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Lattice Green's Function for the Face Centered Cubic Lattice

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An expression for the Green's function (GF) of face centered cubic (FCC) lattice is evaluated analytically and numerically for a single impurity problem. The density of states (DOS), phase shift and scattering cross section are expressed in terms of complete elliptic integrals of the first kind.

KEY WORDS: FCC lattice; impurity; Green's function.

1. INTRODUCTION

The lattice Green's function (LGF) is defined as (Economou, 1983)

$$G(E) = \frac{\Omega}{(2\pi)^d} \int_{\text{IBZ}} \frac{F(\vec{k})}{E - E(\vec{k})}\, d\vec{k} \tag{1.1}$$

$E(\vec{k})$ is a dispersion relation, $F(\vec{k})$ is an appropriate function, Ω is the volume of the crystal in real space, d is the dimension, and IBZ denotes that the integration is restricted to the first Brillouin zone (Economou, 1983; Katsura *et al.*, 1971).

Many quantities of interest in solid state physics can be expressed in terms of LGF, for example, statistical model of ferromagnetism such as Ising model (Brout, 1960), Heisenberg model (Mattis, 1965), and spherical model (Berlin and Kac, 1952); lattice dynamics (Montroll, 1956), random walk theory (Montroll and Wiess, 1965; Domb and Joyce, 1972), and band structure (Li *et al.*, 1989). In a recent work we have evaluated analytically and numerically GF, density of states (DOS), phase shift, and scattering cross section for the following

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cases:

(i) One and two dimensional lattices (Sakaji *et al*., submitted),
(ii) Glasser cubic lattice (Sakaji *et al*., 2002a),
(iii) Body Centered Cubic lattice (Sakaji *et al*., 2002b),
(iv) General Glasser case (Hijjawi and Khalifeh, 2002).

In this paper we report on the single impurity LGF. The paper is organized as follows: Section 2 is devoted to the general definition of the diagonal LGF and its form inside and outside the band for the FCC lattice in terms of complete elliptic integrals of the first kind. This section also contains the formulae for the DOS, phase shift and scattering cross section for the point defect case. In Section 3 we present the results and discussion.

2. THE FCC LATTICE GREEN'S FUNCTION

The diagonal GF for the FCC lattice with nearest neighbor interaction is defined as (Joyce, 1971; Morita and Horiguci, 1971a; Morita and Horiguci, 1971b; Inoue, 1974; Mano, 1975; Mano, 1974; Doniach and Sondheimer, 1974)

$$G^0(L,L;E) = \frac{1}{\pi^3}\int_0^\pi\int_0^\pi\int_0^\pi \times \frac{dk_x\,dk_y\,dk_z}{E-\cos(k_x)\cos(k_y)-\cos(k_x)\cos(k_z)-\cos(k_y)\cos(k_z)}, \quad E>3 \tag{2.1}$$

Integrating the above equation and using the method of analytic continuation (Inoue, 1974; Mano, 1975; Mano, 1974), the diagonal GF outside the band has the form

$$G^0(L,L;E) = \frac{4}{\pi^2(E+1)}K(k_+)\,K(k_-), \quad E>3 \tag{2.2}$$

where

$$k_\pm^2 = \frac{1}{2}\left(1 \mp \frac{4\sqrt{E}}{(E+1)^{3/2}} - \frac{(E-1)\sqrt{(E-3)}}{(E+1)^{3/2}}\right), \tag{2.3}$$

GF outside and inside the band can be written as (all mathematical Manipulations are given in Appendix A).

$$G^0(L,L,;E) = \left\{ \begin{array}{l} \frac{4}{\pi^2(E+1)}K(k_+)K(k_-), \quad E>3 \\ \frac{2}{\pi^2(E+1)}[(Z_+^2+1)(Z_-^2+1)]^{\frac{-1}{4}}(K(v_+)K(u_-)+K(v_-)K(u_+)+i[K(v_+)K(u_+)-K(v_-)K(u_-)]), \quad -1<E<0 \end{array} \right\}, \tag{2.4}$$

where

$$Z_{\mp}^2 = \frac{4\sqrt{-E}}{(E+1)^{3/2}}\left(-\frac{(E-1)}{4}\sqrt{\frac{-E+3}{-E}} \mp 1\right), \tag{2.5}$$

and

$$\nu_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{Z_-^2}{Z_-^2+1}}\right) \tag{2.6}$$

$$\mu_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{Z_+^2}{Z_+^2+1}}\right) \tag{2.7}$$

Therefore, the DOS is

$$\begin{aligned}\mathrm{DOS}^{\mathrm{o}}(E) = \frac{2}{\pi^3(E+1)}\left[(Z_-^2+1)(Z_+^2+1)\right]^{\frac{-1}{4}}\left[K(\nu_+)K(u_+)\right. \\ \left. -K(\nu_-)K(u_-)\right], \quad -1 < E < 0\end{aligned} \tag{2.8}$$

where $K(\nu_{\pm})$ and $K(\underline{u}_{\pm})$ are the complete elliptic integrals of the first kind.

Consider the case of a tight-binding Hamiltonian whose perfect periodicity is destroyed due to the presence of the point defect at the L site. This situation can be thought of physically as arising by substituting the host atom at the L-site by a foreign atom (Economou, 1983; Doniach and Sondheimer, 1974) having a level lying ε' higher than the common level of the host atoms (L). Normally, this atom is close to the host in the same series of the periodic table.

Thus, our diagonal GF of the FCC lattice for the single impurity case can be written as

$$G(L,L,E) = \left\{ \begin{array}{l} \frac{4K(k_+)K(k_-)}{\pi^2(E+1)-4\varepsilon' K(k_+)K(k_-)};\ E > 3 \\ \\ \frac{\frac{\pi^2}{2}(E+1)[(Z_+^2+1)(Z_-^2+1)]^{\frac{1}{4}}K[(\nu_+)K(\mu_-)+K(\nu_-)K(\mu_+)+i(K(\nu_+)K(\mu_-)-(\nu_+)K(\mu_+))]-2\varepsilon'[K^2(\nu_+)+K^2(\nu_-)][K^2(\mu_+)+K^2(\mu_-)]}{[\frac{\pi^2}{2}(E+1)((Z_+^2+1)(Z_-^2+1))^{\frac{1}{4}} - \varepsilon'(K(\nu_+)K(\mu_-)+K(\nu_-)K(\mu_+))]^2+\varepsilon^2[K(\nu_+)K(\mu_+)-K(\nu_-)K(\mu_-)]^2} \\ \\ -1 < E < 0 \end{array} \right\}, \tag{2.9}$$

and the corresponding DOS can be written as:

$$\mathrm{DOS}(E) = \frac{\frac{\pi^2}{2}(E+1)[(Z_+^2+1)(Z_-^2+1)]^{\frac{1}{4}}(K(\nu_+)K(\mu_-)-K(\nu_+)K(\mu_+))}{[\frac{\pi^2}{2}(E+1)((Z_+^2+1)(Z_-^2+1))^{\frac{1}{4}} - \varepsilon'(K(\nu_+)K(\mu_-)+K(\nu_-)K(\mu_+))]^2+\varepsilon^2[K(\nu_+)K(\mu_+)-K(\nu_-)K(\mu_-)]^2}, \tag{2.10}$$

$$-1 < E < 0$$

The S-wave phase shift, $\delta_{0,}$ is defined as (Doniach and Sondheimer, 1974):

$$\tan\delta_{\mathrm{o}} = \frac{\pi \mathrm{DOS}^0(E)}{\frac{1}{\varepsilon'} - \mathrm{Re}G^0(E)}, \tag{2.11}$$

Here, $\mathrm{Re}G^0(E)$ refers to the real part the GF inside the band. After some mathematical manipulations, we obtain:

$$\tan\delta_0 = \frac{K(v_+)K(u_+) - K(v_-)K(u_-)}{\frac{\pi^2(E+1)[(Z_+^2+1)(Z_-^2+1)]^{\frac{1}{4}}}{2\varepsilon'} - (K(v_+)K(u_-) + K(v_-)K(u_+))}, \tag{2.12}$$

The cross section, $\sigma_{,}$ is defined as (Doniach and Sondheimer, 1974):

$$\sigma = \frac{4\pi}{P^2} \frac{\pi^2[\mathrm{DOS}^0(E)]^2}{\left[\mathrm{Re}G^0(E) - \frac{1}{\varepsilon'}\right]^2 + \pi^2[\mathrm{DOS}^0(E)]^2}, \tag{2.13}$$

Here, P refers to the electron momentum.

Therefore, the cross section becomes

$$\sigma = \frac{4\pi}{P^2} \times \frac{[K(v_+)K(u_+) - K(v_-)K(u_-)]^2}{\left[K(v_+)K(u_-) + K(v_-)K(u_+) - \frac{\pi^2(E+1)[(Z_+^2+1)(Z_-^2+1)]^{\frac{1}{4}}}{2\varepsilon'}\right]^2 + [K(v_+)K(u_+) - K(v_-)K(u_-)]^2}. \tag{2.14}$$

3. RESULTS AND DISCUSSION

Our results for the face centered cubic lattice are shown in Figs. 1–9. Figures 1 and 2 show real and imaginary parts of GF for the pure lattice. It diverges as E goes to minus one. Figure 3 shows the DOS for the pure lattice. The DOS has the

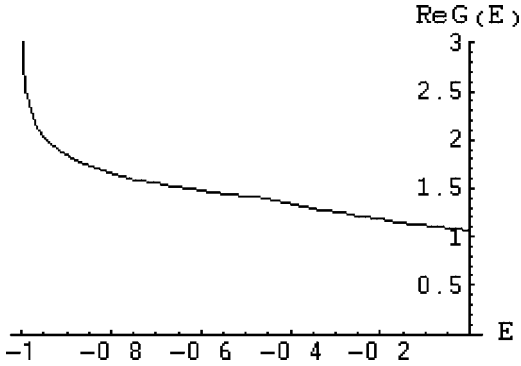

Fig. 1. Real part of Green's function for the perfect FCC lattice.

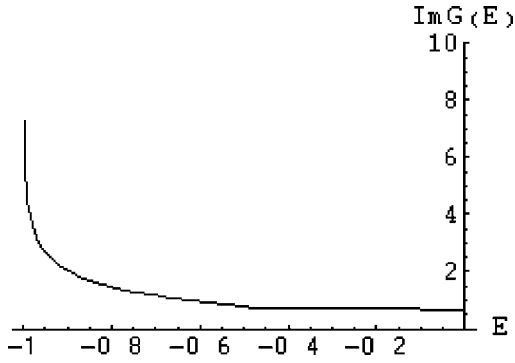

Fig. 2. Imaginary part of Green's function for the perfect FCC lattice.

same behavior as above apart from a constant. Figure 4 shows the DOS for the face centered cubic lattice with single impurity for different potential strengths ε' (-0.6, $-$ 0.2,0.0,0.2, and 0.6). For $\varepsilon' = 0.0$ it diverges as E goes to minus one. The peak value varies with the potential strengths and reaches its maximum at $\varepsilon' = 0.2$. We see from the above figure that the divergence of the DOS is removed by adding point defects due to the presence of additional terms in the denominator coming from the impurity potential. For ε' enclosed between 0.5 to 0.7 and -1 to -0.2, the curves inflect around $E = -0.5$. Figure 5 shows the DOS for the FCC in three-dimensions with one axis representing potential strengths ε' varying between -1 and 1 (arbitrary units) whereas the second axis is energy scale varying between -1 and 0 as indicated in the formalism.

The phase shift, $\delta_{0,}$ is defined as the shift in the phase of the wave function due to the presence of the impurity potential. Figure 6 displays, $\delta_{0,}$ for the FCC with

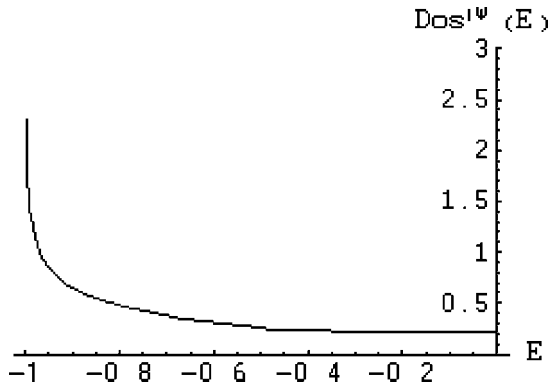

Fig. 3. The density of states (DOS) for the perfect FCC lattice.

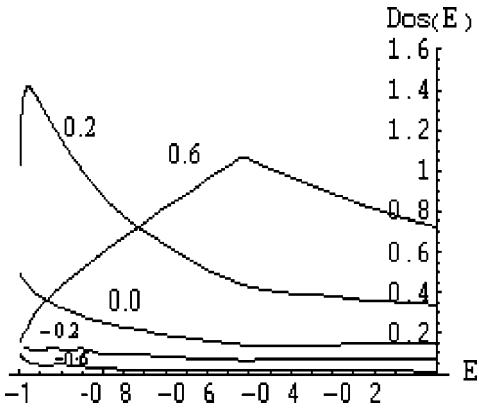

Fig. 4. The density of states (DOS) for the FCC lattice with single impurity for different potential strengths ε' (-0.6, -0.2, 0.0, 0.2, and 0.6).

single impurity for different potential strengths ε' (-0.6, -0.2, 0.0, 0.2, and 0.6). For $\varepsilon' = 0.0$, δ_0, vanishes as the potential is turned off (perfect lattice). The phase shift is always negative for all negative potential strengths ε' the same behavior occurs for $\varepsilon' \geq 0.95$. In the range between $\varepsilon' = 0.0$ and $\varepsilon' = 0.4$, δ_0, is positive. In the range ε' between 0.4 and 0.94 we have discontinuity as shown in Fig. 6. The phase shift is separated into two regions around the discontinuity point: a right hand region where δ_0 is positive and decreases as E increases and a left hand region

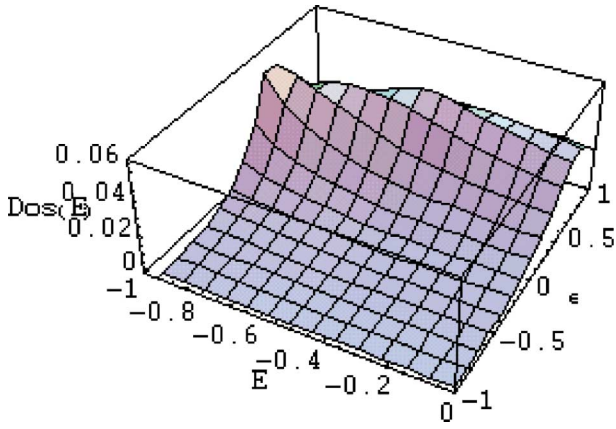

Fig. 5. Three-dimensional density of states (DOS) for the FCC lattice with single impurity for different potential strengths ε' varying between -1 and 1(arbitrary units).

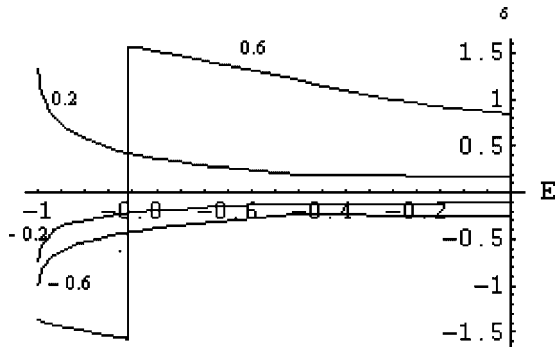

Fig. 6. The phase shift, δ_0, for the FCC lattice with single impurity for different potential strengths ε' (-0.6, -0.2, 0.0, 0.2, and 0.6).

in which δ_0 is negative and increases as E increases (the discontinuity point moves to the right by increasing ε').

Figure 7 shows the phase shift, δ_0, in three dimensions for the face centered cubic lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

The cross section, σ, is defined as the area an impurity atom presents to the incident electron. Figure 8 shows the cross section for single substitutional impurity with different potential strengths, ε'. The peak value varies with the

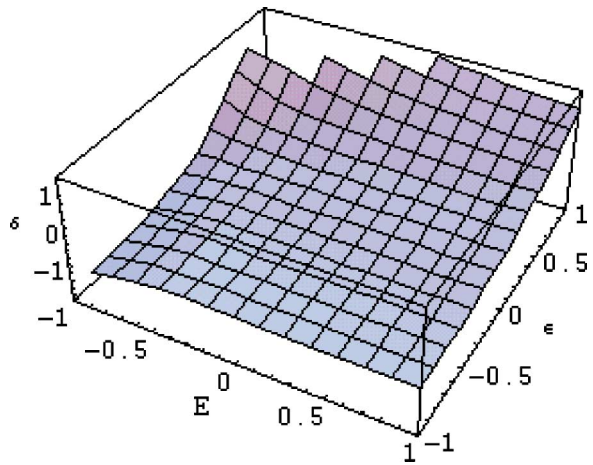

Fig. 7. The phase shift, δ_0, in three dimensions for the FCC lattice with single impurity for different potential strengths ε' varying between -1 and 1(arbitrary units).

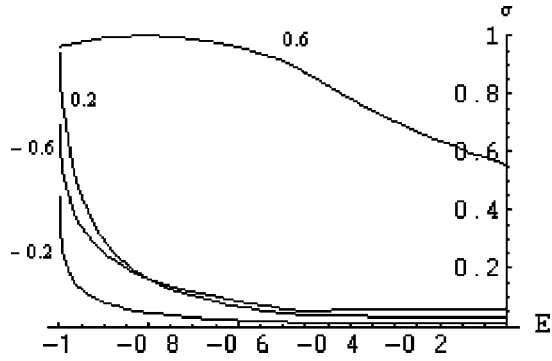

Fig. 8. The cross section, σ, for the FCC lattice with single impurity for different potential strengths ε' (-0.6, -0.2, 0.0, 0.2, and 0.6).

potential strength, it increases as ε' increases in range between $0.0 < \varepsilon' < 1.0$ and increases as ε' decreases in range between $-1.0 < \varepsilon' < 0.0$. The cross section is related to some physical quantities such as the mobility and resistivity in metals. Figure 9 shows the cross section, σ, in three dimensions for the face centered cubic lattice with single impurity for different potential strengths ε' varying between -1 and 1(arbitrary units).

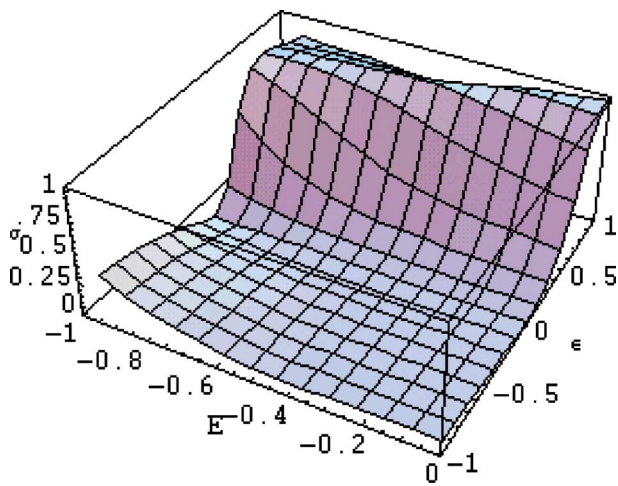

Fig. 9. The cross section, σ, in three dimensions for the FCC lattice with single impurity for different potential strengths ε' varying between -1 and 1(arbitrary units).

APPENDIX A: DERIVATION OF GREEN'S FUNCTION FOR THE FACE CENTERED CUBIC LATTICE INSIDE THE BAND

In this Appendix we derive an expression for GF inside the band in terms of complete elliptic integral of the first kind.

GF for the face centered cubic lattice outside the band is given by (Joyce, 1971; Morita and Horiguci, 1971; Morita and Horiguci, 1971; Inoue, 1974; Mano, 1975; Mano, 1974):

$$G^0(L, L; E) = \frac{4}{\pi^2(E+1)} K(k_+) K(k_-), \tag{A1}$$

where

$$k_\pm^2 = \frac{1}{2}(1 + X_\mp), \tag{A2}$$

$$X_\mp = \mp \frac{4\sqrt{E}}{(E+1)^{3/2}} - \frac{(E-1)\sqrt{(E-3)}}{(E+1)^{3/2}}, \tag{A3}$$

Or in the range E enclosed between -1 and 0

$$k_\pm^2 = \frac{1}{2}(1 + Z_\mp), \quad -1 < E < 0 \tag{A4}$$

where

$$Z_\mp = \frac{4i\sqrt{-E}}{(E+1)^{3/2}} \left(-\frac{(E-1)}{4} \sqrt{\frac{-E+3}{-E}} \mp 1 \right), \tag{A5}$$

The complete elliptic integral of the first kind is expressed as

$$K(k) = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}, 1, k^2\right) \tag{A6}$$

where

${}_2F_1(\frac{1}{2}, \frac{1}{2}, 1, k^2)$ is the Gauss hypergeometric function
Substituting (A6) in (A1) we have

$$G^0(E) = \frac{{}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; k_+^2\right) {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; k_-^2\right)}{E+1} \tag{A7}$$

Using the following transformations (Bateman Manuscript Project, 1963):

$$\begin{aligned} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{1+Z_\mp}{2}\right) = {} & \frac{\Gamma\left(\frac{1}{2}\right)}{\left(\Gamma\left(\frac{3}{4}\right)\right)^2} {}_2F_1\left(\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; Z_\mp^2\right) \\ & + 2Z_\mp \frac{\Gamma\left(\frac{1}{2}\right)}{\left(\Gamma\left(\frac{1}{4}\right)\right)^2} {}_2F_1\left(\frac{3}{4}, \frac{3}{4}; \frac{3}{2}; Z_\mp^2\right), \end{aligned} \tag{A8}$$

With

$$ {}_2F_1(a,b;c;Z_{\mp}^2) = (1-Z_{\mp}^2)^{-a}\,{}_2F_1\left(a,c-b;c;\frac{Z_{\mp}^2}{Z_{\mp}^2-1}\right) \tag{A9} $$

$$ \frac{2\Gamma\left(\frac{1}{2}\right)}{\left(\Gamma\left(\frac{3}{4}\right)\right)^2}\,{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};\frac{Z_{\mp}^2}{Z_{\mp}^2-1}\right) = {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2-1}}\right)\right) $$

$$ +\,{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2-1}}\right)\right), \tag{A10} $$

$$ \frac{2\Gamma\left(-\frac{1}{2}\right)}{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2-1}}\,{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};\frac{Z_{\mp}^2}{Z_{\mp}^2-1}\right) = {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2-1}}\right)\right) $$

$$ -\,{}_2F_1\left(x\frac{1}{2},x\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2-1}}\right)\right), \tag{A11} $$

Substituting (A8), (A9), (A10) and (A11) in (A7) we obtain

$$ G^0(L,L,E) = \frac{2}{\pi^2(E+1)}\left[(Z_+^2+1)(Z_-^2+1)\right]^{\frac{-1}{4}}\left(K(v_+)K(u_-)\right. $$

$$ \left. +\,K(v_-)K(u_+) + i(K(v_+)K(u_+) - K(v_-)K(u_-))\right), \tag{A12} $$

where

$$ v_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{Z_-^2}{Z_-^2+1}}\right) \tag{A13} $$

$$ u_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{Z_+^2}{Z_+^2+1}}\right) \tag{A14} $$

If we have a single impurity then GF is defined as (Economou, 1983):

$$ G(L,L,E) = \frac{G^0(L,L,E)}{1-\varepsilon' G^0(L,L,E)} \tag{A15} $$

After some mathematical manipulation Eq. (A15) becomes.

$$ G(L,L,E) $$

$$ = \frac{\frac{\pi^2}{2}(E+1)\left[(Z_+^2+1)(Z_-^2+1)\right]^{\frac{1}{4}}\left[K(v_+)K(\mu_-)+K(v_-)K(\mu_+)+i(K(v_+)K(\mu_-)-K(v_+)K(\mu_+))\right] - 2\varepsilon'\left[K^2(v_+)+K^2(v_-)\right]\left[K^2(\mu_+)+K^2(\mu_-)\right]}{\left[\frac{\pi^2}{2}(E+1)((Z_+^2+1)(Z_-^2+1))^{\frac{1}{4}} - \varepsilon'(K(v_+)K(\mu_-)+K(v_-)K(\mu_+))\right]^2 + \varepsilon^2\left[K(v_+)K(\mu_+)-K(v_-)K(\mu_-)\right]^2}. $$

(A16)

Thus, the *S*-phase shift and scattering cross section can be evaluated in terms of complete elliptic integrals of the first kind as shown in the text.

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