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Lattice Green's Function for the Body-Centered Cubic Lattice

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An expression for the Green's function (GF) of Body-Centered Cubic (BCC) lattice is evaluated analytically and numerically for a single impurity lattice. 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: body-centered cubic lattice; Green's function.

1. INTRODUCTION

Green's function for the cubic lattices has been the object of an extensive study for many years. This method has proved to be very powerful for quantitative studies of a variety of problems in solid-state physics. Extensive investigations have been made to evaluate analytically as well as numerically for different crystal structures (Economou, 1983).

The lattice Green's function is defined as

$$G(E) = \frac{\Omega}{(2\pi)^d} \int_{1\mathrm{BZ}} \frac{F(\vec{k})}{E - E(\vec{k})}\, d\vec{k} \tag{1.1}$$

$E(\vec{k})$ 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 1BZ denotes that the integration must be restricted to the first Brillouin zone (Economou, 1983; Watson, 1939).

Many quantities of interest in solid-state physics can be expressed in terms of lattice Green's function (LGF), for example, statistical model of ferromagnetism such as Ising model (Brout, 1960), Heisenberg model (Dalton and Wood, 1967), spherical model (Tax, 1955), lattice dynamics (Dederichs *et al.*, 1980), random

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walk theory (Hughes, 1986; Montroll, 1956), and band structure (Koster and Slater, 1954; Li *et al.*, 1989).

In this work we report on the lattice Green's function. The paper is organized as follows: Section 2 is devoted to the general definition of the diagonal lattice Green's function and its form inside and outside the band for the BCC lattice in terms of complete elliptic integrals of the first kind. This section also contains the formulae for the density of states, phase shift, and scattering cross section for a point defect case. In Section 3 we present the results and discussion.

2. THE BODY-CENTERED CUBIC LATTICE GREEN'S FUNCTION

The diagonal Green's function for the BCC lattice with nearest neighbor interaction is defined as (Inoue, 1975; Joyce, 1971a,b; Katsura and Horiguchi, 1971; Mano, 1975; Morita, 1971; Morita and Horiguci, 1971)

$$G^0(L, L; E) = \frac{1}{N(2\pi)^d} \int\int\int_{1\mathrm{BZ}} \frac{d\vec{k}}{E - \varepsilon - 8V \cos(k_x(a/2)) \cos(k_y(a/2)) \cos(k_z(a/2))}, \tag{2.1}$$

where Ω/N is the volume of the unit cell of the lattice, V is the potential, that is, the hopping integral in the tight-binding approximation.

Or

$$G^0(L, L; E) = \frac{1}{\pi^3} \int_0^\pi \int_0^\pi \int_0^\pi \frac{dk_x\, dk_y\, dk_z}{E - \cos(k_x)\, \cos(k_y)\, \cos(k_z)}, \quad |E| > 1. \tag{2.2}$$

Integrating the above equation and using the method of analytic continuation (Joyce, 1971a), the diagonal Green's function outside the band will have the form

$$G^0(L, L; E) = \frac{4}{\pi^2 E} K^2(k), \quad |E| > 1 \tag{2.3}$$

where

$$k^2 = \frac{1}{2}\left[1 - (1 - E^{-2})^{1/2}\right]. \tag{2.4}$$

Green's function outside and inside the band can be written as (Sakaji, 1994) (mathematical manipulations are given in Appendix).

$$G^0(L, L; E) = \left\{ \begin{array}{ll} \frac{4}{\pi^2 E} K^2(k), & |E| > 1 \\ \frac{4}{\pi^2} K(k_+) K(k_-) + \frac{2i}{\pi^2}[K^2(k_+) - K^2(k_-)], & |E| < 1 \end{array} \right\}. \tag{2.5}$$

Therefore, the density of states is

$$\mathrm{DOS}^0(E) = \frac{2}{\pi^3}[K^2(k_+) - K^2(k_-)], \quad |E| < 1, \tag{2.6}$$

where

$$k_{\pm}^2 = \left[\frac{1}{2} \pm (1 - E^2)^{1/2}\right]. \tag{2.7}$$

$K(k_{\pm})$ is the complete elliptic integral of the first kind.

Consider the case of a tight-binding Hamiltonian whose perfect periodicity is destroyed due to the presence of a 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) having a level lying ε' higher than the common level of the host atoms (L).

Thus our diagonal Greens function of the BCC lattice for the single impurity case can be written as (Doniach and Sondheimer, 1974; Sakaji, 1994)

$$G(L, L; E) = \begin{cases} \frac{4K^2(k)}{\pi^2 E - 4\varepsilon' K^2(k)}, & |E| > 1 \\ \frac{4\pi^2 K(k_+)K(k_-) - 8\varepsilon'[K(k_+)K(k_-)]^2 - 4\varepsilon'[K^4(k_+) + K^4(k_-)] + 2\pi^2 i[K^2(k_+) - K^2(k_-)]}{[\pi^2 - 4\varepsilon' K(k_+)K(k_-)]^2 + 4\varepsilon'^2[K^2(k_+) - K^2(k_-)]^2}, & |E| < 1, \end{cases} \tag{2.8}$$

and the density of states can be written as (Doniach and Sondheimer, 1974; Sakaji, 1994)

$$\mathrm{DOS}(E) = \left\{ \frac{2\pi[K^2(k_+) - K^2(k_-)]}{[\pi^2 - 4\varepsilon' K(k_+) - K(k_-)]^2 + 4\varepsilon'^2[K^2(k_+) - K^2(k_-)]^2} \right\}. \tag{2.9}$$

The S-wave phase shift, δ_0, is defined as (Doniach and Sondheimer, 1974)

$$\tan\delta_0 = \frac{\pi \mathrm{DOS}^0(E)}{\frac{1}{\varepsilon'} - \mathrm{Re}G^0(E)}. \tag{2.10}$$

Here $\mathrm{Re}G^0(E)$ refers to the real part the Green's function inside the band. After some mathematical manipulations, we obtain (Doniach and Sondheimer, 1974; Sakaji, 1994)

$$\tan\delta_0 = 2\frac{K^2(k_+) - K^2(k_-)}{\frac{\pi^2}{\varepsilon'} - 4K(k_+)K(k_-)}. \tag{2.11}$$

The cross section, σ, is defined as (Doniach and Sondheimer, 1974)

$$\sigma = \frac{4\pi}{P^2} \frac{\pi^2[\mathrm{DOS}^0(E)]^2}{\left[\mathrm{Re}G^0(E) - \frac{1}{\varepsilon'}\right]^2 + \pi^2[\mathrm{DOS}^0(E)]^2}. \tag{2.12}$$

Here P refers to the electron momentum.

Therefore, the cross section becomes

$$\sigma = \frac{4\pi}{P^2} \frac{[K^2(k_+) - K^2(k_-)]^2}{\left[2K(k_+)K(k_-) - \frac{\pi^2}{2\varepsilon'}\right]^2 + [K^2(k_+) - K^2(k_-)]^2}. \tag{2.13}$$

3. RESULTS AND DISCUSSION

Our results for the body-centered cubic lattice are shown in Figs. 1–8. Figures 1 and 2 show real and imaginary parts of Green's function for the pure lattice. The figures show exponential falloff behavior. Figure 3 shows the density of states for the pure lattice. The density of states has the same behavior as above apart from a constant. The figure shows that the function is symmetric (even function).

Figure 4 shows the density of states for the BCC lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7). For $\varepsilon' = 0.0$ it falls off exponentially. The peak value varies with the potential strengths and reaches its maximum at $\varepsilon' = 0.3$. We see that the divergence of Green's function and density of states is removed by adding impurities. A different behavior is found in the case of the Glasser lattice (Sakaji *et al.*, in press). Figure 5 shows the density of states for the body-centered cubic lattice (DOS) 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 1 as indicated in the formalism.

The phase shift, δ_0, is defined as the shift in the phase of the wave function due to the presence of the impurity potential. Figure 6 displays δ_0 for the body-centered cubic lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7). For $\varepsilon' = 0.0$, δ_0 vanishes as potential is turned off (perfect

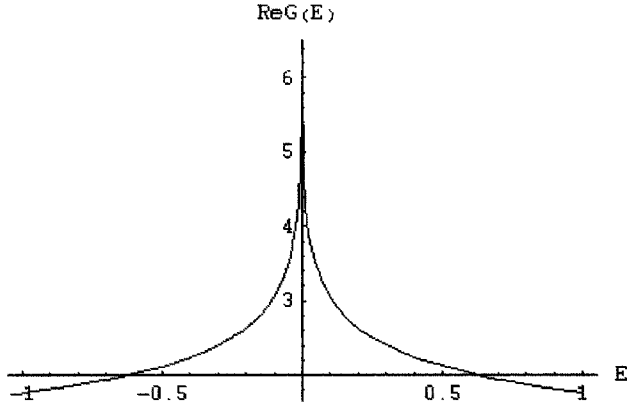

Fig. 1. Real part Green's function for the perfect BCC lattice.

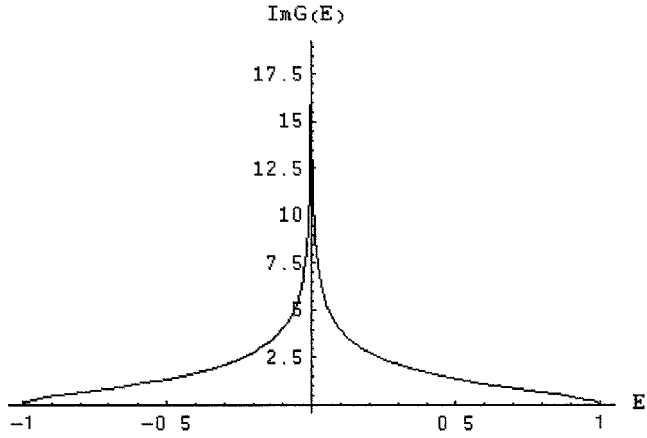

Fig. 2. Imaginary part Green's function for the perfect BCC lattice.

lattice). The phase shift is always negative for all negative potential strengths ε' and for $\varepsilon' = 0.57$. In the range between $\varepsilon' = 0.00$ and $\varepsilon' = 0.17$, δ_0 is continuous and positive. For ε' enclosed between 0.17 and 0.20 a singular behavior occurs at $E = 0.00$. In the range where ε' varies between 0.20 and 0.57 we have discontinuity as shown in Fig. 6 for $\varepsilon' = 0.30$. Two regions around the discontinuity point characterize the phase shift: a right-hand region in which δ_0 is positive and its value decreases as ε' increases and a left-hand region in which δ_0 is negative and its value increases as ε' decreases. That is the discontinuity point moves to the

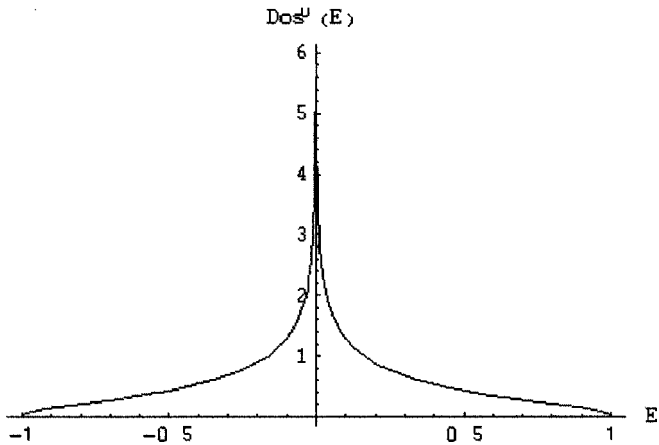

Fig. 3. The density of states (DOS) for the perfect BCC lattice.

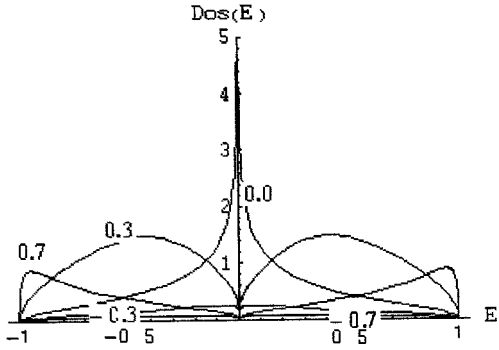

Fig. 4. The density of states (DOS) for the BCC lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

right as ε' increases. A similar behavior occurs for negative E. Figure 7 shows the phase shift, δ_0, in three dimensions for the BCC 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 potential strength and reaches its maximum at $\varepsilon' = 0.30$ and decreases in the range between $\varepsilon' < 0.20$ and $\varepsilon' > 0.30$. The values are all positive since σ can be

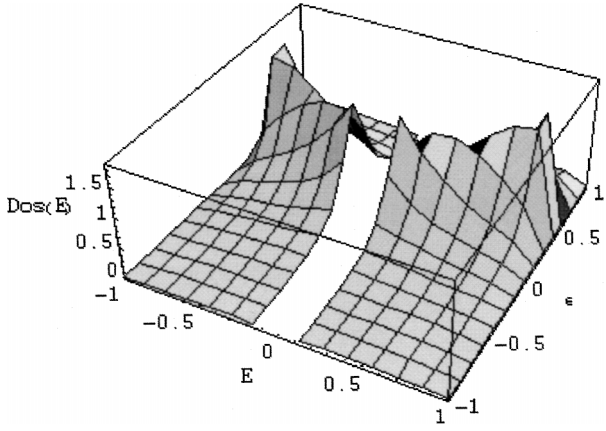

Fig. 5. Three-dimensional density of states (DOS) for the BCC lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

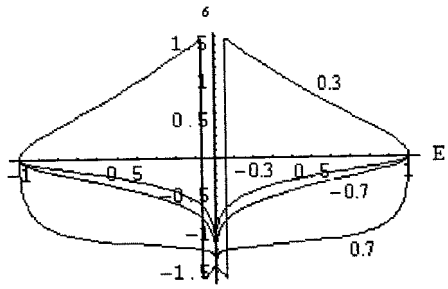

Fig. 6. The phase shift, δ_0, for the BCC lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

viewed as a sort of probability. It is related to some physical quantities such as the conductivity in metals. Figure 9 shows the cross section, σ, in three dimensions for the BCC lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

The Fermi energy is defined as the energy of highest occupied level and is calculated through the equation $\int_{-\infty}^{E_f} \mathrm{DOS}(E)\, dE = n =$ number of particles, where n represents the number of electrons per lattice ($n = 2$), and E_f is the Fermi energy.

The Fermi energy for a single substitutional impurity with different potential strengths are calculated, and the results in arbitrary units are given in Table I (Sakaji, 1974).

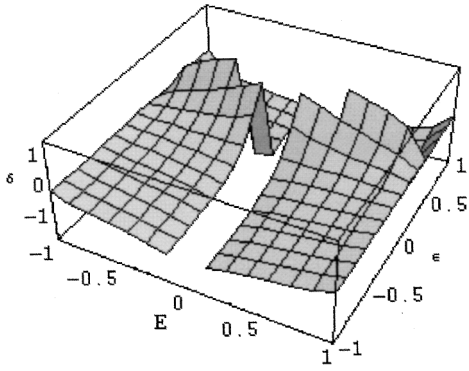

Fig. 7. The phase shift, δ_0, in three dimensions for the BCC lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

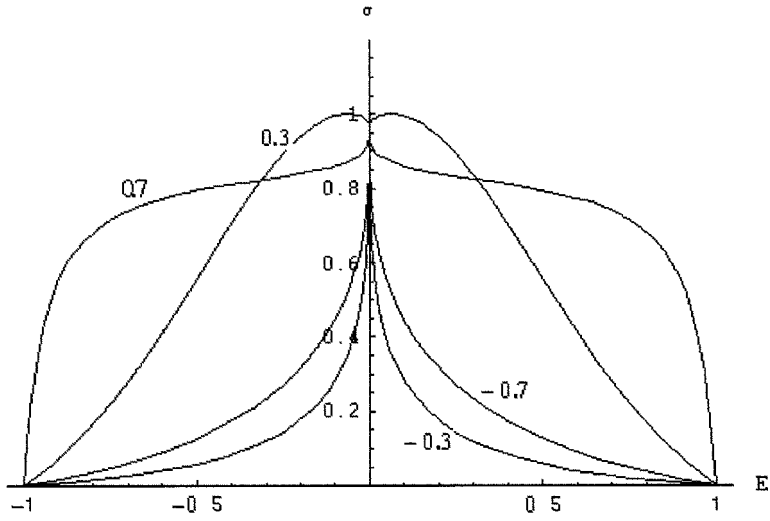

Fig. 8. The cross section, σ, for the BCC lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

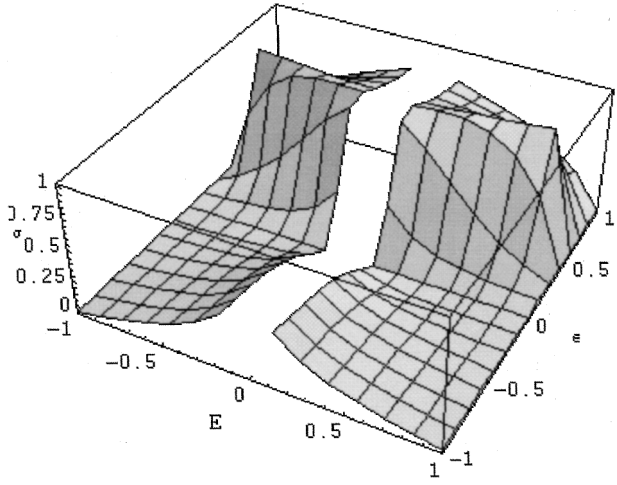

Fig. 9. The cross section, σ, in three dimensions for the BCC lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

Table I. The Fermi Energy for a Single Substitutional Impurity With Different Potential Strength

Potential strength	Fermi energy
0	2.00
0.1	1.91
0.3	1.67
0.4	1.43

APPENDIX: DERIVATION OF GREEN'S FUNCTION FOR THE BODY-CENTERED CUBIC LATTICE INSIDE THE BAND

In this Appendix we devoted to derive expression for Green's function inside the band in terms of complete elliptic integral of the first kind.

Green's function for the body-centered cubic lattice outside the band is given by (Inoue, 1975; Joyce, 1971a,b; Morita and Horiguci, 1971)

$$G^0(E) = \frac{4K^2(k)}{\pi^2 E}, \tag{A1}$$

where

$$k = \sqrt{\frac{1}{2}\left(1 - \sqrt{1 - E^{-2}}\right)}, \quad E > 1.$$

The complete elliptic integral of the first kind is expressed as

$$K(k) = \frac{\pi}{2}\,{}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; k^2\right), \tag{A2}$$

where ${}_2F_1(\frac{1}{2}, \frac{1}{2}; 1; k^2)$ is the Gauss hypergeometric function.

Kummer's identity is defined as (Sakaji *et al.*, in press)

$${}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; E^{-2}\right) = {}_2F_1\left[\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2}\left(1 - \sqrt{1 - E^{-2}}\right)\right]. \tag{A3}$$

Substituting (A3) in (A1) we have

$$G^0(E) = \frac{\left[{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; E^{-2}\right)\right]^2}{E}. \tag{A4}$$

Using the following transformations (Gradshteyn and Ryzhik, 1965)

$$\begin{aligned} {}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; E^{-2}\right) = E^{1/2}\Bigg[&\frac{\left[\Gamma\left(\frac{1}{4}\right)\right]^2}{2\pi^{3/2}}\,{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; 1 - E^2\right) \\ &+ 2\frac{\pi^{1/2}\sqrt{E^2 - 1}}{\left[\Gamma\left(\frac{1}{4}\right)\right]^2}\,{}_2F_1\left(\frac{3}{4}, \frac{3}{4}; \frac{3}{2}; 1 - E^2\right)\Bigg], \end{aligned} \tag{A5}$$

with

$$\frac{\left[\Gamma\left(\frac{1}{4}\right)\right]^2}{\pi^{3/2}}{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-E^2\right)$$
$$={}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{1-E^2}\right)\right]+{}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{1-E^2}\right)\right], \quad \text{(A6)}$$

and

$$\frac{4\pi^{1/2}\sqrt{1-E^2}}{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-E^2\right)$$
$$={}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{1-E^2}\right)\right]-{}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{1-E^2}\right)\right]. \quad \text{(A7)}$$

Substituting (A6) and (A7) in (A5) then we obtain

$${}_2F_1\left(\frac{1}{4},\frac{1}{4};1;E^{-2}\right)=\frac{1}{2}E^{1/2}\left\{(1+i){}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{1-E^2}\right)\right]\right.$$
$$\left.+(1-i){}_2F_1\left[\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{1-E^2}\right)\right]\right\}, \quad \text{(A8)}$$

or in terms of complete elliptic integral of the first kind

$${}_2F_1\left(\frac{1}{4},\frac{1}{4};1;E^{-2}\right)=\frac{E^{1/2}}{\pi}[(1+i)K(k_+)+(1-i)K(k_-)], \quad \text{(A9)}$$

where

$$k_\pm=\frac{1}{2}\left(1\pm\sqrt{1-E^2}\right).$$

Substituting (A9) in (A4) then we obtain

$$G^0(E)=\frac{1}{\pi^2}[(1+i)K(k_+)+(1-i)K(k_-)]^2, \quad \text{(A10)}$$

then

$$G^0(E)=\frac{2}{\pi^2}[2K(k_+)K(k_-)+i(K^2(k_+)-K^2(k_-))]. \quad \text{(A11)}$$

If we have a single impurity then Green's function is defined as

$$G(L,E)=\frac{G^0(E)}{1-\varepsilon' G^0(E)}. \quad \text{(A12)}$$

After some mathematical manipulation Eq. (A12) becomes

$$G(L,E) = \{[4\pi^2 - 2\varepsilon' K(k_+)K(k_-)]K(k_+)K(k_-) + i2\pi^2[K^2(k_+) - K^2(k_-)] - 4\varepsilon'[K^4(k_+) + K^4(k_-)]/\{[\pi^2 - 4\varepsilon' K(k_+)K(k_-)]^2 + 4\varepsilon'^2[K^2(k_+) - K^2(k_-)]^2\}. \quad \text{(A13)}$$

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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