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1999 J. Phys.: Condens. Matter 11 5505

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Application of the screened Korringa–Kohn–Rostoker method

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Received 21 October 1998, in final form 10 May 1999

Abstract. In the familiar Korringa–Kohn–Rostoker (KKR) or Green function method, wave propagation between scattering sites is described by the so-called structure constants of the lattice (KKR structure constants), where these quantities are treated as having infinite spatial extent. In a recent development, it has been shown that the KKR method can be formulated in terms of screened structure constants that are of finite range (the screened KKR method). Here, we present an alternative formulation of the screened KKR method that is derived from simple manipulations of the multiple-scattering equations. We carry out density-of-states and total-energy calculations for spin-polarized and non-spin-polarized materials using the method. We point out possible unphysical features of the method.

1. Introduction

The Korringa–Kohn–Rostoker (KKR) or, as it is alternatively referred to, the Green function method has been used extensively in the study of materials properties connected to the electronic structure. Among its most notable successes, the calculation of the electronic structure of ordered elemental solids (the standard KKR method) [1, 2], substitutionally disordered alloys, the KKR coherent potential approximation (KKR-CPA) [3, 4], and impurities [5] can be mentioned. Based on the multiple-scattering theory (MST) [6], the KKR method calculates the system Green function which leads directly to the calculation of observable quantities such as the electron density and the ground-state energy of the system. Application of MST relies heavily on the construction of the structure constants which describe free-particle propagation between scattering sites. Even though these structure constants can be calculated straightforwardly using Ewald's method [7], they remain computationally cumbersome.

Therefore, it is sensible to search for the development of MST within a framework that would keep intact its advantages while also reducing the difficulties associated with the infinite extent of the structure constants of the lattice. Such a framework has been proposed recently based on ideas originally put forth by Braspenning and Lodder [8, 9] for developing multiple-scattering theory in the presence of a reference medium rather than free space (see [10, 11] and references therein). The formalism leads to the construction of screened structure constants whose extent often does not reach beyond a few nearest neighbours (nn) in a lattice. This formalism has been successfully applied not only to bulk materials but to surfaces as well [10, 12].

In this paper, we present an alternative formulation of the screened KKR method that is more transparent than previous ones. We use the method to calculate self-consistently the

electronic structure and the density of states (DOS) for the ordered paramagnetic materials, fcc copper and bcc molybdenum, and the ferromagnetic bcc iron and fcc nickel. We compare results with those obtained from the standard (\mathbf{k} -space) Green function method and with calculations from reference [12]. We also point out unphysical behaviour that may arise in such calculations. The remainder of the paper takes the following form. In section 2, we present the derivation of the screened KKR equations. In section 3, we illustrate the formal expressions derived in section 2 by means of numerical examples. Spin-polarized calculations are presented in section 4. A final discussion containing our conclusions is given in section 5.

2. Formulation of the screened KKR method

The formal equations leading to effective, short-ranged structure constants for use within the Green function method can be derived from simple manipulations of the multiple-scattering equations.

The site-diagonal elements of the Green function can be written as [13]

$$G(\mathbf{r}, \mathbf{r}') = \sum_{L, L'} Z_L^n(\mathbf{r}) \tau_{LL'}^{nn} Z_{L'}^n(\mathbf{r}') - \sum_{L, L'} Z_{L'}^n(\mathbf{r}) J_{L'}^n(\mathbf{r}') \quad (1)$$

where the functions $Z_L^n(\mathbf{r})$ and $J_L^n(\mathbf{r})$ are solutions of the Schrödinger equation in the n th Wigner–Seitz cell. The points \mathbf{r} and \mathbf{r}' are in that cell. The superscripts on the elements of the scattering path operator [14], $\tau_{LL'}^{ij}$, refer to the cells centred at the lattice sites \mathbf{R}_i and \mathbf{R}_j , and the subscripts are the angular momentum indices. The $\tau_{LL'}^{ij}$ depend on the energy, and are obtained from the inverse of the matrix

$$\mathbf{M} = \mathbf{m} - \mathbf{g}. \quad (2)$$

The non-zero elements of \mathbf{m} are blocks \mathbf{m}^i corresponding to $i = j$. The matrix \mathbf{m}^i is the inverse of the scattering t -matrix for the atom on site i , and, for the special case of muffin-tin potentials, is given by

$$m_{LL'}^i = (t_{LL'}^i)^{-1} = (-\kappa \cot \eta_i^l + i\kappa) \delta_{LL'} \quad (3)$$

where $\kappa = \sqrt{\epsilon}$ and the η_i^l are the scattering phase shifts. The elements of \mathbf{g} are the propagators for electrons in free space, which are

$$g_{LL'}^{ij} = -4\pi\kappa i^{l-l'+1} \sum_{l''} i^{l''} C_{LL'}^{L''} h^+(\kappa|\mathbf{R}_{ij}|) Y_{L''}(\mathbf{R}_{ij}) \quad (4)$$

where $\mathbf{R}_{ij} = \mathbf{R}_j - \mathbf{R}_i$, and the $C_{LL'}^{L''}$ are Gaunt factors. Note that the matrix elements $g_{LL'}^{ij}$ are defined to be zero for $i = j$. It is standard to truncate the angular momentum expansions at some l_{max} . If there are N atoms in the crystal, the dimensions of \mathbf{M} are $N(l_{max} + 1)^2 \times N(l_{max} + 1)^2$. The matrix elements $\tau_{LL'}^{ij}$ are the ij, LL' elements of \mathbf{M}^{-1} , i.e., $\tau = \mathbf{M}^{-1}$. Since the number of atoms in the crystal is infinite, \mathbf{M} is an infinite matrix and taking the inverse is not a well-defined operation.

For the special case in which all of the atoms are the same, \mathbf{m} has a set of identical $(l_{max} + 1)^2 \times (l_{max} + 1)^2$ scattering matrices on the diagonal. Using the matrix \mathbf{U} , with elements

$$U_{LL'}^{ij} = (1/\sqrt{N}) \exp(-i\mathbf{R}_i \cdot \mathbf{k}_j) \delta_{LL'} \quad (5)$$

\mathbf{g} can be transformed into block-diagonal form:

$$[\mathbf{U}^\dagger \mathbf{g} \mathbf{U}]_{LL'}^{ij} = g_{LL'}(\mathbf{k}) \delta_{ij} = \sum_{j=1}^N \exp(i\mathbf{k} \cdot \mathbf{R}_{0j}) g_{LL'}^{0j} \quad (6)$$

which defines the $(l_{max} + 1)^2 \times (l_{max} + 1)^2$ matrices $\mathbf{g}(\mathbf{k})$. It is easy to take the inverse of the transformed matrix one block at a time, and the result, after allowing N to approach infinity, is the standard one [13]:

$$\tau^{ij} = \frac{\Omega}{(2\pi)^3} \int \exp(-i\mathbf{k} \cdot \mathbf{R}_{ij}) [\mathbf{m} - \mathbf{g}(\mathbf{k})]^{-1} d\mathbf{k} \quad (7)$$

where Ω is the volume of the unit cell.

When the atoms in the crystal are not all the same, the block matrices on the diagonal of \mathbf{m} , \mathbf{m}^i , are different and finding \mathbf{M}^{-1} is not as straightforward. A method for dealing with this problem is to write

$$\mathbf{m} = \mathbf{m}^s + (\mathbf{m} - \mathbf{m}^s). \quad (8)$$

The matrix \mathbf{m}^s is chosen to have identical blocks on the diagonal, as was the case with the ordered crystal. It follows that

$$\tau = \tau^s - \tau^s (\mathbf{m} - \mathbf{m}^s) \tau = [1 + \tau^s (\mathbf{m} - \mathbf{m}^s)]^{-1} \tau^s \quad (9)$$

with

$$\tau^s = [\mathbf{M}^s]^{-1} = (\mathbf{m}^s - \mathbf{g})^{-1}. \quad (10)$$

One way to calculate $\tau^{s,ij}$ is to use (7) with \mathbf{m}^s replacing \mathbf{m} .

This method for calculating the scattering path operator has been used frequently in multiple-scattering theory. For one impurity atom embedded in a perfect lattice, the blocks \mathbf{m}^s describe the scattering from the host atoms, $\mathbf{m} - \mathbf{m}^s$ has only one non-zero block, and (9) leads to a simple formula for τ^{ij} . For a cluster of n impurities, n of the blocks in $\mathbf{m} - \mathbf{m}^s$ are non-zero, and it is only slightly more complicated to calculate τ^{ij} [15].

For an arbitrary collection of atoms in the crystal, it is useful to define the scattering matrices \mathbf{m}^s such that the scattering path operators $\tau^{s,ij}$ are essentially zero when $|\mathbf{R}_j - \mathbf{R}_i| \geq R_{max}$. For instance, calculating the τ^{mn} needed for the evaluation of the Green's function in (1), truncated matrices τ^s , \mathbf{m} , and \mathbf{m}^s are obtained from the ones defined above by setting the blocks corresponding to sites for which $|\mathbf{R}_j - \mathbf{R}_i| \geq R_{max}$ equal to zero. Then τ^{mn} is the nn block of the finite matrix

$$\tau = [1 + \tau^s (\mathbf{m} - \mathbf{m}^s)]^{-1} \tau^s. \quad (11)$$

Note that the advantage in transforming the scattering path operator matrix instead of the structure constants, as stated in equation (9) in reference [11], is that the present derivation leads directly to the scattering path operator of the real system from which the physical properties are calculated as will be shown in the next section. Furthermore, it is easy to fit τ^s as a function of energy as opposed to the screened structure constants in reference [11].

The experience gained in the research on the screened structure constants described in references [10–12] suggests a convenient scattering potential to use in the calculation of the \mathbf{m}^s . The potential is a positive constant v^s within the muffin-tin sphere of each cell in the crystal, and zero in the interstitial region. The phase shifts can be calculated quite easily for this potential, and \mathbf{m}^s is obtained from (3). The matrix τ^s is calculated from a truncated version of the matrix defined in (10), rather than using the \mathbf{k} -space formula in (7). A complete real-space calculation of the total energy can be carried out using the τ^{mn} from (11). The ramifications of this approach will be considered elsewhere. In the present paper, we calculate the scattering path operator τ^s in real space and then use it to obtain the total energy and DOS from \mathbf{k} -space integration. The details of these calculations are given in the next section.

3. Calculations

We perform total-energy and DOS calculations for real materials employing the screened KKR method. We compare results of these calculations with those that are obtained using the usual KKR method in which the KKR structure constants are obtained using the Ewald procedure [7]. For the screened KKR method we calculate the screened scattering path matrix (τ^s) in real space, whilst calculation of the scattering path matrix for the system is carried out in \mathbf{k} -space.

The screening medium is constructed by placing the same constant repulsive muffin-tin potential of height v^s on all of the sites of the underlying lattice. An N -site cluster, comprised of the central site (denoted by 0) and its $N - 1$ neighbouring sites, is used to approximate scattering processes within this medium. The calculation of τ^s is performed by inverting the matrix \mathbf{M}^s for the cluster using (10), where \mathbf{m}^s is the inverse of the t -matrix corresponding to the screening potential v^s .

The τ^{00} block of the scattering path matrix for the system is obtained using

$$\tau^{00}(\epsilon) = (1/\Omega_{BZ}) \int_{\Omega_{BZ}} [1 + \tau^s(\mathbf{k})(\mathbf{m} - \mathbf{m}^s)]^{-1} \tau^s(\mathbf{k}) d\mathbf{k} \quad (12)$$

and the Green function is obtained using (1).

In (12), $\tau^s(\mathbf{k})$ is the lattice Fourier transform of $\tau^{s,ij}$ and is given by

$$\tau^s(\mathbf{k}) = \sum_{j=0}^N \exp(i\mathbf{k} \cdot \mathbf{R}_{0j}) \tau^{s,0j}. \quad (13)$$

It should be noted that, unlike the corresponding equations for the free-particle propagator (6), this lattice Fourier transform contains a contribution from the origin since $\tau^{s,00} \neq 0$.

Because we have obtained the elements $\tau^{s,ij}$ using a finite cluster in real space, we must choose the ones to use in the lattice Fourier transform (13). The point is that the use of a finite cluster breaks the translational invariance that exists between elements $\tau^{s,ij}$ and $\tau^{s,mn}$ when the pair of sites i, j and m, n have the same positional relationship to one another. We use the matrix elements $\tau^{s,0j}$ ($j = 1, N$) connecting the central site to its neighbours on the basis that they are better approximation to those of the infinite array of v^s s than are general matrix elements $\tau^{s,ij}$ ($i \neq 0$) connecting sites on the periphery of the cluster.

Once the Green function is determined, the charge density, $\rho(\mathbf{r})$, and the DOS, $n(\epsilon)$, are calculated using

$$\rho(\mathbf{r}) = -(1/\pi) \text{Im} \int_{-\infty}^{\epsilon_F} G(\mathbf{r}, \mathbf{r}, \epsilon) d\epsilon \quad (14)$$

and

$$n(\epsilon) = -(1/\pi) \text{Im} \int_{\Omega_{ws}} G(\mathbf{r}, \mathbf{r}, \epsilon) d\mathbf{r} \quad (15)$$

respectively. In the above, ϵ_F is the Fermi energy.

It should be apparent that the parameters controlling the convergence of the screened KKR method are the usual truncation of the angular momentum at l_{max} used to calculate the Green function from (1), the number of sites in the cluster N , the angular momentum cut-off, l_{scr} ($l_{max} \leq l_{scr}$), retained in the cluster used to calculate $\tau^{s,ij}$, and the height of the screening potential, v^s .

In carrying out calculations, we make extensive use of the complex-energy plane. When performing total-energy calculations, integrations over energy are carried out in the complex-energy plane using a semi-circular contour. In calculations of the density of states, used for display purposes, the energy contour is parallel to the real-energy axis with a small imaginary

part (typically $\text{Im } \epsilon \sim 0.001 \text{ Ryd}$). The self-consistent-field (SCF) total-energy calculations use the local density approximation for the exchange–correlation potential and are carried out at zero temperature. We use the muffin-tin approximation for magnetic Fe and Ni, and the atomic sphere approximation for Cu and Mo. This is to test the method for the most commonly used approximations for the atomic potentials. The BZ integration required in (12) is performed using the direction (prism) method [16].

In figure 1 we show the DOS obtained with the screened KKR for fcc Cu with lattice parameter $a = 6.83 \text{ Bohr radii}$. The dashed curve corresponds to SCF potentials obtained using the screened KKR, and the solid curve to the standard KKR method. Figure 1 also shows the error in the DOS (in Ryd) that is obtained by taking the difference between the DOS calculated at each energy point using the two methods. Figure 2 shows similar results obtained for bcc Mo with lattice constant $a = 5.80 \text{ Bohr radii}$.

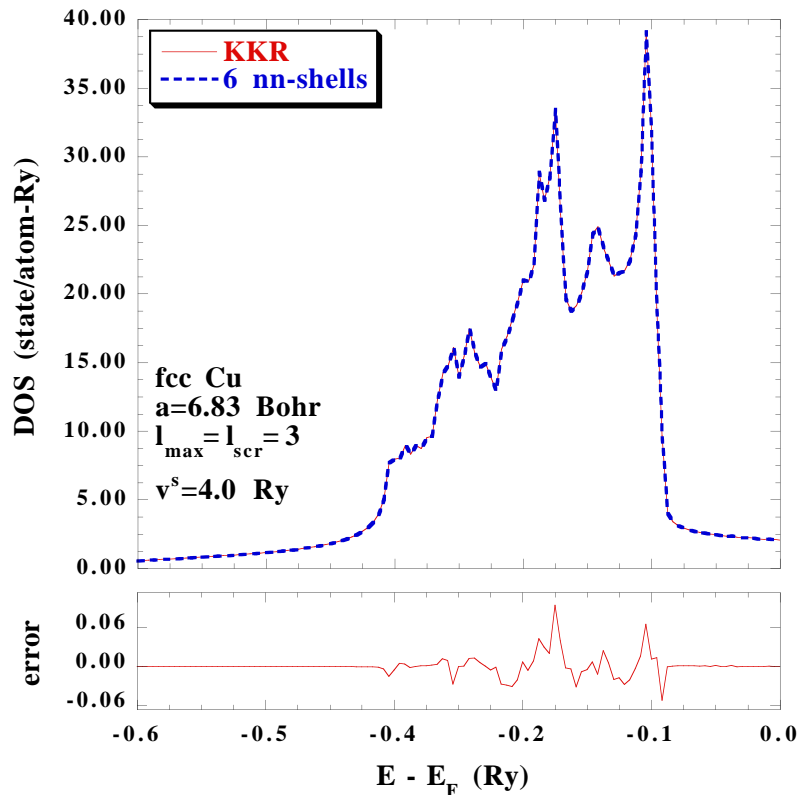


Figure 1. Comparison of KKR (solid curve) and screened KKR (dashed curve) DOS for fcc Cu. The error in the DOS with respect to the standard KKR is also shown.

It can be seen from figures 1 and 2 that for both Cu and Mo the densities of states obtained using the different techniques are essentially identical. The corresponding total energies differ by 0.03 and 0.006 mRyd respectively. In the calculation of the screened structure constants, we used $l_{\text{scr}} = 3$ and $v^s = 4.0 \text{ Ryd}$ for both structures. For the fcc structure we used $N = 87$ (six nn shells), while for bcc we used $N = 89$ (seven nn shells). In both cases, $l_{\max} = 3$ was used in the KKR calculations. Clearly, for these parameters the screened structure constants are converged.

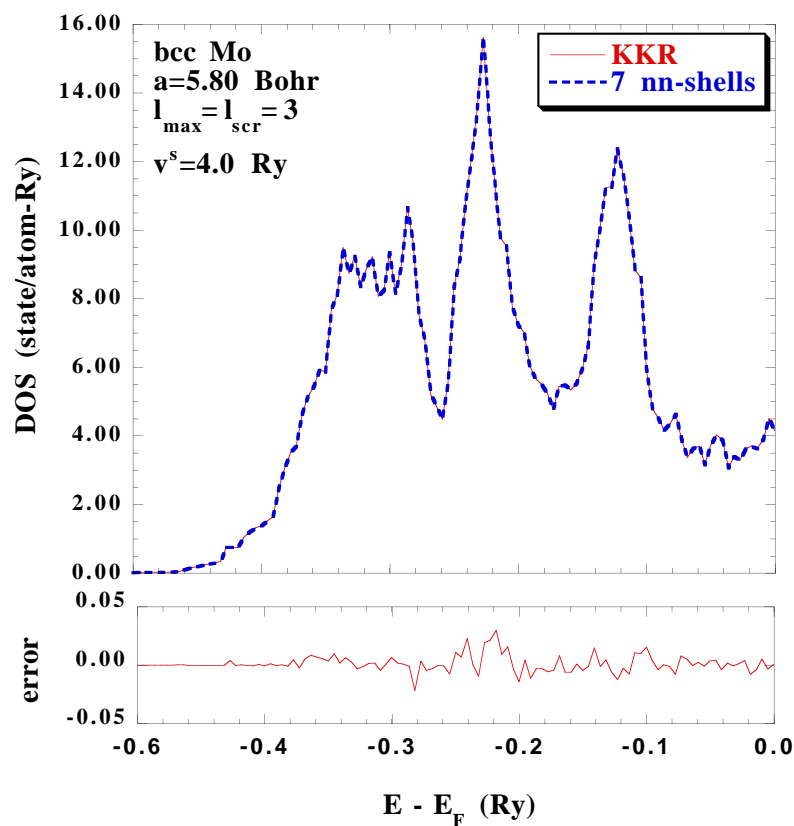


Figure 2. A comparison of the DOS of bcc Mo. The KKR DOS is represented by the solid curve and the screened KKR DOS is shown by the dashed curve. The error in the DOS with respect to the standard KKR is also shown.

In table 1 we show the effect of truncation of the cluster size on the total energy. The screened structure constants were calculated with fixed values of $l_{scr} = 3$ and $v^s = 4.0$ Ryd. Again, $l_{max} = 3$ was used in the KKR calculations. Columns 2 and 3 show the errors in the total energy using the screened KKR method with clusters containing various numbers of

Table 1. Calculated errors in total energy at different numbers of nn shells used in the calculation of the screened structure constants. The table is for fcc Cu and bcc Mo at the respective lattice parameters $a = 6.83$, $a = 5.80$ Bohr radii, $l_{scr} = l_{max} = 3$, and $v^s = 4.0$ Ryd.

	Cu error in energy (mRyd)	Mo error in energy (mRyd)
1 nn shell	-2.95	*
2 nn shells	0.75	*
3 nn shells	0.26	-0.400
4 nn shells	-0.02	*
5 nn shells	0.03	-0.100
6 nn shells	0.03	-0.002
7 nn shells		-0.006

nearest-neighbour shells. The errors are measured with respect to total energies obtained using the standard KKR method. For Cu, an accuracy of ~ 0.03 mRyd is obtained for five nn shells. For bcc Mo, an accuracy of 0.002 is attained for six nn shells. An asterisk in the table indicates that no SCF solution was obtained using the above parameters. Adjusting the height of the screened potential to $v^s = 1.0$ Ryd, we were able to obtain a SCF total energy for Mo with one nn shell that differs from the KKR result by 8 mRyd. For two nn shells, adjustment of the screening potential to $v^s = 8.0$ Ryd resulted in a SCF total energy with an error of 0.5 mRyd. Adjustment of the v^s did not yield a SCF total energy in the case of four nn shells. It is not clear why, in some instances, adjustment of the height of v^s led to self-consistency and in other instances it did not. It is not surprising that an approximation to the Green function using screened structure constants that are not fully converged may result in a non-analytic Green function.

There are differences between the calculations in this paper and those reported by Zeller in reference [12]. For example, he uses direct sampling for the BZ integrations, the exchange–correlation potential of Alder and Ceperley, and the full-potential MST. The calculated errors in the total energy for fcc Cu listed in table 1 above show the same trend as those listed in table I of reference [12]. The reason is that the differences in the total energies cancel out. The primary difference between the calculations described here and those in reference [12] is that Zeller calculates the total energy and the DOS at finite electron temperature. This enables him to avoid problems that arise in zero-temperature calculations, which will be discussed.

Next, we show the effect that the height of the screened potential v^s has on the total energy as a function of the number of shells used in the calculation of the screened structure constants. In figure 3, we plot the error in total energy of fcc Cu with lattice parameter $a = 6.83$ versus the number of nearest-neighbour shells. The screened KKR calculations were done at two different screening potentials $v^s = 4$ and 8 Ryd, with $l_{scr} = l_{max} = 3$.

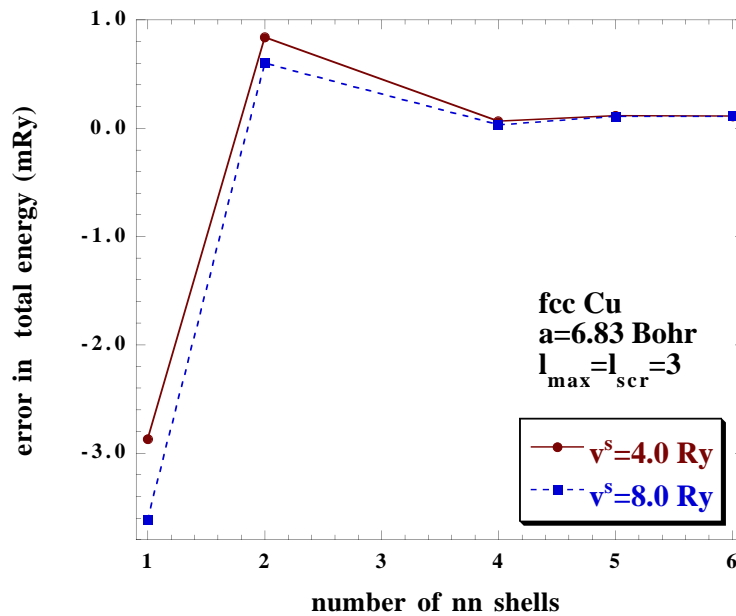


Figure 3. The errors in total energy calculated at two values of v^s are plotted as functions of the number of nearest-neighbour shells used to calculate the screened structure constants. The calculations were done at $l_{scr} = l_{max} = 3$.

From figure 3, it is evident that for four and more nn shells, the strength of the screened potential has essentially no effect on the total energy. Empty-lattice DOS calculations using the screened KKR method are reported in reference [12]. These, however, do not address the problems that arise in DOS calculations for real materials.

In figure 4 we show the calculated DOS of Cu at $l_{scr} = l_{max} = 2$ and $v^s = 2.0$ Ryd where only one nn shell has been used in the calculation of the screened structure constants.

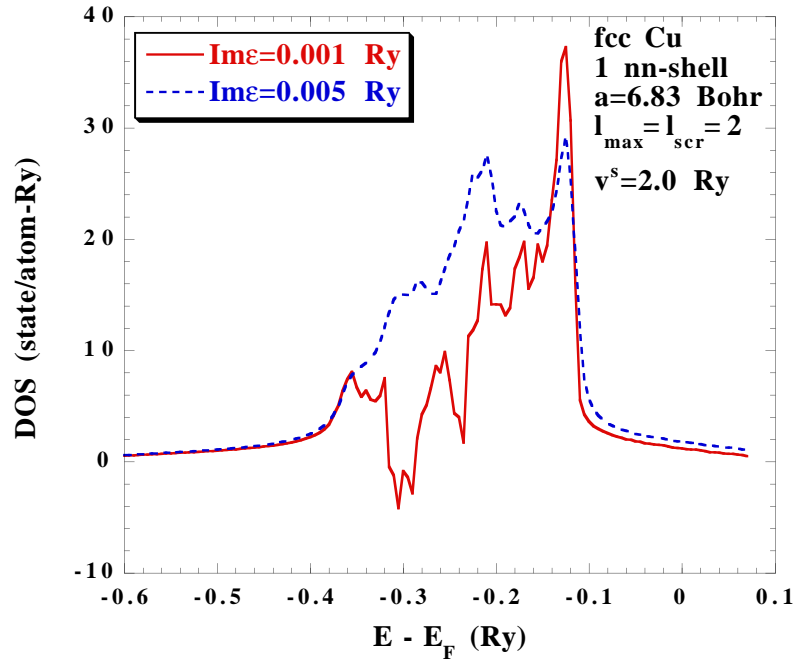


Figure 4. The screened KKR DOS for fcc Cu for one nn shell. The calculations were done at $l_{scr} = l_{max} = 2$, and $v^s = 2.0$ Ryd. The solid curve is the DOS calculated along a contour parallel to the real axis that is 0.001 Ryd off in the complex plane. The dashed curve represents the DOS calculated along a similar contour 0.005 Ryd off in the complex plane.

It can be seen that, for the above parameters, the DOS (solid curve) is negative in the middle of the d bands. This is indicative of a non-analytic Green function. Recall that when we perform SCF calculations we determine ϵ_F and calculate the charge density by integrating over a contour in the complex-energy plane. Thus, any non-analytic behaviour in the Green function will give rise to spurious results. The solid curve represents the DOS calculated along a contour parallel to the real axis that is 0.001 Ryd off in the complex plane ($\text{Im } \epsilon = 0.001$ Ryd). The negative DOS are indicative of a spurious pole (or cut) in the Green function that is further off in the complex plane than this. The density of states calculated along a contour for which $\text{Im } \epsilon = 0.005$ Ryd (dashed curve) does not exhibit unphysical behaviour. Thus the effect of this non-analytic behaviour will not be seen if calculations are performed at finite electron temperature, $T > 700$ K.

From the above studies it is clear that the screened KKR produces results that are essentially identical to the standard KKR ones if six (seven) nn shells are used for fcc (bcc) structures, but truncation of the inversion to include ≤ 4 nn shells may lead to unreliable DOS, and, in some instances, can lead to non-analytic behaviour.

4. Spin-polarized calculations

It is interesting to apply the screened KKR method to magnetic materials and investigate the validity of the method in such calculations. We present total-energy calculations for bcc Fe and fcc Ni in the ferromagnetic state using the screened KKR method. In the standard KKR calculations used as a reference, the structure constants are obtained from a polynomial fit rather than the Ewald method. In these calculations, we obtain the screened structure constants at $l_{scr} = 3$ and $v^s = 4.0$ Ryd. As before, the KKR calculations were done with $l_{max} = 3$. Figures 5 and 6 show total energies as functions of lattice parameters. The screened KKR calculations for Ni were done with $N = 13$ (one nn shell), and those for Fe with $N = 27$ (three nn shells).

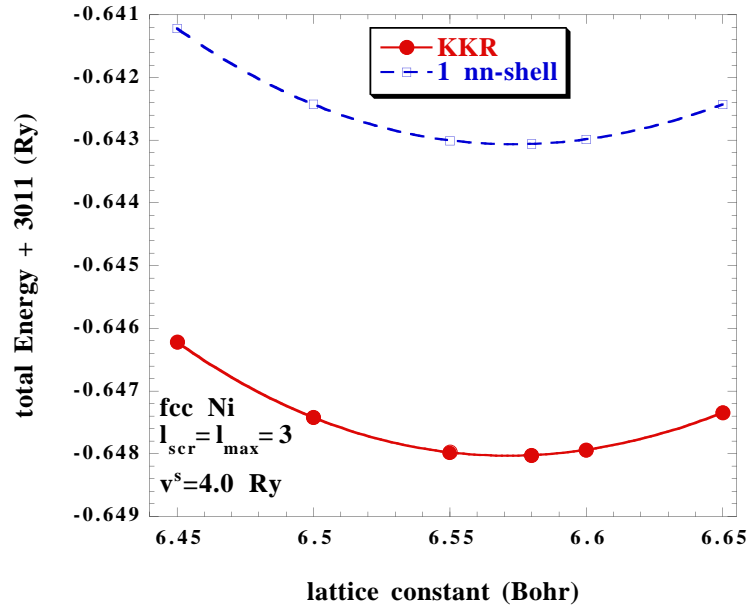


Figure 5. The total energy of fcc Ni as a function of the lattice parameter is shown. The solid curve represents the standard KKR and the dashed curve the screened KKR total energies. The calculations were done at $l_{scr} = l_{max} = 3$, and $v^s = 4.0$ Ryd. Only one nn shell was included in the cluster to calculate the screened structure constants.

The total energies were fitted to a third-degree polynomial to obtain the equilibrium lattice constant a_0 , total energy E_0 , and bulk modulus B_0 . Table 2 shows the results.

Table 2. The equilibrium lattice constant a_0 , total energy E_0 , and bulk modulus B_0 were obtained for nickel and iron at $l_{scr} = l_{max} = 3$ and $v^s = 4.0$ Ryd. $N = 13$ for nickel and 27 for iron. The corresponding standard KKR values are also listed. The zero of energy for Ni is -3011 and that of Fe is -2522 Ryd.

	fcc Ni		bcc Fe	
	Standard KKR	Screened KKR ($N = 13$)	Standard KKR	Screened KKR ($N = 27$)
a_0 (Bohr radii)	6.572	6.573	5.281	5.280
E_0 (Ryd)	-0.64803	-0.64307	-0.82884	-0.82924
B_0 (Mbar)	2.20	2.29	2.21	2.16

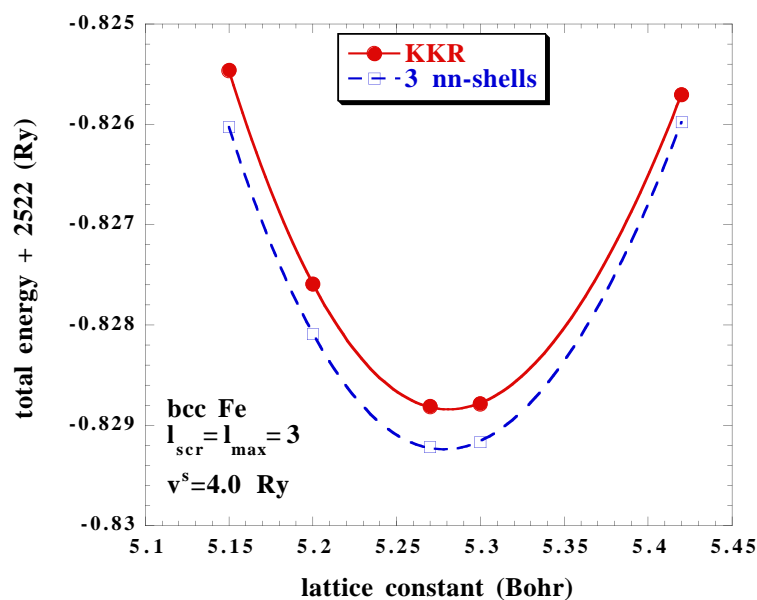


Figure 6. The total energy of bcc Fe is shown for five lattice parameters. The screened KKR calculations were done at $N = 27$, $l_{scr} = l_{max} = 3$, and $v^s = 4.0$ Ryd.

From table 2, the equilibrium lattice constants and bulk moduli agree well with the corresponding KKR values. The equilibrium total energies differ from the standard KKR values by about -5.0 mRyd for Ni and 0.4 mRyd for Fe. Also, magnetic moments calculated for the two systems using the screened KKR method yield values that are different from those obtained from the standard KKR calculations by -0.002 Bohr magneton (μ_B) for Ni and 0.005 μ_B for Fe. Errors in the total energy and magnetic moment reduce considerably when the number of sites N used in the calculation of the screened structure constants is increased. For nickel at $a = 6.65$ Bohr radii, $N = 55$ (four nn shells for fcc structure) and iron at $a = 5.27$ Bohr radii, $N = 65$ (six nn shells for bcc structure), the errors in the total energy are about 0.004 and 0.03 mRyd respectively. The corresponding errors in the magnetic moment are -0.0003 and 0.00007 μ_B .

5. Conclusions

We have presented an alternative formulation of the screened KKR method that is derived from simple manipulations of the multiple-scattering equations. The derivation focuses on transformation of the scattering τ -matrix rather than the Green function, and leads to an expression for the τ -matrix for the system that is more transparent than previous ones. To illustrate how the formalism works in practice, we performed total-energy and DOS calculations for copper and nickel in fcc phases and molybdenum and iron in bcc phases. It was found that the method yields total energies that are within tens of μ Ryd of the standard KKR results. The high degree of accuracy is obtained only when the screened structure constants are calculated with ≥ 5 nearest-neighbour shells of repulsive scatterers. The effect of the height of the repulsive potentials on the total energy was shown to be minimal using converged screened structure constants. However, when the screened structure constants are not converged, the total energy is more sensitive to variations in the strength of the screening

potential. We have demonstrated unphysical features (negative DOS) that may arise in the calculations when the maximum angular momentum, the number of neighbouring shells, and the height of repulsive potentials are not chosen properly. The negative DOS, we believe, are mainly due to spurious poles in the Green function. The poles appear at energies close to the real axis ($\text{Im } \epsilon \sim 0.001 \text{ Ryd}$), when the system's Green function is obtained from the screened structure constants that are not converged. We also pointed out that non-analytic behaviour is not seen when calculations are done at finite electron temperature, $T > 700 \text{ K}$.

The equilibrium total energies calculated for Fe and Ni with ≤ 3 nn shells were shown to be in reasonable agreement with their standard KKR counterparts (a few mRyd). For these systems the magnetic moments differ by only a few thousandths of μ_B from the standard KKR results. We pointed out that the total energy and the magnetic moment improve considerably as more sites are used in the calculation of the screened structure constants. The method may be used for tight-binding and near-tight-binding purposes to obtain accurate magnetic moments, and good equilibrium lattice constants and bulk moduli.

Acknowledgments

This work was supported by BES–DMS, and OCTR–MICS, US DOE, under subcontract DEAC05–96OR22464 with Lockheed–Martin Energy Research Corporation.

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