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# On the ‘screened’ Korringa–Kohn–Rostoker (KKR) method for calculating the electronic structure of solids

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**Abstract.** We demonstrate how the screening procedure works in a one-dimensional application of the KKR method by constructing an explicit analytic expression for the full scattering path matrix for the reference system. As an example of where screening renders novel calculations possible, we discuss the Friedel oscillations in a one-dimensional chain of potential wells with broken crystal symmetry.

## 1. Introduction

Computational methods for solving Schrödinger-like equations are central to the study of the electronic structures of condensed matter. Normally, these evolve smoothly as more efficient algorithms are implemented or more realistic features of the crystal potential are included. However, sometimes, a new idea changes not only the way we do things but also the way we think about certain problems and render new classes of problems tractable. Screening in the LMTO and KKR methods is one such idea. It was pioneered by Andersen and collaborators largely in the context of LMTO calculations [1, 2], and was adopted, in its present form, for the KKR method by Szunyogh *et al* [7] and Zeller *et al* [9]. In the present paper we wish to illustrate the idea in the context of a very simple, one-dimensional model to display its principal features more directly than is possible in a full three-dimensional calculation.

The multiple scattering approach to solving the Schrödinger equation for an array of spherical non-overlapping potentials (KKR formalism) has been formulated for one spatial dimension in a very elegant paper by Butler [3]. Formally, this one-dimensional model is nearly identical to its three-dimensional counterpart but is computationally much simpler. Therefore it is very well suited to investigate features of the KKR method.

In the above context, screening refers to the fact that the structure constants in a multiple scattering theory can be made short ranged in real space by using a suitably chosen reference system other than the vacuum [1, 7, 9].

For clarity and later convenience we recall the one-dimensional KKR method in section 2. In a slight generalization of Butler’s results [3] the analytic expression for the scattering path matrix is given and its site dependence discussed. The understanding of this site dependence is crucial in order to understand the screening effect that occurs by using a suitable reference system. In section 3 we describe a reference system explicitly and demonstrate screening. To illustrate the power of multiple scattering theory with screened structure constants to solve problems without translational symmetry, we have chosen to investigate the charge oscillations around an interface between two semi-infinite solids. We

find the expected connection between the wavelength of the oscillation and the extremal bulk  $k$ -vector of the Fermi surface.

Furthermore we show results for the dependence of the charge oscillation amplitude on the smoothness of the boundary. Surprisingly it turns out that smearing out the boundary can lead to an enhancement of the oscillation amplitudes.

## 2. The KKR for a one-dimensional model

For the sake of introducing notation and references we will give here a short introduction to the one-dimensional KKR method [3, 4].

The general problem we face is solving the one-dimensional Schrödinger equation

$$\left\{ - \left( \frac{d}{dx} \right)^2 + V(x) \right\} \psi(x) = E \psi(x) \quad (1)$$

where we assume that the potential  $V$  can be written as a sum of localized contributions  $V_i$  in such a way that the Schrödinger equation with  $V_i$  instead of  $V$  (the single site problem) can be solved readily. Furthermore, we assume that there is no overlap between the different potentials  $V_i$  and that there is a (eventually infinitesimally small) region around every potential  $V_i$  where the total potential is zero. This region is usually referred to as the interstitial region.

It is a main feature of the KKR and similar multiple scattering based methods that the whole problem is split into two parts. First the Schrödinger equation for a given energy  $E$  is solved for every individual potential  $V_i$ . It is important to note that there exist solutions for every (even complex) energies because in this first step there are no boundary conditions imposed. In a second step these solutions have to be matched smoothly. The matched solution is now subject to some boundary conditions which lead to an eigenvalue equation—the KKR equation.

### 2.1. Coordinates and basis functions

When we face the problem of finding the solution of the single site problem for the potential  $V_i$  which is nonzero around a point  $R_i$  it is appropriate to introduce a local coordinate system.

So let  $R_i$  be a point on the real axis. We can then describe every point  $x$  by giving its distance  $r_i = |x - R_i|$  and the direction  $\hat{x}_i = (x - R_i)/r_i$  with respect to  $R_i$ .  $\hat{x}_i$  is the one-dimensional analogue to the angles  $\Theta$  and  $\phi$  in three-dimensional polar coordinates. With this convention we can write for every  $x$ :

$$x = r_i \hat{x}_i + R_i. \quad (2)$$

Every function  $f(x)$  can be written as a sum of an even and an odd contribution with respect to  $R_i$ :

$$f(x) = f_0(r_i) Y_0(\hat{x}_i) + f_1(r_i) Y_1(\hat{x}_i) \quad (3)$$

with

$$\begin{aligned} f_0(r_i) &= \frac{1}{\sqrt{2}} (f(R_i + r_i) + f(R_i - r_i)) \\ f_1(r_i) &= \frac{1}{\sqrt{2}} (f(R_i + r_i) - f(R_i - r_i)) \end{aligned} \quad (4)$$

and

$$Y_0(\hat{x}_i) = \frac{1}{\sqrt{2}} \quad Y_1(\hat{x}_i) = \frac{\hat{x}_i}{\sqrt{2}}. \quad (5)$$

This expansion is unique and can be viewed as the analogue to the angular momentum expansion in three dimensions.

A complete set of solutions to the free Schrödinger equation is given by the following regular

$$j_0(\sqrt{Er}) = \cos(\sqrt{Er}) \quad j_1(\sqrt{Er}) = \sin(\sqrt{Er}) \quad (6)$$

and irregular

$$n_0(\sqrt{Er}) = \sin(\sqrt{Er}) \quad n_1(\sqrt{Er}) = -\cos(\sqrt{Er}) \quad (7)$$

special solutions. Furthermore it is useful to introduce the functions

$$\begin{aligned} h_0(\sqrt{Er}) &= j_0(\sqrt{Er}) + in_0(\sqrt{Er}) = e^{i\sqrt{Er}} \\ h_1(\sqrt{Er}) &= j_1(\sqrt{Er}) + in_1(\sqrt{Er}) = -ie^{i\sqrt{Er}}. \end{aligned} \quad (8)$$

These linear combinations are characterized by the fact that they decay with large  $r$  whenever  $\sqrt{E}$  has a positive imaginary part. Normally, all these functions will appear in connection with the corresponding one-dimensional spherical harmonic  $Y_l$ . Therefore, we will use the notation

$$j_l(E, x) = j_l(\sqrt{Er})Y_l(\hat{x}) \quad (9)$$

and similar for  $n$  and  $h$  when appropriate.

When complex energies are encountered the sheet of the square root  $\sqrt{E}$  is to be taken such that its imaginary part is positive. That means that the branch cut is along the positive real axis. For real and positive  $E$ ,  $\sqrt{E}$  is then defined as  $\lim_{\epsilon \searrow 0} \sqrt{E + i\epsilon}$ , which is the usual positive square root.

## 2.2. The KKR equation

Now that we have clarified the notation we can return to the Schrödinger equation (1). For  $x$  in the interstitial region around the potential at  $R_i$  every solution of the Schrödinger equation can be expressed as a linear combination of the  $j_l$  and the  $h_l$  centred at  $R_i$ :

$$\Psi(x) = \sum_l a_l^i j_l(E, x_i) + \sum_l b_l^i h_l(E, x_i). \quad (10)$$

For  $x$  inside the range of the potential  $V_i$ ,  $\Psi(x)$  is meant to be the solution of the single site Schrödinger equation with potential  $V_i$  which fits smoothly to  $\Psi$  given by (10). Requiring  $\Psi$  to be continuously differentiable at  $x = R_i$  results in two linear equations connecting the coefficients  $a_l$  and  $b_l$  have to fulfil:

$$b_l^i = \frac{1}{i\sqrt{E}} \sum_{l'} t_{ll'}^i a_{l'}^i. \quad (11)$$

$t^i$  is called the scattering matrix of the potential centred at site  $i$  and is determined by this potential alone. When the potential is symmetric the scattering matrix is diagonal, i.e. a complete set of solutions with pure symmetry can be constructed. Once the scattering matrix for every site is known the coefficients  $a$  can be expressed by the  $b$ .

So far we have gained a set of solutions which for  $x$  in the interstitial region around  $R_i$  have the form:

$$\Psi(x) = \sum_{l'} i\sqrt{E} t_{ll'}^{-1} b_{l'}^i j_l(E, x_i) + \sum_l b_l^i h_l(E, x_i). \quad (12)$$

By construction these solutions are regular at the cell centres  $x = R_i$  but for arbitrary  $b$  they will be discontinuous at the cell boundaries.

On the other hand, parametrizing  $\Psi$  by

$$\Psi(x) = \sum_i \sum_l c_l^i h_l(E, x_i) \quad (13)$$

for  $x$  in the whole interstitial region guarantees proper matching at the cell boundaries and also the right behaviour at infinity (i.e. exponential decay whenever  $\sqrt{E}$  has a positive imaginary part). The KKR equation now follows from requiring that (12) and (13) describe the same function which will then have all the correct matching and regularity properties. While for  $x$  in the interstitial region around site  $i$   $\Psi$  is expressed in (12) by functions centred at the site  $i$ ,  $\Psi$  in (13) is written as a superposition of functions  $h_l$  centred at different sites. However, as  $h_l(r_j)$  for  $j \neq i$  is a regular function for  $x$  around  $R_i$  it can be expanded in terms of  $j$  centred at  $R_i$ :

$$h_l(E, x_j) = i\sqrt{E} \sum_{l'} j_{l'}(E, x_i) g_{ll'}^{ij}(E). \quad (14)$$

The coefficients  $g_{ll'}^{ij}(E)$  are called structure constants. Explicit expressions for them are given below. In the interstitial region around the  $i$ th scatterer,  $\Psi$  given by (13) can now be rewritten such that only functions centred at  $R_i$  are involved:

$$\Psi(x) = \sum_l c_l^i h_l(E, x_i) + i\sqrt{E} \sum_{j(\neq i)} \sum_{l'} j_l(E, x_i) g_{ll'}^{ij}(E) c_{l'}^j. \quad (15)$$

Comparing this expression with equation (12) one can read off immediately

$$c_l^i = b_l^i \quad (16)$$

$$\sum_{l'} (t^i)_{ll'}^{-1} b_{l'}^i = \sum_{j(\neq i)} \sum_{l'} g_{ll'}^{ij}(E) b_{l'}^j. \quad (17)$$

Putting the pairs  $(l, i)$  together under one index and considering the scattering matrix  $t$  as a matrix diagonal in the site index  $i$ , the second equation can be written as a matrix equation:

$$(t^{-1} - g)b = 0 \quad (18)$$

showing that the eigenvalues are given by the zeros of the determinant of the matrix  $t^{-1} - g$ , often called the KKR matrix.

One way of calculating physical quantities such as charge density would be to find the solutions of this equation for all eigenenergies smaller than the Fermi energy and to construct from the eigenfunctions the quantity in question [6].

A different way to proceed is to calculate the Green's function of the system. This can be done without explicitly constructing the eigenfunctions as it can be expressed by the inverse of the KKR matrix

$$\tau = (t^{-1} - g)^{-1} \quad (19)$$

and solutions of the single site problem. The derivation of this expression is completely analogous to the three-dimensional case [5] and it reads

$$G^{ij}(x, x'; E) = \sum_{l'} \left\{ Z_l(x_i; E) \tau_{ll'}^{ij}(E) Z_{l'}(x_j; E) - \delta_{ij} \delta_{ll'} Z_l(x_{<}; E) J_l(x_{>}; E) \right\}. \quad (20)$$

Here  $x$  is assumed to be located around  $R_i$  and  $x'$  around  $R_j$ .  $Z_l(x_i; E)$  is the solution of the single site problem with potential  $V_i$ , which has the asymptotic form

$$Z_l(E, x) = \sum_{l''} t_{l'l''}^{-1}(E) j_{l''}(E, x) - \frac{i}{\sqrt{E}} h_{l'}(E, x) \quad (21)$$

for  $x$  inside the interstitial region around  $R_i$ . From the definition of the scattering matrix  $t$ , equations (10) and (11), it is clear that this solution is regular.  $J$ , the second solution involved, is characterized by

$$J(x; E) = j(x; E) \quad (22)$$

for  $x$  inside the interstitial region around  $R_i$  and will be irregular for a nonvanishing potential.

Given the Green's function  $G$  the local density of states  $\rho^i$  can be calculated via

$$\rho^i(E) = -\frac{1}{\pi} \text{Im} \int dx G^{ii}(x, x; E) \quad (23)$$

and the number of particles in the Wigner–Seitz cell of the  $i$ th potential is

$$n^i = \int dE \rho^i(E). \quad (24)$$

The energy integral here is a contour integral in the upper complex energy plane starting at some real energy lower than the lowest eigenenergy and ending at the Fermi energy.

One has to note that  $\tau$  is defined by (19) only for energies different from any eigenenergy because only in this case is the matrix inversion defined. For energies inside the band,  $\tau$  is defined by using energies with a small positive imaginary part and letting this imaginary part go to zero.

### 2.3. Structure constants and scattering path matrix

One of the nice features of the one-dimensional KKR is the possibility of giving an explicit expression for the structure constants:

$$g^{ij}(E) = \frac{e^{i\sqrt{E}|R_{ji}|}}{i\sqrt{E}} \begin{pmatrix} 1 & -i \operatorname{sgn} R_{ji} \\ i \operatorname{sgn} R_{ji} & 1 \end{pmatrix} \quad \text{for } i \neq j \quad (25)$$

where  $R_{ij} = R_j - R_i$ . For given site indices  $i$  and  $j$ , the  $g^{ij}$  are  $2 \times 2$  matrices because of the two possible values of  $l$ . By convention, for  $i = j$  the structure constants are set to zero. This expression follows from (14) and the definitions of  $h$ ,  $j$  and  $Y$  by straightforward calculation.

Equation (25) shows that the structure constants are an oscillating, nondecaying function of the lattice site distance  $R_{ji}$ . (The structure constants in three dimensions decay as  $1/|R_{ji}|$ .)

For the case of a periodic lattice with lattice constant  $a$  and site independent scattering matrices the site dependence of the KKR matrix enters only via the difference  $R_{ji} = a(j-i)$  so it can be diagonalized in the site indices by a lattice Fourier transformation:

$$g^k = \sum_{d=-N}^N e^{ikd} g^{(j+d)j} \quad k = \frac{2\pi(-N)}{2N+1}, \frac{2\pi(-N+1)}{2N+1}, \dots, \frac{2\pi N}{2N+1} \quad (26)$$

where periodic boundary conditions (period  $2N+1$ ) are assumed. By the assumption of lattice periodicity this expression is independent of  $j$ . The inverse transformation reads

$$g^{(j+d)j} = \frac{1}{2N+1} \sum_k e^{-ikd} g^k. \quad (27)$$

The sum in (26) with  $g$  given by (25) can be split into geometric sums and can therefore be easily performed with the result ( $N \rightarrow \infty$ )

$$g^k(E) = \frac{1}{i\sqrt{E}} \begin{pmatrix} -1 + \frac{i \sin a\sqrt{E}}{\cos k - \cos a\sqrt{E}} & \frac{\sin k}{\cos k - \cos a\sqrt{E}} \\ -\frac{\sin k}{\cos k - \cos a\sqrt{E}} & -1 + \frac{i \sin a\sqrt{E}}{\cos k - \cos a\sqrt{E}} \end{pmatrix}. \quad (28)$$

As the scattering matrix  $t$  is diagonal in the site indices and assumed to be site independent, its lattice Fourier transform is just  $t$  itself independent of  $k$ . We now restrict ourselves to symmetric potentials, so the scattering matrix becomes diagonal in  $l$  and we use its representation

$$t_l^{-1} = \frac{-1}{i\sqrt{E}}(1 + i \cot \delta_l) \quad (29)$$

in terms of the phase shifts  $\delta_l$ . The KKR matrix in  $k$ -space now reads

$$t^{-1} - g^k(E) = \frac{1}{i\sqrt{E}} \frac{1}{\cos k - \cos a\sqrt{E}} \times \begin{pmatrix} -i \cot \delta_0 (\cos k - \cos a\sqrt{E}) - i \sin a\sqrt{E} & -\sin k \\ \sin k & -i \cot \delta_1 (\cos k - \cos a\sqrt{E}) - i \sin a\sqrt{E} \end{pmatrix}. \quad (30)$$

The determinant of this matrix can be evaluated analytically and its zeros determine the dispersion relation:

$$\cos k = \frac{\cos(\sqrt{E}a + \delta_0 + \delta_1)}{\cos(\delta_0 - \delta_1)} =: x. \quad (31)$$

The abbreviation  $x$  for the right-hand side of the dispersion relation has been introduced for further reference. To find an expression for the  $\tau$ -matrix the  $2 \times 2$  matrix (equation (30)) has to be inverted and the result has to be back-Fourier-transformed. As we are interested not only in the site diagonal elements of  $\tau$ , we present here the calculation in a slightly generalized version compared to Butler [3]. In the Fourier transformation integrals of the form

$$I_d = \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-idk} \frac{\cos k - f_l}{\cos k - x} dk \\ \tilde{I}_d = \frac{i}{2\pi} \int_{-\pi}^{\pi} e^{-idk} \frac{\sin k}{\cos k - x} dk \quad (32)$$

occur where

$$f_l = \cos(\sqrt{E}a) - \tan \delta_l \sin(\sqrt{E}a) \quad (33)$$

and  $x$  stands for the right-hand side of the dispersion relation (31). These integrals can be transformed into contour integrals along a unit circle by the substitution  $z = e^{ik}$ . After this substitution the integrands have poles at  $z = 0$  and at the solutions  $z_1, z_2$  of  $z^2 - 2zx + 1 = 0$ :

$$z_{1,2} = x \pm \sqrt{x^2 - 1}. \quad (34)$$

One can easily check that  $z_1 z_2 = 1$ . The integrals (32) are well defined only when the poles are away from the integration contour, i.e. when  $|z_1| \neq 1$  and this is the case whenever  $E$  is not an eigenenergy. When, on the other hand,  $E$  is an eigenenergy then (31) has to have a real  $k$  as the solution so  $|x| \leq 1$ . This now implies  $z_1 = z_2^*$  and therefore  $|z_1|^2 = z_1 z_1^* = z_1 z_2 = 1$ . Of course this just reflects the fact that the KKR matrix

is invertible only for energies different from eigenenergies. When we now number the solutions  $z_1$  and  $z_2$  such that  $|z_1| < 1 < |z_2|$  the above integrals become

$$I_d = \delta_{d0} + \frac{2(x - f_l)}{z_1 - z_2} z_1^{|d|} \quad \text{and} \quad \tilde{I}_d = -\text{sgn}(d) z_1^{|d|} \quad (35)$$

where the signum function  $\text{sgn}$  is defined to be

$$\text{sgn}(d) = \begin{cases} +1 & d > 0 \\ 0 & d = 0 \\ -1 & d < 0. \end{cases}$$

Using these integrals we arrive at the following expression for the  $\tau$  matrix:

$$\tau^{ij} = \frac{-\sqrt{E} z_1^{|i-j|}}{1 + \tan \delta_0 \tan \delta_1} \begin{pmatrix} \tan \delta_0 (\delta_{ij} + I(x, 1)) & \tan \delta_0 \tan \delta_1 \text{sgn}(i - j) \\ -\tan \delta_0 \tan \delta_1 \text{sgn}(i - j) & \tan \delta_1 (\delta_{ij} + I(x, 0)) \end{pmatrix} \quad (36)$$

with

$$I(x, l) = \frac{2(x - f_l)}{z_1 - z_2}. \quad (37)$$

As  $|z_1| < 1$  the prefactor  $z_1^{|i-j|}$  causes an exponential damping of the matrix elements with distance from the diagonal. When, however, the limit to eigenenergies is taken,  $|z_1|$  approaches 1 and there is no more damping. In this case the matrix elements just oscillate according to  $z_1^{|i-j|} = e^{ik|i-j|}$ , where  $k = k(E)$  is the solution of (31) with positive imaginary part. Evidently, this long range effect of  $\tau^{ij}$  is the consequence of the long range effect of  $g^{ij}$  in (25). The screening procedure, which we shall introduce in the next section, is a transformation of the above representation of the problem to another, computationally much more convenient form, where the matrices  $\tau^{ij}$  and  $g^{ij}$  are almost diagonal.

### 3. Reference system and screening

Since the number of sites determines the size of the KKR matrix, the calculation of  $\tau$  by directly inverting the KKR matrix is only feasible for small systems. On the other hand Fourier transformation is useful only for periodic systems. We shall now show that by using an unperturbed Hamiltonian reference system other than the free electron case above, we can transform the problem at hand to one which is more widely tractable. As will be clear presently one has to choose a reference system with the same underlying structure as the system under consideration so that the structure constants of both systems are the same. If this is done we have from (19)

$$\tau^{-1} - (\tau^r)^{-1} = t^{-1} - (t^r)^{-1} = \delta m \quad (38)$$

where the matrix  $\delta m$  is introduced as an abbreviation and the superscript  $r$  refers to the reference system. Note that the matrix  $\delta m$  is diagonal in the site indices. The  $\tau$  matrix of the system under consideration can now be expressed by the  $\tau$  matrix of the reference system  $\tau^r$ :

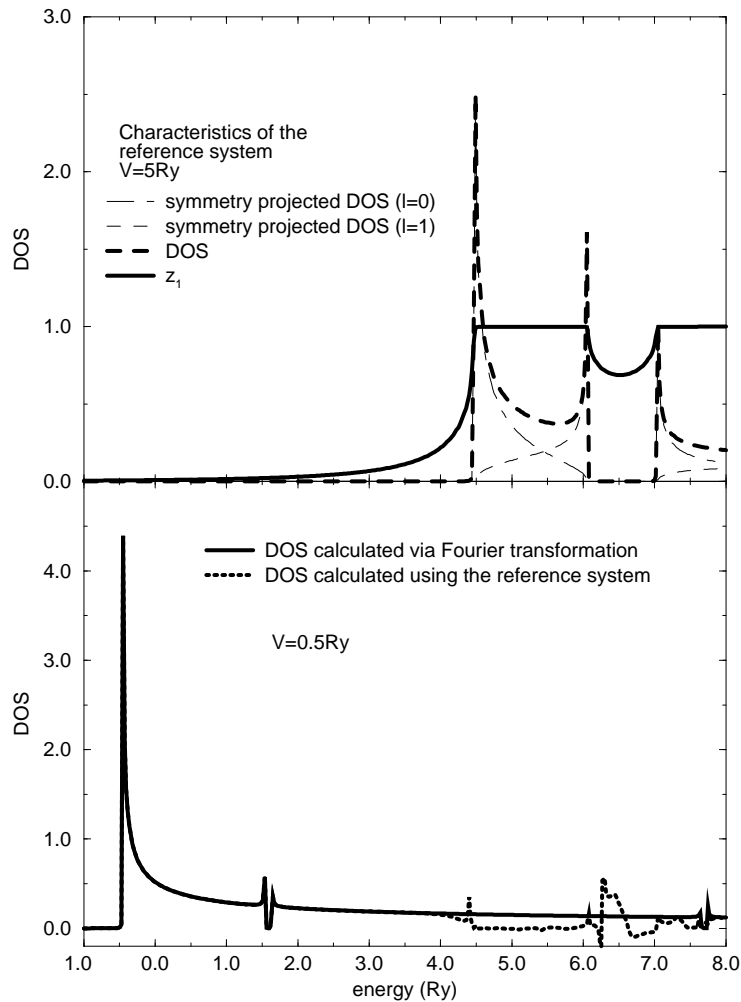
$$\tau = ((\tau^r)^{-1} + \delta m)^{-1}. \quad (39)$$

This equation can be transformed by simple algebraic manipulations to

$$\tau = (\delta m)^{-1} - (\delta m)^{-1} \{ \tau^r + (\delta m)^{-1} \}^{-1} (\delta m)^{-1}. \quad (40)$$

When the reference system is now chosen such that it has no states in the energy range of interest, the matrix elements of  $\tau^r$  decrease exponentially with distance from the diagonal as





**Figure 1.** In the upper panel the density of states for the reference system is shown (thick broken line) together with its decomposition into two symmetry projected parts (thin broken lines). The full line shows the factor  $|e^{ik}|$  (called  $z_1$  in the figure) which governs the decay of the site off-diagonal  $\tau$  matrix elements of the reference system. In the lower panel the exact density of states for the chain of square potential wells (0.5 Ryd deep) is compared with the result from the calculation with screening.

was shown in the previous section. Hence the matrix  $\{\tau^r + (\delta m)^{-1}\}$  can be approximated by a block tridiagonal matrix and as such can be inverted numerically using e.g. the decimation technique described in [7] and in the book by Turek *et al* [8]. Thus screening has rendered a whole new class of problems tractable.

In order to obtain, by this method, the inverse of the infinite dimensional KKR matrix in a finite number of steps, use of the so-called removal invariance is made. Therefore with this method problems can only be solved where a finite chain of arbitrary single site potentials lies between two half infinite homogeneous potential chains.

The formulation of the screening procedure described here is very close to that by Zeller *et al* [9]. While they expressed the so-called structural Green's function  $\hat{G}$  by its counterpart

of the reference system, we have chosen to deal with the multiple scattering matrix  $\tau$ . Since those two quantities are closely related according to

$$\tilde{G} = t^{-1}\tau t^{-1} - t^{-1} \quad (41)$$

these two procedures are essentially the same.

As a first illustration we investigate a periodic chain of identical square potential wells. As was shown in the previous section the  $\tau$  matrix for this system can be calculated analytically using lattice Fourier transformation. On the other hand we can also invert the KKR matrix in real space by the screening procedure just described. As the reference system we have chosen repulsive square potential wells (5 Ryd high) of the same width (2 au) and lattice constant (2.2 au) as the potential chain under consideration which was 0.5 Ryd deep. In the screened  $\tau$  matrix we neglected third and higher nearest neighbours. From both  $\tau$  matrices we calculated the density of states via (23). The results are shown in figure 1. In the upper panel the density of states of the reference system together with  $|e^{ik}|$ , the factor which governs the decay of  $\tau$ , are displayed. As expected  $|e^{ik}| = 1$  for energies inside the bands where  $k$  is the real wavevector and  $|e^{ik}| < 1$  outside. In the lower panel of the figure the density of states obtained by using a reference system and the exact results obtained by Fourier transformation are compared. For energies smaller than about 4 Ryd the two curves cannot be distinguished. This is the region where  $|e^{ik}|$  has values smaller than  $\sim 0.2$ . For the same reference system the energy range in which both curves coincide can be slightly improved by taking more distant neighbours into account. Including up to ninth nearest neighbours leads to coincidence of both curves up to about 4.4 Ryd corresponding to  $|e^{ik}| \approx 0.5$ . In contrast to the three-dimensional case the energy range for which the screening works could be increased to an arbitrary extent by simply choosing the reference potentials as high as necessary. This is because there are no problems with angular momentum convergence as we only have to deal with two different symmetries.

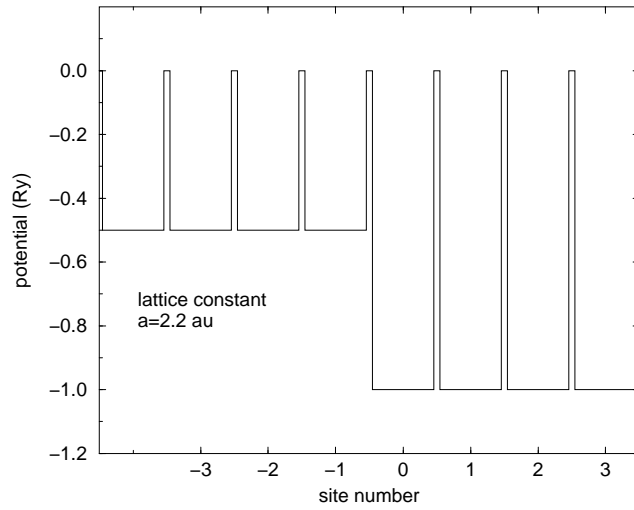
#### 4. The interface problem

One class of condensed matter systems where screening is especially helpful are systems composed of two half infinite crystals separated by a few interlayers [7, 8]. Translational invariance is then given only in two dimensions, whereas it is broken in the direction perpendicular to the interlayers. Lattice Fourier transformation in the symmetry plane reduces the problem to one with one spatial dimension. Therefore the resulting problem for a given in-plane wavevector ( $k_{\parallel}$ ) is now very similar to the one-dimensional model discussed here. Screening, in particular, simplifies the problem of inverting the KKR matrix to the problem of inverting a banded matrix much in the same way as we have discussed for the one-dimensional model in the previous section.

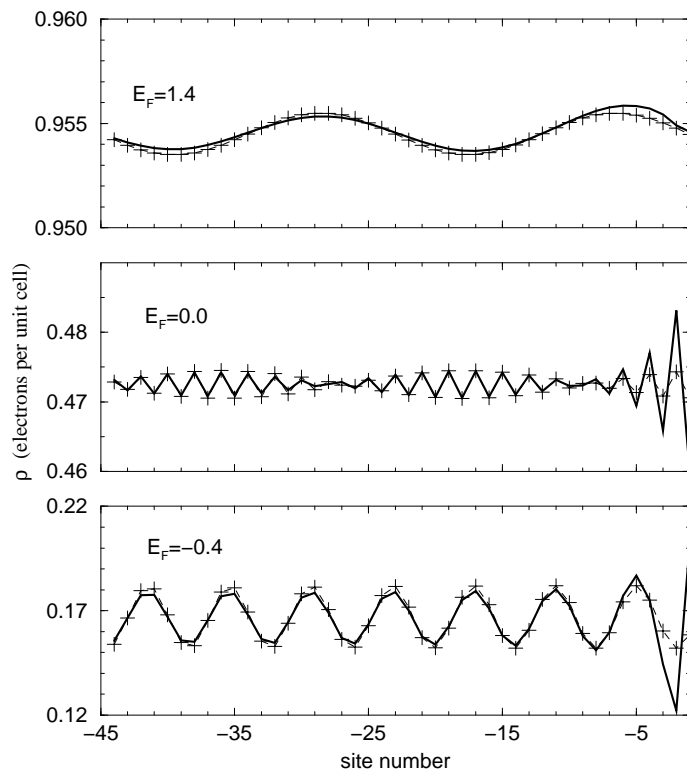
##### 4.1. Charge oscillations

In order to model the broken symmetry we have chosen a chain of square potential wells which are 0.5 Ryd deep on the left-hand side and 1.0 Ryd deep on the right-hand side (see figure 2). The underlying one-dimensional lattice, however, is chosen to have perfect lattice symmetry ( $a = 2.2$  au) because it is only in this case that we can use the analytic expression (36) for the  $\tau$  matrix of the reference system.

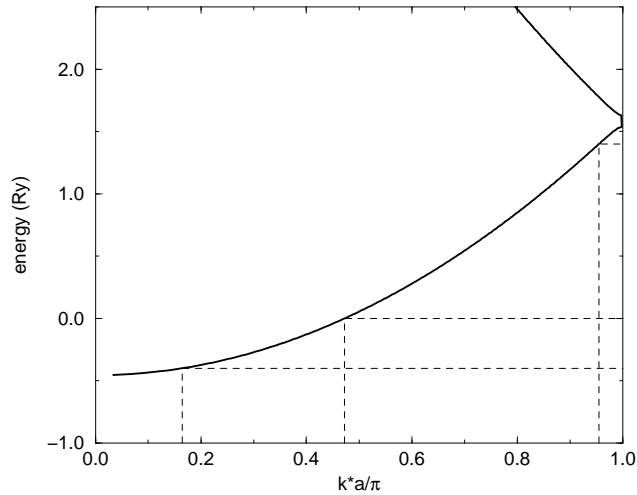
In this system the charge per unit cell is site dependent and oscillates around the value of the corresponding periodic system (Friedel oscillations). A special feature of the one-dimensional case is that there is no damping of this oscillation with distance from the



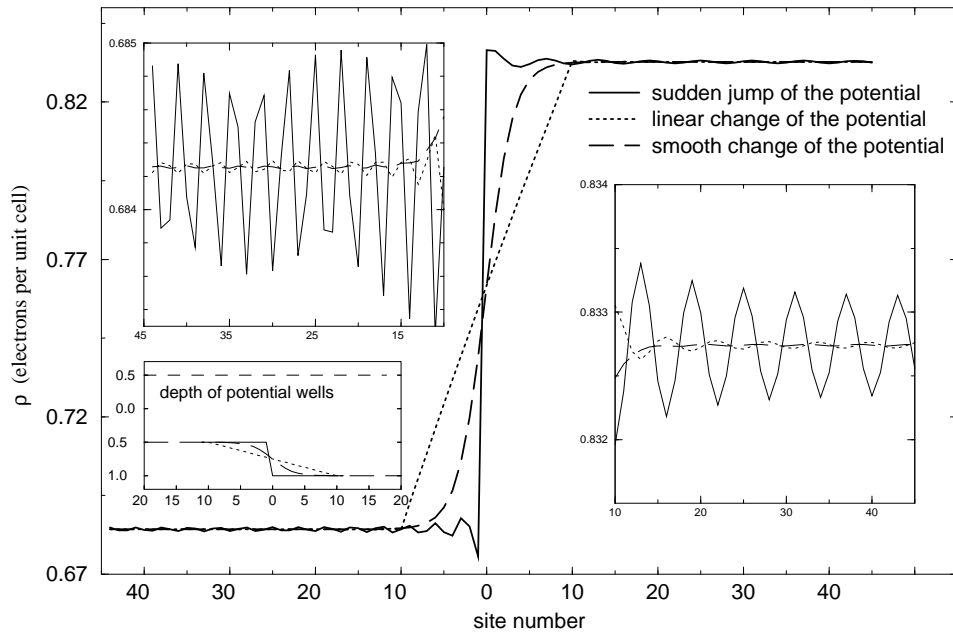
**Figure 2.** Here we show a part of the infinitely extended model potential we have used.



**Figure 3.** The charge per unit cell as a function of site number is shown (heavy line). The potential used is shown in figure 2. The crosses show the sinus curves which oscillate with the wavevector  $k = 2k_F$ , where  $k_F$  can be read from figure 4.

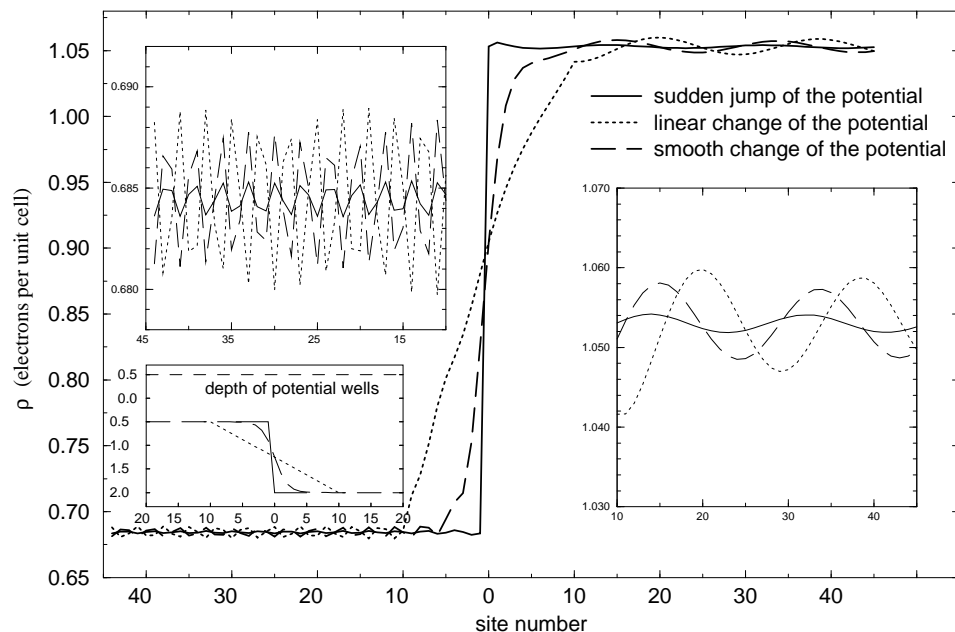


**Figure 4.** The dispersion relation for the translationally invariant chain of square potential wells (0.5 Ryd deep,  $a = 2.2$  au) is shown. The dashed lines mark the values of  $k$  for  $E = -0.4, 0.0, 1.4$  respectively which are used in figure 3.



**Figure 5.** The calculated charge per unit cell is shown here for three different chains of potential wells. The depth of the wells as a function of site number is shown in the lower left inset. The two other insets show a magnification of the main curves.

boundary. The wavevector describing this oscillation is given by  $2 \times k_F$  where  $k_F$  is the electron wavevector at the Fermi energy for the periodic system. This is well known from perturbation theory and we show here that this behaviour can be reproduced numerically in our calculations. As the reference system we again use the chain of repulsive potential



**Figure 6.** As figure 5 except for the depth of the potential wells which here equals 2 Ryd for the sites on the right.

wells characterized in figure 1. Again the analytic expression (36) can be used for the  $\tau$ -matrix of the reference system  $\tau^r$  and (40) yields the  $\tau$ -matrix describing the system under consideration. Finally from (23) and (24) the charge is obtained.

In figure 3 the result of this calculation for three differently chosen Fermi energies is shown for the sites on the left (see figure 2). The heavy line shows the result of the full calculation as described above, whereas the crosses are given for site number  $i$  by  $\alpha \sin(2k_F ai + \phi)$  with fitted amplitude  $\alpha$  and phase  $\phi$  and the  $k$ -vector  $k_F$  is taken from the dispersion relation (figure 4) of the fully crystal symmetric chain with 0.5 Ryd deep potentials. Obviously the oscillations have exactly the expected frequency. Be aware that the curves are only defined for integer site numbers (the line between the points serves only as a guide for the eye) and therefore the charge oscillates fastest for  $ka = 0.5\pi$ .

#### 4.2. Influence of the sharpness of the boundary on the amplitude of the charge oscillations

Finally, to illustrate the power of the above screened KKR method to deal with interesting surface problems we want to make use of the possibility of choosing single site potentials arbitrarily in a finite region between two half infinite chains. A natural question to ask in the present context is how the amplitude of the charge oscillations changes when the boundary between the two kinds of potential is smeared out. In figure 5 we show the results for a potential which is the same as that shown in figure 2 apart from a few layers around site 0, where the potential depth is either a linear function of the site number or a Fermi-distribution-like function. The inset on the bottom left in figure 5 shows the depth of the potential wells as a function of the site index. The dashed line in this inset marks the Fermi energy which is chosen to be 0.5 Ryd. The insets on the top left and on the right show a magnification of the charge per unit cell. All the full lines correspond to sudden jumps

of the potential depth; all the dotted lines correspond to a linear change of the potential; and all the dashed lines correspond to the Fermi-distribution-like behaviour of the potential depth. The curves show a clear drop of the oscillation amplitudes when going from the sharp to the smooth interface as one would naturally expect.

Surprisingly, this is not generally the case as demonstrated by figure 6. The only difference to the calculation just described is the potential depth on the right-hand side which is chosen here to be 2 Ryd. The difference between the potential on the left and the potential on the right is now much greater. Here the full line which shows the result for the sharp boundary is the one with the smallest oscillation amplitude.

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