1 \leq E \leq 1$. The complex energy $\zeta = z = E + i\theta$ has θ non-zero but small to avoid the singularities on the real axis. A non-zero θ is also required for the iteration procedure to converge. In our calculations we use $\theta = 10^{-8}$.

(b) Initialise all parameters to $\varepsilon(j) = 0$ and $V(j, j + 1) = 0.5$. Redefine the parameters within the strip κ which have different values as indicated by (41).

(c) Iterate equations (21) and test for convergence of the complex parameter $\varepsilon^{(n)}(0)$ at each iteration n.

(d) The DOS $\rho(z; 0)$ at the site m ($j = 0$) is given by (8) and (27).

Outside the region of extended states in the bulk we have $\mathrm{Im}(G(N, H, E; 0)) = 0$ unless E corresponds to a local mode, when $[\mathrm{Re}(G(N, H; E; 0))]^{-1} = 0$. Alternatively we could write

$$\det(zI - H) = \det(zI - H_0) \det(I - G_0 H_1) \tag{42}$$

where H_0 and G_0 are the Hamiltonian and Green's function, respectively, of the homogeneous system and $H_1 = H - H_0$. Because the homogeneous system has no localised states, the roots of

$$\det(I - G_0 H_1) = 0 \tag{43}$$

are the localised states, which are invariant under the transformation. For comparatively simple systems (Southern *et al* 1983a) it is not difficult to find these roots and obtain the reduced set of recurrence relations governing their behaviour within the invariant subspace of the localised states. For more complicated systems, this strategy vitiates the simplicity of the numerical methods proposed in this paper.

5. Results

For the homogeneous system where there is no surface or impurity present the local Green's function $G(N, H; z; j)$ is equal to the site average $g(H; z)$ for all j. The DOS can be obtained from the imaginary part of (36) and there is an inverse square-root singularity at the band edges $|E| = 1$. This singular behaviour can also be deduced using standard scaling arguments (Southern *et al* 1983b, Niemeijer and van Leeuwen 1976) for the generating function F in a neighbourhood of the fixed point $t = 1$ of (32a) which corresponds to the band edge $E = 1$. In the presence of a small number of inhomogeneities, the site average Green function $g(H; z)$ remains unchanged but the local Green's functions $G(N, H; z; j)$ are no longer equal to it. The LDOS at a site m lattice spacings into the bulk is obtained from the limiting value ($n \to \infty$) of $\varepsilon^{(n)}(m)$ under the rescaling transformation. For a site located deep in the bulk ($m \to \infty$), the limiting value is that for the homogeneous system

$$\varepsilon^\infty(\infty) = \begin{cases} E + (E^2 - 1)^{1/2} & E < -1 \\ E + i\tau(z)(1 - E^2)^{1/2} & |E| < 1 \\ E - (E^2 - 1)^{1/2} & E > 1. \end{cases} \tag{44}$$

For sites near the surface, however, $\varepsilon^{(n)}(m)$ does not iterate to these forms and the square-root divergence of the imaginary part of the local Green's function is absent except for the special values of the interaction parameters, referred to below. Instead it approaches zero as a square root at the band edges. We now discuss the results of some sample calculations.

5.1. No impurity in the bulk (p = 0)

This simple case where we have an adatom and a surface but no impurities in the bulk
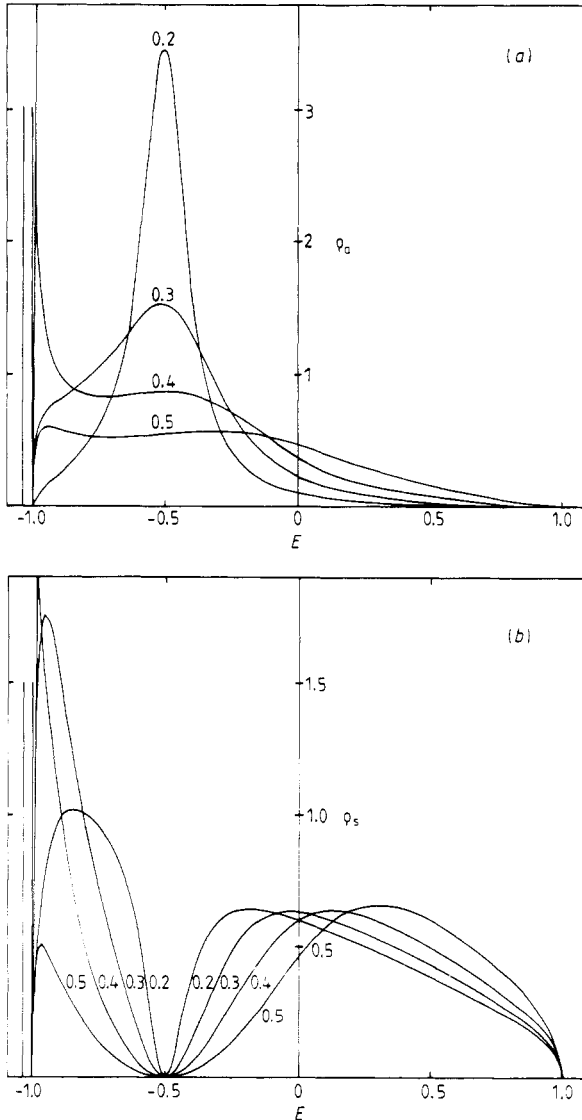
Figure 2. (*a*) Adatom densities of states ρ_a, (*b*) surface densities of states ρ_s, where $\varepsilon_a = -0.5$, $\varepsilon_s = -0.2$, $V_s = 0.5$. The curves are labelled with their values of V_a and the localised state in each case appears only for $V_a > 0.387$.

has been discussed in detail by Ueba (1980). However, his expressions contain a minor error, which we discovered by comparing his results with those obtained using the numerical procedure outlined in § 4. If the surface–bulk interaction $V_s = V = 0.5$ the correct condition for the existence of a local mode in the adatom density of states (ADOS) is $V_a^2 > (\varepsilon_s \mp \tfrac{1}{2})(\varepsilon_a \mp 1)$, where the upper/lower sign refers to the region above/below the band edge of bulk states. The appearance of the local mode is preceeded by a singularity at the band edge when $V_a^2 = (\varepsilon_s \mp \tfrac{1}{2})(\varepsilon_a \mp 1)$. For Ueba's choice of $\varepsilon_a = -0.5$ and $\varepsilon_s = -0.2$ a local mode will appear below the band if $|V_a| > 0.387$. Figure 2(a) shows our results for the ADOS ρ_a for different values of V_a. As indicated above we used $\theta = 10^{-8}$ and for this value approximately 30 iterations are required for convergence of ρ_a at each value of E. The local mode below the band appears only for the cases $V_a = 0.4, 0.5$, since only in these cases is the critical value of $|V_a|$ exceeded. In the case $V_a = 0.4$ the local mode is very close to the band edge and within the band the DOS has a steep maximum close to the edge. The local mode shown in figure 2(a) at $E = -1.04$ is for $V_a = 0.5$. Apart from this minor discrepancy between our results and those of Ueba (1980), our numerical calculations for ρ_a are in exact agreement with the corrected expressions obtained using the standard approach. The surface atom density of states (SDOS) is shown in figure 2(b) for the same parameter values as in figure 2(a). The SDOS is modified by the presence of the adatom and vanishes inside the band at $E = \varepsilon_a$. The condition for a local mode to appear in the SDOS outside the band is the same as for the
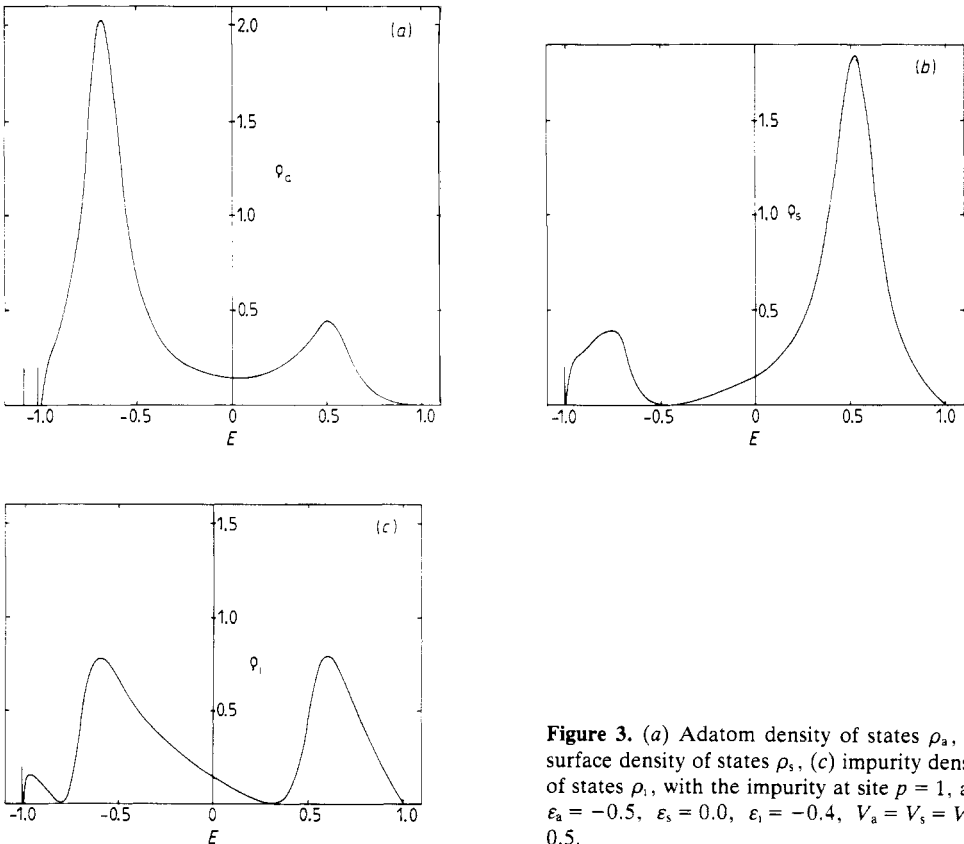
Figure 3. (a) Adatom density of states ρ_a, (b) surface density of states ρ_s, (c) impurity density of states ρ_i, with the impurity at site $p = 1$, and $\varepsilon_a = -0.5$, $\varepsilon_s = 0.0$, $\varepsilon_i = -0.4$, $V_a = V_s = V_i = 0.5$.
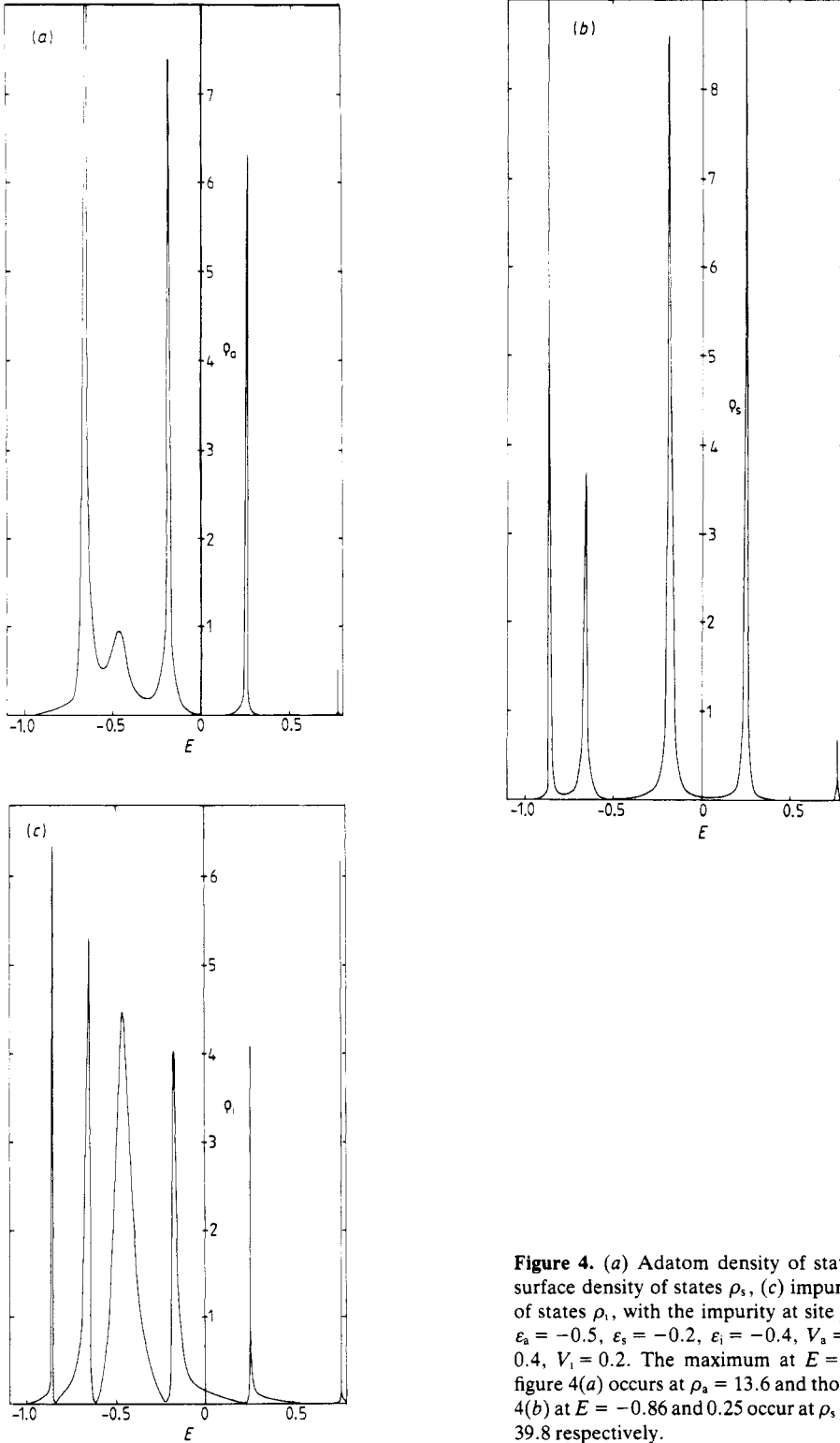
Figure 4. (*a*) Adatom density of states ρ_a, (*b*) surface density of states ρ_s, (*c*) impurity density of states ρ_i, with the impurity at site $p = 4$, and $\varepsilon_a = -0.5$, $\varepsilon_s = -0.2$, $\varepsilon_i = -0.4$, $V_a = 0.3$, $V_s = 0.4$, $V_i = 0.2$. The maximum at $E = -0.656$ in figure 4(*a*) occurs at $\rho_a = 13.6$ and those in figure 4(*b*) at $E = -0.86$ and 0.25 occur at $\rho_s = 67.0$ and 39.8 respectively.

ADOS and in figure 4(b) for $V_a = 0.4$ the local mode is again close to the edge with that for $V_a = 0.5$ at $E = -1.04$. Ueba (1980) did not include the effect of the adatom in calculating ρ_s and the appearance of a second local mode in his calculation of the ADOS is spurious.

5.2. *Impurity one site from surface ($p = 1$)*

Figures 3(a) to (c) show the ADOS ρ_a, the SDOS ρ_s and the impurity atom density of states (IDOS) ρ_i respectively, calculated using our rescaling method for $\varepsilon_a = -0.5$, $\varepsilon_s = 0.0$, $\varepsilon_i = -0.4$ and $V_a = V_s = V_i = V = 0.5$, where the impurity is located next to the surface atom. The two peaks in ρ_a inside the band can be identified with the adatom and surface atom by comparing figures 3(a) and (b). Again it should be noted that the SDOS shown in Ueba (1980) figure 4(b) is for $V_a = 0.0$, thereby excluding the effect of the adatom.

5.3. *Impurity displaced four sites from the surface ($p = 4$)*

When the impurity is situated deeper in the bulk, the standard techniques to solve the problem become algebraically complicated. However, the rescaling procedure is just as simple in this case as in §5.1 and §5.2 above. Figures 4 show some sample results for ρ_a, ρ_s and ρ_i when the impurity is located four sites from the surface and the parameters in (41) have the values $\varepsilon_a = -0.5$, $\varepsilon_s = -0.2$, $\varepsilon_i = -0.4$, $V_a = 0.3$, $V_s = 0.4$ and $V_i = 0.2$. By comparing figures 4(a) to (c) we can determine how the surface and impurity atoms affect the adatom electronic properties.

6. Conclusions

In summary the procedure outlined in § 4 can be used to study the effects of impurities and surface properties on the adatom density of states. Additional impurities can also be treated easily and the problem of an adatom adsorbed on to a randomly disordered material could be examined using an approach similar to that described by Langlois *et al* (1983). The virtues of our method lie both in the fact that it is exact and in its computational simplicity.

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