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Green's function and a generalized Lloyd formula for the density of states in disordered muffin-tin alloys

S. Kaprzyk* and A. Bansil
Department of Physics, Northeastern University, Boston, Massachusetts 02115

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We consider the Korringa-Kohn-Rostoker coherent-potential-approximation Green's function for a disordered system of muffin-tin potentials and evaluate its integral over the Wigner-Seitz cell rigorously throughout the complex energy plane. The resulting expression is shown to possess a perfect derivative form, provided the angular-momentum summations are extended to infinity; for a finite angular-momentum cutoff this result is valid to a good approximation. For real energies our expression constitutes a generalization of the Lloyd formula for the density of states. The conventional Lloyd formula contains unphysical singularities that are not only unsatisfactory from a formal viewpoint, but also make its use increasingly cumbersome in multicomponent alloys as the number of atoms in the unit cell becomes larger. Our expression, on the other hand, is free from such singularities, and thus provides a useful basis for evaluating density of states and its energy integral in muffin-tin systems.

I. INTRODUCTION

The Lloyd formula for the density of states, $\rho(E)$, has proven very useful in discussing properties of the muffin-tin Hamiltonian.[1] In the Korringa-Kohn-Rostoker coherent-potential-approximation (KKR-CPA) theory of alloys, this formula expresses $\rho(E)$ as a perfect derivative of energy, and thus permits an evaluation of the Fermi energy without requiring an explicit computation of $\rho(E)$ over the occupied states.[2-4] The Lloyd formula in the literature is based essentially on the use of the scattering operator rather than the Green's function, and contains spurious singularities (e.g., at free-electron energies, and at energies where one of the phase shifts for any of the atoms vanishes), which must be subtracted in an *ad hoc* manner in order to apply the formula. Such a procedure is not only unsatisfactory from a formal viewpoint, but furthermore becomes increasingly cumbersome to implement in multicomponent alloys as the number of atoms in the unit cell increases. We emphasize that the full KKR-CPA Green's function $G(z)$ of course does not possess any unphysical poles,[5-10] and that the difficulty arises because some terms in $G(z)$ are dropped in the conventional derivation of the Lloyd formula.

With this motivation, we consider for the first time the full KKR-CPA Green's function and its real-space integral in an analytically rigorous manner throughout the complex energy plane; the usefulness of complex energies has become increasingly apparent in exploring the properties of muffin-tin systems in recent years.[11-15] In our treatment, all terms in $G(z)$ are kept, including in particular terms which are real for real energies. These latter terms do not contribute to $\rho(E)$ [proportional to the imaginary part of $G(z)$], but if dropped they lead to an unsatisfactory generalization of $G(z)$ in the complex plane.

We find that the exact integral of KKR-CPA Green's function over the Wigner-Seitz cell can be expressed as a perfect derivative for all z, provided the angular-momentum (L) summations are extended to infinity; for finite L cutoff, this form holds to a good approximation. On the real energy axis, our expression for $G(z)$ yields an analytically satisfactory extension of the Lloyd formula for $\rho(E)$. This generalized formula contains no unphysical poles, and constitutes a useful basis for evaluating density of states and its energy integral in muffin-tin systems. We have made extensive numerical tests with our formula in binary alloys, as well as in complex multicomponent perfect crystals and alloys containing many atoms per unit cell, and found the results to be reasonable in all cases.

An outline of this article is as follows. The real-space integral of the KKR-CPA Green's function is considered in Sec. II. A discussion of our results is presented in Sec. III. The Appendix outlines the derivation of one of the relations used in Sec. II.

II. GENERALIZED LLOYD FORMULA FOR CONCENTRATED ALLOYS

For the random binary alloy A_xB_y (with $y\equiv 1-x$) of nonoverlapping muffin-tin potentials, the $(\mathbf{r},\mathbf{r})$ matrix element of the ensemble averaged KKR-CPA Green's function $G(z)$ is given in the zeroth Wigner-Seitz (WS) cell by[16,17]

$$\begin{aligned}\langle \mathbf{r}|G(z)|\mathbf{r}\rangle = &-\sum_{L} Y_L(\hat{\mathbf{r}})[xZ_l^A(r_<)J_l^A(r_>)+yZ_l^B(r_<)J_l^B(r_>)]Y_L(\hat{\mathbf{r}})\\ &+\sum_{LL'} Y_L(\hat{\mathbf{r}})\{xZ_l^A(r)[T_{00}^{0=A}]_{LL'}Z_{l'}^A(r)+yZ_l^B(r)[T_{00}^{0=B}]_{LL'}Z_{l'}^B(r)\}Y_{L'}(r)\ . \qquad (1)\end{aligned}$$

Here, $L\equiv(l,m)$ is a composite angular and magnetic quantum number index, and $Y_L(\hat{\mathbf{x}})$ is a real spherical harmonic. $Z_l^{A\,(B)}$ and $J_l^{A\,(B)}$ are the regular and irregular solutions of the radial Schrödinger equation, respectively, in the A (B) muffin-tin sphere, normalized such that

$$Z_l^{A\,(B)}(r)=j_l(\kappa r)(\tau_l^{A\,(B)})^{-1}-i\kappa h_l(\kappa r)\ , \tag{2a}$$

$$J_l^{A\,(B)}(r)=j_l(\kappa r)\quad\text{for } r\geq R_m\ , \tag{2b}$$

where R_m is the muffin-tin sphere radius, $\kappa\equiv\sqrt{E}$, $j_l(x)$ and $h_l(x)\equiv j_l(x)+in_l(x)$ are the spherical Bessel and Hankel functions, respectively, and $\tau_l^{A\,(B)}$ is the on-the-energy-shell matrix element of the A (B) t matrix, related to the corresponding phase shift $\delta_l^{A\,(B)}$ by the equation

$$\tau_l^{A\,(B)}=-\kappa^{-1}\exp(i\delta_l)\sin\delta_l\ . \tag{3}$$

The matrix $T_{00}^{0=A\,(B)}$ in Eq. (1) denotes the (00) path operator (in the lattice-site representation) for an A (B) impurity placed in the KKR-CPA effective medium and is related to the medium path operator T_{00}:[3,4]

$$T_{00}^{0=A\,(B)}=[1-(\tau_{A\,(B)}^{-1}-\tau_c^{-1})T_{00}]^{-1}T_{00}\ , \tag{4}$$

where τ_c is the CPA scattering matrix. It is useful to write $T_{LL'}^{00}$ as

$$T_{LL'}^{00}=\left[\frac{1}{\tau_c^{-1}-B}\right]_{LL'} \tag{5}$$

in terms of the matrix B, related to the free-electron Green's function G_0:

$$\begin{aligned}G_0(\mathbf{r}+\mathbf{R}_n,\mathbf{r}+\mathbf{R}_{n'})=&-i\kappa\sum_L j_l(\kappa r_<)h_l(\kappa r_>)\\&\times Y_L(\hat{\mathbf{r}})Y_L(\hat{\mathbf{r}})\delta_{nn'}\\&+\sum_{LL'}Y_L(\hat{\mathbf{r}})j_l(\kappa r)\\&\times B_{LL'}^{nn'}j_{l'}(\kappa r)Y_{L'}(\hat{\mathbf{r}})\ .\end{aligned} \tag{6}$$

Here, $\{\mathbf{R}_n\}$ is the set of lattice vectors. The Fourier transform of the matrix B in the (nn') space gives the usual KKR structure function matrix.

Our purpose is to derive an expression for

$$G(z)\equiv\int_{\mathrm{WS}}d\mathbf{r}\langle\mathbf{r}|G(z)|\mathbf{r}\rangle\ , \tag{7}$$

where the integral extends over the zeroth WS cell. By defining

$$F_{L'L}^{A\,(B)}=\int_{\mathrm{WS}}d\mathbf{r}\,Y_L(\hat{\mathbf{r}})Z_L^{A\,(B)}(r)Z_{L'}^{A\,(B)}(r)Y_{L'}(\hat{\mathbf{r}})\ , \tag{8a}$$

$$I_{L'L}^{A\,(B)}=\int_{\mathrm{WS}}d\mathbf{r}\,Y_L(\hat{\mathbf{r}})Z_L^{A\,(B)}(r_<)J_{L'}^{A\,(B)}(r_>)Y_{L'}(\hat{\mathbf{r}})\ , \tag{8b}$$

and keeping Eqs. (1) and (7) in mind, we obtain

$$\begin{aligned}G(z)=\mathrm{Tr}[&-xI^A(z)-yI^B(z)\\&+xF^A(z)T_{00}^{0=A}+yF^B(z)T_{00}^{0=B}]\ ,\end{aligned} \tag{9}$$

where the trace is over the angular-momentum indices.

By using the regularity of the solution $Z^{A\,(B)}$ and the Green's theorem to convert volume integral to a surface integral, it can be shown that (suppressing angular-momentum indices)

$$F^A(z)=d\tau_A^{-1}/dz+\tau_A^{-1}P\tau_A^{-1}+\tau_A^{-1}Q+Q^T\tau_A^{-1}+R\ , \tag{10}$$

with a similar equation for F^B. The matrices P, Q, and R can be written in terms of the free-electron solutions j_l and h_l:

$$P_{LL'}=\int_S d\mathbf{S}\cdot\mathbf{W}[Y_L(j_l(\kappa r))',Y_{L'}j_{l'}(\kappa r)]\ , \tag{11a}$$

$$Q_{LL'}=\int_S d\mathbf{S}\cdot\mathbf{W}[Y_L(j_l(\kappa r))',-i\kappa Y_{L'}h_{l'}(\kappa r)]\ , \tag{11b}$$

$$R_{LL'}=\int_S d\mathbf{S}\cdot\mathbf{W}[-i(\kappa h_l)'Y_L,-i\kappa h_{l'}(\kappa r)]\ . \tag{11c}$$

Here, the integrations over the surface of the WS cell, a prime on the small parentheses denotes an energy derivative, and the "Wronskian" $\mathbf{W}[f,g]$ is defined as

$$\mathbf{W}[f(\mathbf{r}),g(\mathbf{r})]\equiv f(\mathbf{r})\nabla g(\mathbf{r})-g(\mathbf{r})\nabla f(\mathbf{r})\ . \tag{12}$$

We now invoke the relation (see Appendix)

$$\begin{aligned}xF^AT_{00}^{0=A}&+yF^BT_{00}^{0=B}\\&=x(P\tau_A^{-1}+Q)+y(P\tau_B^{-1}+Q)+Q^T+x\frac{d\tau_A^{-1}}{dz}T_{00}^{0=A}\\&\quad+y\frac{d\tau_B^{-1}}{dz}T_{00}^{0=B}-\frac{d\tau_c^{-1}}{dz}T_{00}\\&\quad+\frac{1}{N}\sum_{\mathbf{k}}\frac{d}{dz}\ln[\tau_c^{-1}-B(z,\mathbf{k})]\ .\end{aligned} \tag{13}$$

Using (13), and the CPA condition

$$xT_{00}^{0=A}+yT_{00}^{0=B}=T_{00}\ , \tag{14}$$

the right-hand side of (9) may be written as

$$G(z)=G_1(z)+G_2(z)+G_3(z)\ , \tag{15}$$

where we have defined

$$G_1(z)=\mathrm{Tr}(Q)\ , \tag{16a}$$

$$\begin{aligned}G_2(z)=\mathrm{Tr}\Bigg\{&N^{-1}\sum_{\mathbf{k}}\frac{d}{dz}\ln[\tau_c^{-1}-B(z,\mathbf{k})]\\&+\frac{d}{dz}\ln(\tau_A^{-1}-\tau_B^{-1})-y\frac{d}{dz}\ln(\tau_c^{-1}-\tau_A^{-1})\\&-x\frac{d}{dz}\ln(\tau_c^{-1}-\tau_B^{-1}\Bigg\}\ .\end{aligned} \tag{16b}$$

$$G_3(z)=\mathrm{Tr}[x(-I^A+P\tau_A^{-1}+Q)+y(-I^B+P\tau_B^{-1}+Q)]\ . \tag{16c}$$

$G_2(z)$ is now in the form of a perfect derivative. To manipulate $G_3(z)$, using Eqs. (11a) and (11b), and keeping asymptotic form (2a) in mind, we write the part $(P\tau_{A\,(B)}^{-1}+Q)$ in Eq. (16c) as

$$(P\tau_{A\,(B)}^{-1}+Q)_{LL'}=\int_S d\mathbf{S}\cdot\mathbf{W}[Y_L(j_l(\kappa r))',Y_{L'}Z_{l'}^{A\,(B)}(r)]\ . \tag{17}$$

Equation (17) can be combined with expression (8b) for $I^{A\,(B)}$ to obtain

$$(-I^{A\,(B)}+P\tau^{-1}_{A\,(B)}+Q)_{LL'} = \lim_{S_\epsilon\to 0}\int_{S_\epsilon} d\mathbf{S}\cdot\mathbf{W}[Y_L(J_l^{A\,(B)}(r))',Y_{L'}Z_{l'}^{A\,(B)}(r)]\ . \tag{18}$$

The right-hand side of (18) arises from the singularity in (8b) at the origin from the irregular solution $J^{A\,(B)}$. We now write the regular wave function $Z_l^{A\,(B)}$ as

$$Z_l^{A\,(B)}(r,z)\equiv\phi_l^{A\,(B)}(z)\psi_l^{A\,(B)}(r,z)\ , \tag{19}$$

where $\phi_l^{A\,(B)}(z)$ is an energy-dependent renormalization factor independent of r such that $\psi_l^{A\,(B)}\to r^l$ for $r\to 0$.[18] The integral in (18) can then be evaluated, and the result is

$$\lim_{S_\epsilon\to 0}\int_{S_\epsilon} d\mathbf{S}\cdot\mathbf{W}[Y_L(J_l^{A\,(B)}(r))',Y_{L'}Z_{l'}^{A\,(B)}(r)] = \frac{d}{dz}\ln\phi_l^{A\,(B)}(z)\delta_{LL'}\ . \tag{20}$$

Using (20), (18), and (16) yields

$$G_3(z)=-\frac{d}{dz}\mathrm{Tr}(x\ \ln\phi^A+y\ \ln\phi^B)\ . \tag{21}$$

The form of $G(z)$ obtained by substituting (21) and (16b) into (15) deserves some comment. For real energies, $\mathrm{Im}G_3(E)$ is real, and thus gives a vanishing contribution to $\mathrm{Im}G(E)$. Note that the individual terms $G_1(E)$, $G_2(E)$, and $G_3(E)$ possess spurious singularities which cancel against each other. In particular, $G_1(E)$ and $G_2(E)$ both contain free-electron poles, the latter arising from singularities in the KKR structure functions $B(E,\mathbf{k})$ at free-electron energies. Similarly, both $G_2(E)$ and $G_3(E)$ are individually singular when $\delta_{A\,(B)}\to 0$. The Lloyd formula for integrated density of states in disordered alloys in the literature has been based essentially on the use of $\mathrm{Im}[G_2(E)]$, which is justified provided the free electron and other unphysical contributions in $G_2(E)$ are properly subtracted. We emphasize that $G_2(z)$ does not possess the properties of a physical Green's function, and is thus difficult to extend into the complex plane. With this motivation, we will now manipulate $G_1(z)$ and rewrite $G(z)$ in a form in which the individual contributions are properly behaved.

For this purpose, we introduce the A (B) logarithmic derivatives at the muffin-tin radius

$$D_l^{A\,(B)}(z)=r^2\frac{\partial}{\partial r}\ln Z_l^{A\,(B)}(z,r)|_{r=R_m}\ , \tag{22}$$

related to the corresponding τ matrices by

$$\tau^{-1}_{A\,(B)}=\frac{1}{j_l(\kappa R_m)}\frac{1}{D_l^{A\,(B)}-D_l^{(j)}}\frac{1}{j_l(\kappa R_m)}+i\kappa\frac{h_l(\kappa R_m)}{j_l(\kappa R_m)}\ , \tag{23}$$

where $D_l^{(j)}$ is the logarithmic derivative for the spherical Bessel function, defined via (22) by replacing Z_l by $j_l(\kappa r)$. We also require the angular-momentum representation of the free-electron Green's function

$$G_0^{LL'}(z,\mathbf{k})=\frac{1}{D_l^{(h)}-D_l^{(j)}}\delta^{LL'} +j_l(\kappa R_m)B_{LL'}(z,\mathbf{k})j_{l'}(\kappa R_m)\ , \tag{24}$$

where $D_l^{(h)}$ denotes the logarithmic derivative for the spherical Hankel function h_l. Finally, by manipulating (11b), we write $G_1(z)$ as

$$G_1(z)=\sum_L\left[-i\kappa\int_{\mathrm{WS}}d\mathbf{r}\,h_l(\kappa r)j_l(\kappa r)Y_L(\hat{\mathbf{r}})Y_L(\hat{\mathbf{r}}) +\frac{d\ln\kappa^l}{dz}\right]\ . \tag{25}$$

Equations (22)–(24) can be used to eliminate the τ and B matrices in (16b) in favor of the D and G_0 matrices, respectively. The resulting expression for $G_2(z)$ together with Eqs. (16c) and (25) for $G_3(z)$ and $G_1(z)$ can be shown to yield

$$G(z)=-\frac{d}{dz}\mathrm{Tr}\left[\frac{1}{N}\sum_{\mathbf{k}}\ln[G_0^{-1}(z,k)+D^{(j)}-D^c]^{-1} +x\ \ln\{\psi^A(R_m)[1-G_c(D^A-D^c)]\} +y\ \ln\{\psi^B(R_m)[1-G_c(D^B-D^c)]\}\right] +X(z)\ , \tag{26}$$

where

$$X(z)\equiv\sum_L\left[-i\kappa\int_{\mathrm{WS}}d\mathbf{r}\,h_l(\kappa r)j_l(\kappa r)Y_L(\hat{\mathbf{r}})Y_L(\hat{\mathbf{r}}) -\frac{d}{dz}\ln\frac{j_l(\kappa R_m)}{\kappa^l}+\frac{1}{N}\frac{d}{dz}\sum_{\mathbf{k}}[\ln G_0(z,\mathbf{k})]_{LL}\right]\ , \tag{27}$$

and the KKR-CPA Green's function G_c and the associated "logarithmic derivatives" D^c are the self-consistent solutions of the CPA equation:

$$xG_A+yG_B=G_c\ , \tag{28}$$

where

$$G_c=N^{-1}\sum_{\mathbf{k}}[G_0^{-1}(z,\mathbf{k})+D^{(j)}-D^c]^{-1}\ , \tag{29a}$$

$$G_{A\,(B)}=(G_c^{-1}+D^c-D^{A\,(B)})^{-1}\ . \tag{29b}$$

The quantity $X(z)$, Eq. (27), can be shown to vanish in the limit of $l\to\infty$. We have computed $X(z)$ in $3d$ metals for different l values and energy ranges, and estimate that in most cases of interest with $l\leq 2$, $X(z)$ is quite small.[19] By neglecting $X(z)$ in (26), and keeping (29) in mind, we obtain our final formula[20]

$$G(z)=-\frac{d}{dz}\mathrm{Tr}\left[\frac{1}{N}\sum_{\mathbf{k}}\ln[G_0^{-1}(z,k)+D^{(j)}-D^c]^{-1} +x\ \ln\{[\psi^A(R_m)]^{-1}G_A\} +y\ \ln\{[\psi^B(R_m)]^{-1}G_B\}-\ln G_c\right]\ . \tag{30}$$

It is interesting to consider limiting forms of Eq. (30). For a perfect A crystal, setting $G_A = G_B = G_c$, $D^A = D^B = D^c$, and $\psi^A = \psi^B$, yields

$$G(z) \to \frac{d}{dz} \mathrm{Tr} \left[\ln \psi^A(R_m) - \frac{1}{N} \sum_{\mathbf{k}} \ln \frac{1}{G_0^{-1}(z,\mathbf{k}) + D^{(j)} - D^A} \right] . \quad (31)$$

In the free-electron limit, $G_A = G_B = G_c = G_0$, $D^{(j)} = D^c$, $\psi^A = \psi^B = j_l$, and $G(z) \to G_0(z)$.

We emphasize that the Green's function $[G_0^{-1}(z,\mathbf{k}) + D^{(j)} - D^c]^{-1}$ possesses the Herglotz property

$$\mathrm{Im}[G_0^{-1}(z,\mathbf{k}) + D^{(j)} - D^c] \geq 0 \quad (32)$$

in the upper half plane, and therefore it is especially suited for extension into the complex plane.

Finally, we note that the preceding formalism is easily generalized to treat the case of a multicomponent alloy containing many atoms per unit cell; we avoid giving an explicit expression for the Green's function and the related Lloyd formula for the sake of brevity.

III. DISCUSSION

For a finite $L_{\max}$ in the angular-momentum summation, the exact result (26), keeping (27) in mind, does not naturally possess the form of a perfect derivative, although as noted above, in the limit $L_{\max} \to 0$, the part $X(z)$ vanishes, and the perfect derivative form [(30)] is obtained. Equation (30), while it is expected to be a good approximation, is not exact for finite $L_{\max}$. In numerical tests, we find that for a given $L_{\max}$, (30) will in general possess unphysical free-electron singularities, which move to higher energies with increasing values of $L_{\max}$.

Concerning the extension of various quantities into the complex plane, it is noteworthy that much of the existing KKR-CPA literature proceeds by writing the Green's function in terms of the scattering operator T defined by

$$G = G_0 + G_0 T G_0 .$$

We emphasize that the scattering operator T does not possess the physical properties of a Green's function in the complex plane. In particular, the path operators associated with $T(z)$ are not Herglotz, and do not possess a proper spectral representation. Our experience is that $T(z)$ is a poorly behaved quantity for extending the KKR-CPA theory into the complex plane.

The physical essence of Eqs. (26) and (3) is that they allow us to evaluate the real-space integral of the KKR-CPA Green's function in a formal manner. The density of states and the integrated density of states in the alloy is straightforwardly related to imaginary part of the right-hand side of these equations. These quantities can also of course be computed directly by carrying out the real-space integral in Eq. (7) numerically. The latter procedure, however, is cumbersome and becomes more so in complex systems, and furthermore, since there are many equivalent ways of dividing the volume of the unit cell into contributions from individual atoms in a multicomponent alloy, it will lead to ambiguities in defining the density of states. Formulas (26) and (30), on the other hand, are free from such complications, and form a natural basis for discussing densities of states in muffin-tin systems.

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APPENDIX: DERIVATION OF EQ. (13)

The expansion (6) for G_0, when used in the operator relation

$$\frac{dG_0}{dz} = -G_0^2(z) , \quad (\mathrm{A1})$$

can be shown to yield, for $n \neq m$ (suppressing angular-momentum indices),

$$-\frac{d}{dz} B^{nm} = \sum_{s \neq n,m} B^{ns} P B^{sm} + B^{nm} Q + Q B^{nm} , \quad (\mathrm{A2})$$

where the matrices P and Q are defined by Eqs. (11a) and (11b), respectively. By using (A2) for dB/dz, together with the multiple scattering equation for the path operators,[3,4]

$$T^{nm} = \tau_n \delta_{nm} + \tau_n \sum_{s \neq m} B^{ns} T^{sm} , \quad (\mathrm{A3})$$

it is straightforward to obtain the identity

$$\frac{1}{N} \left[\sum_n \frac{d\tau_n^{-1}}{dz} T^{nn} - \sum_{n \neq m} \frac{dB^{nm}}{dz} T^{mn} \right] = \frac{1}{N} \sum_s F^s T^{ss} - \frac{1}{N} P \sum_s \tau_s^{-1} - Q - Q^T , \quad (\mathrm{A4})$$

valid for a general system of muffin-tin potentials. Here, F^s is defined by Eq. (10). Equation (13) follows upon averaging both sides of (A4) within the CPA, and rearranging terms.

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[*] Permanent address: Academy of Mining and Metallurgy, Institute of Physics and Nuclear Techniques, Krakow, Poland.

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[18] ψ_l is thus the energy-independent wave function commonly generated in muffin-tin calculations, when the radial Schrödinger equation is integrated starting with the form r^l for $r \rightarrow 0$.

[19] Note that the correction term $X(z)$ in (26) does not depend on the potentials, and is a universal function for a specific lattice and a particular choice of the muffin-tin radii. $X(z)$ can be computed straightforwardly by numerical integration.

[20] Exact result (26) can be used to obtain approximate forms other than Eq. (30). One useful possibility is to extend the L summation in the first term on the right-hand side of (27) to infinity (without doing so in other terms), so that this term can then be evaluated via a direct integral of the real-space free-electron Green's function.