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Numerical Evaluation of the Free-Electron Lattice Green's Function*

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A method is described for the fast and efficient numerical evaluation of the general free-election lattice Green's function in the **r** representation. This is useful for the solution of the general unrestricted energy-band problem and for applying the coherent-potential approximation in obtaining the electronic structure of realistic models of substitutionally disordered alloys.

1. INTRODUCTION

The most familiar use of the free-electron lattice Green's function is in the multiple scattering approach to electronic band structure calculations [1, 2]. In the usual procedure the crystal potential is approximated in the "muffin tin" manner, i.e., only the spherical contributions around each atomic site are kept. The potential is then spherically symmetric within the inscribed sphere of the atomic polyhedra and constant outside these spheres. Using this approximation, the Schroedinger equation can be integrated. The results are cast into the form of a determinant which is a function of the energy, and the zeroes of this determinant yield the band energies. The muffin-tin approximation yields a tractable numerical problem and the procedure works well for metals, including *d*-band transition metals [3]. However, for compounds which have a large amount of covalency involved in their bonding, the muffin-tin approximation is not expected to be valid and a more general approach is necessary. A general approach incorporating the free-electron lattice Green's function may involve iterative methods [4] or the use of a basis set [5]. The advantage of a general Green's function method is apparent when a basis set is used, because the basis set need be only large enouth to describe the states in the energy range of interest and the core states can be ignored.

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Another application for which the free-electron lattice Green's function is necessary is in the application of the coherent-potential approximation in substitutional alloys [6]. The need for the general Green's function is independent of any approximation made in the potential.

The disadvantage of using the general Green's function is that it is a complicated function of the energy, which must be searched for the location of roots which yield the eigen-energies of the problem. The Green's function must be evaluated many times in a computationally fast and efficient way for a tractable numerical scheme to be developed. This paper presents a method of calculating the free-electron lattice Green's function in the **r** representation. It is fast and efficient enough to make the other problems mentioned tractable. Section II of this paper contains the form of the Green's function that will be used. Section III presents the evaluation techniques and Section IV the results including error analysis and timing on a Control Data 6400 computer.

2. THE GREEN'S FUNCTION

The Green's function is defined by

$$(-\nabla_r^2 - E)\, G(\mathbf{r}, \mathbf{r}') = -\delta(\mathbf{r} - \mathbf{r}') \tag{2.1}$$

so

$$\Psi(\mathbf{r}) = \int_v G(\mathbf{r}, \mathbf{r}')\, V(\mathbf{r}')\, \Psi(\mathbf{r}')\, d^3r' \tag{2.2}$$

where $\Psi(\mathbf{r})$ is the wavefunction for the crystal and satisfies the Bloch condition

$$\Psi(\mathbf{r} + \mathbf{R}_s) = e^{i\mathbf{k}\cdot\mathbf{R}_s}\Psi(\mathbf{r}), \tag{2.3}$$

$V(\mathbf{r})$ is the periodic crystal potential,

$$V(\mathbf{r} + \mathbf{R}_s) = V(\mathbf{r}), \tag{2.4}$$

v is the volume of the unit cell in **r** space, **k** is the crystal momentum and $\mathbf{R}_s$ is a direct lattice vector. The Green's function can be written

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{v}\sum_n \frac{\exp[i(K_n + \mathbf{k})\cdot(\mathbf{r} - \mathbf{r}')]}{(\mathbf{K}_n + \mathbf{k})^2 - E}, \tag{2.5}$$

where K_n are reciprocal lattice vectors, or in the alternative form

$$G(\mathbf{r}, \mathbf{r}') = -\frac{1}{4\pi}\sum_s \frac{\exp[i\kappa\,|\,\mathbf{r} - \mathbf{r}' - \mathbf{R}_s\,|]}{|\,\mathbf{r} - \mathbf{r}' - \mathbf{R}_s\,|} \exp(ik\cdot\mathbf{R}_s). \tag{2.6}$$

Here

$$\begin{aligned} \kappa &= +E^{1/2}, \qquad E > 0 \\ \kappa &= i(-E)^{1/2}, \qquad E < 0 \end{aligned} \tag{2.7}$$

It is also apparent from (2.5) or (2.6) that

$$G(\mathbf{r}, \mathbf{r}') = G(\mathbf{r} - \mathbf{r}') \tag{2.8}$$

and that

$$G(\mathbf{r}' - \mathbf{r}) = G^*(\mathbf{r} - \mathbf{r}'), \tag{2.9}$$

the Hermitian property.

It is evident that neither (2.5) or (2.6) is an appropriate form for the numerical evaluation of $G(\mathbf{R})$, $(\mathbf{R} = \mathbf{r} - \mathbf{r}')$, because of the slow convergence of either series. Recognizing this, Ham and Segall [7] applied the Ewald technique [8] to improve the convergence and obtained

$$G(\mathbf{R}) = G_1(\mathbf{R}) + G_2(\mathbf{R}) \tag{2.10}$$

where

$$G_1(R) = -\frac{1}{v}\sum_m \frac{\exp[i(\mathbf{k} + \mathbf{K}_m) \cdot \mathbf{R}] \exp\{-[(\mathbf{k} + \mathbf{K}_m)^2 - E]/\eta\}}{(\mathbf{k} + \mathbf{K}_m)^2 - E} \tag{2.11}$$

and

$$G_2(R) = -\frac{\pi^{-3/2}}{2} \sum_s e^{ik\cdot\mathbf{R}_s} I(E, |\mathbf{R} - \mathbf{R}_s|) \tag{2.12}$$

where

$$I(E, |\mathbf{R} - \mathbf{R}_s|) = \int_{\frac{1}{2}\sqrt{\eta}}^{\infty} \exp[-|\mathbf{R}_s - \mathbf{R}|^2 p^2 + E/4p^2]\, dp \tag{2.13}$$

and $\eta > 0$ is the Ewald parameter which is chosen to minimize computation time as will be seen later. Equations (2.10), (2.11), and (2.12) give the form in which the Green's function will be evaluated here. The integral $I(E, |\mathbf{R} - \mathbf{R}_s|)$ given by 2.13) is the most difficult quantity to evaluate rapidly. It is encountered in each term of the sum on $\mathbf{R}_s$ and its rapid evaluation is at the core of any fast Green's function evaluation method. Its appearance in the sum over $\mathbf{R}_s$ and the necessity of calculating $G(R)$ over a large grid of $\mathbf{R}$ values (for each E value) for numerical integration, make essential the separation of the E and $\mathbf{R}$ dependences and the extremely rapid evaluation of I for a given $\mathbf{R}$. The other terms require only the evaluation of the exponential function and algebraic manipulations.

3. Evaluation Technique

In this section we consider the integral $I(E, | \mathbf{R} |)$, given by (2.13). This can be rewritten

$$I(x, y) = \frac{\sqrt{\eta}}{2} \int_1^\infty \exp[-x^2\xi^2 + y/\xi^2]\, d\xi \tag{3.1}$$

where $x = \frac{1}{2} \sqrt{\eta} | \mathbf{R} - \mathbf{R}_s |$ and $y = E/\eta$. This integral can be evaluated exactly in terms of the complex complimentary error function [9]:

$$I(x, y) = \frac{\sqrt{\pi\eta}}{8x} \{e^{2bx}[\mathrm{erfc}(x + b)] + e^{-2bx}[\mathrm{erfc}(x - b)]\} \tag{3.2}$$

where

$$\begin{aligned} b = i\sqrt{y}, \qquad & y > 0 \\ \sqrt{-y}, \qquad & y < 0 \end{aligned} \tag{3.3}$$

Note that

$$\lim_{x \to 0} I(x, y) = \frac{\sqrt{\pi\eta}}{4x} \tag{3.4}$$

This displays the singularity of the Green's function which occurs when

$$\mathbf{r} - \mathbf{r}' = \mathbf{R}_s \tag{3.5}$$

If the range of integration over $\mathbf{r}$ and/or $\mathbf{r}'$ is restricted to the first primitive cell as in (2.2) the singularity occurs only in the $R_s = 0$ or first term of the sum in (2.12) and only for $\mathbf{r} = \mathbf{r}'$. This situation can be handled by volume averaging as described below.

Since (3.2) is not a suitable form for the rapid numerical evaluation of $I(x, y)$ because of the complex arithmetic and the mixing of x and y dependences, a different, more direct method has been divised. When working in the $\mathbf{r}$ representation the Green's function will need to be evaluated most frequently as a function of $| \mathbf{R} | = \mathbf{r} - \mathbf{r}'$(or x) and as a function of E (or y). The method adopted was to use a Taylor series expansion in x about a suitable number of expansion points $\{x_i\}$. The method for choosing the $\{x_i\}$ will be described later. The coefficients at one of the expansion points are functions of y and x, but the dependences on these parameters can be separated and much of the calculation can be done once and for all after the set $\{x_i\}$ is chosen. The details of this technique are now given.

The Taylor series expansion was made of the function $J(x, y)$, defined by

$$I(x, y) = \frac{\sqrt{\eta}}{2x} e^{-x^2} J(x, y), \tag{3.6}$$

in the form

$$J(x, y) = \sum_{l=0}^{l_{\max}} A_{li}(x - x_i)^l \tag{3.7}$$

where

$$\frac{x_i + x_{i-1}}{2} \leqslant x < \frac{x_{i+1} + x_i}{2}, \qquad i = 0, 1, 2, \ldots, i_{\max}, \tag{3.8}$$

$$A_{l,i} = \frac{J^{(l)}(x_i, y)}{l!}, \tag{3.9}$$

and where

$$J^{(l)}(x_i, y) = \left. \frac{d^l J}{dx^l} \right|_{x=x_i} \tag{3.10}$$

For any x the closest x_i is found and the associated expansion is then used. The singularity $(1/x)$ is removed to enable an expansion around $x = 0$ to be made. The exponential term (e^{x^2}) is removed to simplify the procedure for obtaining the derivatives $J^l(x_i)$ as will be seen below and to account somewhat for the asymptotic behavior of the integral and enable the expansion to be more accurate. The point $x = 0$ is always included in the set of points around which the expansions are made, i.e., $x_0 = 0$, even though all the $x \geqslant 0$. This is because behavior of $J(x, y)$ around $x = 0$ is the hardest to approximate accurately. To obtain the derivatives of $J(x, y)$ we just rewrite it in the form

$$J(x, y) = \frac{2x}{\sqrt{\eta}} e^{x^2} I(x, y) \tag{3.11}$$

and use the expression for $I(x, y)$ given by (3.2). Using

$$\frac{d}{df} \operatorname{erfc}(f) = \frac{-2}{\sqrt{\pi}} e^{-f^2} \tag{3.12}$$

we obtain

$$\frac{d^2}{dx^2} [xI(x, y)] = -4y[xI(x, y)] + x\sqrt{\eta}\, e^{-(x^2-y)} \tag{3.13}$$

Using (3.11) this can be transformed into

$$\frac{d^2}{dx^2} J(x, y) - 4x \frac{d}{dx} J(x, y) + 2[2(x^2 + y) - 1]\, J(x, y) = 2xe^y. \tag{3.14}$$

Taking $(l-2)$ derivatives of (3.14) and using the definitions (3.10) and (3.9), we obtain

$$A_{l,i} = \frac{2}{l(l-1)}\{2lx_iA_{l-1,i} - [2(x_i^2 + y - l) + 3]\,A_{l-2,i} - 4(x_iA_{l-3,i} + A_{l-4,i})\} \tag{3.15}$$

for $l \geqslant 4$,

$$A_{3,i} = \frac{4}{3}x_i(A_{2,i} - A_{0,i}) - \frac{1}{3}[2(x_i^2 + y) - 3]\,A_{1,i} + 2e^y, \tag{3.16}$$

and

$$A_{2,i} = 2x_iA_{1,i} - [2(x_i^2 + y) - 1]\,A_{0,i} + x_ie^y \tag{3.17}$$

The initializing values for this set of recursion relations are

$$A_{0,i} = J^{(0)}(x_i y) \qquad \text{and} \qquad A_{1,i} = J^{(1)}(x_i, y). \tag{3.18}$$

Thus the coefficients of the expansion (3.7) can be evaluated at each energy using this recursion technique.

In order to be able to store as much of the calculation as possible in tables, it is useful to effect a separation of the energy and position dependence of the initializing values given in (3.18). A method of doing this first considered by Davis [10] is the method chosen here. The essence of this method is to expand the term involving y in the integral given in (3.1). Using (3.11), we obtain

$$J(x, y) = xe^{x^2} \sum_{m=0}^{\infty} \frac{y^m}{m!} \int_1^{\infty} \frac{e^{-x^2\xi^2}}{\xi^{2m}}\, d\xi \tag{3.19}$$

and

$$\int_1^{\infty} \frac{e^{-x^2\xi^2}}{\xi^{2m}}\, d\xi = \frac{x^{2m-1}}{2}\, \Gamma(1/2 - m, x^2) \tag{3.20}$$

where $\Gamma(1/2 - m, x^2)$ is the incomplete Gamma function [11]. It is convenient to define

$$f(1/2 - m, x^2) = e^{x^2}x^{2m}\Gamma(1/2 - m, x^2) \tag{3.21}$$

so

$$J(x, y) = \frac{1}{2} \sum_{m=0}^{\infty} \frac{y^m}{m!} f(1/2 - m, x^2). \tag{3.22}$$

Now we have the continued fraction expansion [12]

$$f(1/2 - m, x^2) = \frac{x}{x^2+}\,\frac{(m + 1/2)}{1+}\,\frac{1}{x^2+}\,\frac{(m + 3/2)}{1+}\,\frac{2}{x^2+\cdots} \tag{3.23}$$

for $x > 0$, $|1/2 - m| < \infty$. This expansion doesn't converge at $x = 0$; therefore, at that point another procedure must be used. We observe that

$$f(1/2 - m, 0) = \Gamma(1/2)\,\delta_{m,0} = \sqrt{\pi}\,\delta_{m,0} \tag{3.24}$$

so

$$A_{0,0} = \sqrt{\pi}/2. \tag{3.25}$$

To obtain the second initializing value $A_{1,0}$ one must take the derivative of (3.21)

$$\frac{d}{dx} f(1/2 - m, x^2) = \left(1 + \frac{m}{x^2}\right)(2x) f(1/2 - m, x^2) - 2. \tag{3.26}$$

This can be substituted into (3.22) to obtain

$$\frac{d}{dx} J(x, y) = (2x)\,J(x, y) - e^y + \frac{1}{x} \sum_{m=1}^{\infty} \frac{y^m}{(m-1)!} f(1/2 - m, x^2). \tag{3.27}$$

Now using the expansion [13]

$$f(1/2 - m, x^2) = \exp(x^2)\left[\Gamma(1/2 - m)\,x^{2m} - x \sum_{m=0}^{\infty} \frac{(-x^2)^n}{(n + 1/2 - m)\,n!}\right] \tag{3.28}$$

In the last term of (3.27), taking the limit as $x \to 0$ and using the definitions (3.18) and the result (3.25) we obtain the simple expression

$$A_{1,0} = -e^y - \sum_{m=1}^{\infty} \frac{y^m}{(1/2 - m)(m-1)!}\,. \tag{3.29}$$

Equations (3.25) and (3.29) are used to obtain the initializing values of the $A_{l,i}$'s at $x = x_0 = 0$. For the other $x_i \neq 0$, we use (3.23) substituted into (3.22) and (3.27).

The expression (3.23) for $f(1/2 - m, x^2)$ can be simplified for computational purposes by putting it into a sum-of-products form and using a recursion formula. Using standard results [14] (3.23) can be written

$$f(1/2 - m, x^2) = \sum_{i=1} P_i \tag{3.30}$$

where

$$P_i = \prod_{j=1}^{i} \rho_j \tag{3.31}$$

and the recursion relation for ρ_j is

$$1 + \rho_j = \frac{1}{1 + r_k(1 + \rho_{j-1})} \tag{3.32}$$

where

$$r_j = \frac{1}{x^2}(j - 1 + m\delta_{j,\mathrm{even}}) \tag{3.33}$$

for $j > 1$ and the initializing values of ρ^j are

$$\rho_1 = 1/x \tag{3.34}$$

and

$$\rho_2 = \frac{1}{1 + r_2} - 1. \tag{3.35}$$

If the sum in (3.30) is terminated at $i = n$, the relative accuracy is determined by the size of $| P_n/P_{n-1} |$.

Recapitulating, once the set $\{x^i\}$ is chosen the values of $f(1/2 - m, x_i^2)$ are determined by (3.30) using (3.31), (3.32), (3.33), (3.34), and (3.35). These are stored in tables and called when E is changed to determine the coefficients $A_{l,i}$ in (3.7). Thus the time consumed in their calculation is relatively unimportant. Using (3.22) and (3.18) we obtain

$$A_{0,i} = \frac{1}{2} \sum_{m=0}^{\infty} \frac{y^m}{m!} f(1/2 - m, x_i^2), \tag{3.36}$$

where the special case for $A_{0,0}$ is given by (3.25). Also using (3.27) and (3.18)

$$A_{1,i} = (2x_i)\, A_{0,i} - e^y + \frac{1}{x_i} \sum_{m=1}^{\infty} \frac{y^m}{(m-1)!} f(1/2 - m, x_i^2) \tag{3.37}$$

where the special case $A_{1,0}$ is given by (3.10). Note that the sums in (3.36), (3.37), and (3.29) can run concurrently to reduce computational time. Once these initial values are determined (3.15), (3.16), and (3.17) can be used to generate the other $A_{l,i}$. For fixed energy the integral $I(x, y)$ is rapidly calculated using (3.7) and (3.6); for a change in the energy the $A_{l,i}$ must be recalculated but much of this calculation can be looked up in the stored tables.

For the Taylor series of (3.7), $l_{\max} = 8$ yields 6 place accuracy for $I(x, y)$. The number of expansion points, x_i, is determined by the asymptotic behavior of $I(x, y)$ for large x. In the computer program used to generate the tables, expansion points were added until the asymptotic formula indicated a value for $I(x, y)$ which was smaller than 10^{-20}, which gave $i_{\max} = 28$ and a range of $0 \leqslant x \leqslant 6.875$.

The programs, of course, have provisions for modifiying these values. For such values of x, a great deal of latitude in choosing y is possible without sacrificing convergence. The expansion (3.22), however, is an expansion in $y = E/\eta$ and the energy range of interest is $-1Ry \leqslant E \leqslant 1Ry$, so η is somewhat restricted if this series is to converge. In the calculation here (3.22) was truncated after 15 terms; this yielded a relative error of $\leqslant 10^{-9}$ for the worst case, $E = -1.0$. It may seem odd that we regard $E = -1.0$ as worst case, since then the expansion gives an alternating series. The reason for this usage is that in the expansion technique used here, the limit on accuracy is determined by the convergence of the sums giving the initializing values, and these converge must slowly for negative E. We found that these sums ceased to converge in 15 terms for $E = -1$ and η less than about 0.2 or 0.3. With all these considerations an evaluation time for $I(x, y)$ of 109 microseconds was obtained on the CDC 6400.

Since the Green's function is singular as described by (3.4) and (3.5) and the singularity is integrable, its effect in integrals such as (2.2) can be accounted for by simple volume averaging. In any numerical integration scheme each point is assigned a weight which is essentially the volume per point. It is this volume over which the singular term of the Green's function (and the potential if necessary) must be averaged in (2.2). This is quite straightforward for three-dimensional integrals such as (2.2); however, if the integrals become six dimensional, which happens when a basis set is assumed for band structure calculation, the averaging becomes somewhat complicated and is described in detail elsewhere [15].

The evaluation of the runs over the reciprocal lattice in (2.11) and the direct lattice in (2.12) involves the evaluation of the exponential, sine and cosine functions in addition to the integral (2.13). The evaluation time for the exponential was 36 μsec and for the sine and cosine calculated together was 116 μsec on the C.D.C. 6400 using programs especially designed for speed. The number of terms kept in these lattice runs depends on their relative evaluation times and thus on the choice of y and the accuracy to which the Green's function must be evaluated.

The next section contains the results of timing runs for various values of the relevant parameters for several different lattices.

4. RESULTS

Timing runs were made for a number of typical crystal structures. For each structure, one general **k** value was chosen, since the timing doesn't depend on **k**. Then for a number of positions in the primitive cell and for the energies $E = +1$, 0, -1 Ry timing runs were made for a range of η values, $1.2 > \eta > 0.2$. For each position, energy, and η, the number of direct and reciprocal lattice vectors necessary to give the direct and reciprocal lattice partial sums contribution to at least six places were determined as were the separate times for each series. The best η was then chosen on the basis of mjnimum total time. This should represent fairly well the shortest evaluation time for at least six-place accuracy over the whole primitive cell and for the entire energy range of interest, i.e., the range from -1 to $+1$ *Ry*.

TABLE I

Results of Timing Runs

Lattice	Best η	Number direct	Shell	Number reciprocal	Shell	Time (m sec)
sc	.6	57	5	123	8	74
bcc	.8	89	7	177	9	67
fcc	1.0	79	5	137	9	60
hcp	.8	155	15	135	15	90

Column two gives the best η for the most rapid evaluation of the Green's function to obtain at least six-place accuracy anywhere in the primitive cell. Columns three and four give the number of direct lattice vectors, including the origin, and the corresponding number of shells needed, respectively; columns five and six give the same information for the reciprocal lattice vectors; column seven gives the average time to evaluate the Green's function at one position (on the C.D.C. 6400).

Table I gives the results of the timing runs for the various crystal structures considered, simple cubic, body centered cubic (bcc), face centered cubic (fcc), and hexagonal close packed (hcp). The cubic lattice parameter was taken to be 6 atomic units as was the *C*-axis length in the hcp case. Such lattice parameters are typical of those found in real crystals. The direct and reciprocal lattice vectors were obtained with a special program that produced the vectors and arranged them in order of increasing length [16]. The best η for the most rapid evaluation of the Green's function while obtaining at least six-place accuracy at a general point in the primitive cell is given in the second column of the table. The third column gives the number of direct lattice vectors, including the origin, needed for convergence. The fourth column gives the number of shells of vectors of equal length to which this number corresponds. Columns five and six give the same information about the necessary number of reciprocal lattice vectors. The last column of Table I gives the total time in milliseconds needed to evaluate the Green's function at one position. The uncertainty in this number arises from variations in the servicing and accessing periods of the system clock. The numbers in Column 7 are the result of averaging the times of ten calculations of the same numbers. The H.C.P. case takes longer than the rest because the H.C.P. lattice contains two atomic sites in the primitive cell whereas the other lattices contain only one. These times are given for the greatest accuracy that would probably ever be required to, for example, obtain a final value for a band energy. In searching for the rough location of such an energy one would probably need only four-place accuracy. The time necessary for four-place accuracy is on the average about a third of that necessary for six places. The numbers given here for the C.D.C. 6400 computer, of course, are quite machine-dependent, thus timing runs should be redone when using a different machine.

The method of evaluating the free-electron lattice Green's function given here appears to be fast and accurate enough to make numerically tractable calculations on real crystal systems. It is expected that it will be useful in a variety of solid state physics problems.

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16. This program is available from the authors on request.