International Journal of Theoretical Physics, Vol. 45, No. 1, January 2006 (© 2006)
DOI: 10.1007/s10773-005-9012-0

Lattice Green's Function for the Diamond Lattice

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Received December 27, 2004; accepted November 14, 2005

An expression for the Green's function (GF) of diamond lattice is evaluated analytically and numerically for a single impurity interacting with the first nearest-neighboring host atoms. 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: Diamond lattice; impurity; Green's function.

1. INTRODUCTION

The lattice Green's function is defined as (Economou, 1983; Katsura *et al.*, 1971; Sakaji *et al.*, 2002a)

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

$E(\vec{k})$ is a dispersion relation, $F(\vec{k})$ is an appropriate function, Ω is the volume of the crystal in real space, d the dimension, and IBZ denotes that the integration is restricted to the first Brillouin zone (Hijjawi *et al.*, 2004; Hijjawi and Khalifeh, 2002; Morita and Horiguci, 1971; Inoue, 1974; Sakaji *et al.*, 2002b).

In this paper, we report on lattice Green's function and the article 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 diamond 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.

Finally, the details of the green's function derivation inside the band are given in Appendix A.

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2. THE DIAMOND LATTICE GREEN'S FUNCTION

The diagonal Green's function for the diamond lattice with nearest neighbor interaction is defined as (Ishioka and Koiwa, 1978; Koiwa and Ishioka, 1979)

$$G^0(L, L; E) = \frac{1}{\pi^3} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \frac{dx\,dy\,dz}{E - (1 + \cos x \cos y + \cos x \cos z + \cos y \cos z)}, \quad E > 4 \tag{2.1}$$

This case is of practical interest in calculating the correlation factor appearing in the diffusion via a vacancy mechanism (Ishioka and Koiwa, 1978).

Integrating the earlier equation and using the method of analytic continuation, the diagonal Green's function outside the band has the form (Guttmann and Prellberg, 1993; Ishioka and Koiwa, 1978; Joyce, 1973; Koiwa and Ishioka, 1979)

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

where

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

Green's function for the perfect lattice inside and outside the band can be written as (all mathematical manipulations are given in Appendix).

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

where

$$X_{\mp} = \pm \frac{4\sqrt{1-E}}{E^{3/2}} - \frac{(E-2)\sqrt{(4-E)}}{E^{3/2}}, \tag{2.5}$$

and

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

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

Therefore, the density of states is

$$\mathrm{DOS}^0(E) = \frac{2}{\pi^3 E}\frac{[K(v_+)K(u_+) - K(v_-)K(u_-)]}{[(X_-^2+1)(X_+^2+1)]^{1/4}}, \quad 0 < E < 1 \tag{2.8}$$

where $K(v_\pm)$ and $K(u_\pm)$ are the complete elliptic integrals of the first kind.

We consider the case where perfect periodicity is destroyed by modifying just one site (L site). The situation can be thought of physically as arising by substituting the host atom at the L-site by a foreign atom (Doniach and Sondheimer, 1974; Economou, 1983), i.e., a localized zero-range potential of strength ε' is introduced. In the tight-binding model, ε' is proportional to charge difference between the impurity outer electrons and those of the host atom.

Thus, our diagonal Green's function of the diamond lattice for the single impurity case can be written as

$$\begin{aligned} &G(L, L, E) \\ &= \begin{cases} \dfrac{4K(k_+)K(k_-)}{\pi^2 E - 4\varepsilon' K(k_+)K(k_-)}, & E > 4 \\ \tfrac{\pi^2}{2}E[(X_+^2+1)(X_-^2+1)]^{1/4}[K(v_+)K(u_-) + K(v_-)K(u_+) & \\ \quad + i(K(v_+)K(u_+) - K(v_-)K(u_-))] - 2\varepsilon'[K^2(v_+) & \\ \quad + K^2(v_-)][K^2(u_+) + K^2(u_-)]/ & \\ \Big[\tfrac{\pi^2}{2}E((X_+^2+1)(X_-^2+1))^{1/4} - \varepsilon'(K(v_+)K(u_-) & \\ \quad + K(v_-)K(u_+))\Big]^2 + \varepsilon^2[K(v_+)K(u_+) - K(v_-)K(u_-)]^2, & 0 < E < 1 \end{cases} \end{aligned} \tag{2.9}$$

The density of states can be written as (Economou, 1983):

$$\begin{aligned} \mathrm{DOS}(E) = {} & \frac{\pi^2}{2}E[(X_+^2+1)(X_-^2+1)]^{1/4}(K(v_+)K(u_+) - K(v_-)K(u_-))/ \\ & \left[\frac{\pi^2}{2}E((X_+^2+1)(X_-^2+1))^{1/4} - \varepsilon'(K(v_+)K(u_-) + K(v_-)K(u_+))\right]^2 \\ & + \varepsilon^2[K(v_+)K(u_+) - K(v_-)K(u_-)]^2, \quad 0 < E < 1 \end{aligned} \tag{2.10}$$

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

$$\tan\delta_o = \frac{\pi\,\mathrm{Dos}^0(E)}{\frac{1}{\varepsilon'} - \mathrm{ReG}^0(E)}, \tag{2.11}$$

Here, ReG^0 (E) refers to the real part the Green's function inside the band. After some mathematical manipulations, we obtain:

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

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

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

Here, P refers to the electron momentum.

Therefore, the cross-section becomes

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

3. RESULTS AND DISCUSSION

The results for the diamond lattice are shown in Figs. 1–9. Figure 1 shows the density of states for the pure lattice. It diverges as $E = 0$ and falls off exponentially as expected from Eq. (2.4). The real and imaginary parts of Green's Function for the pure lattice are displayed in Figs. 2 and 3, they have the same behavior as

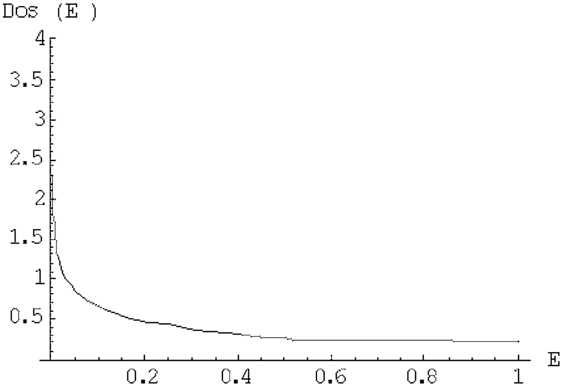

Fig. 1. The density of states for the perfect diamond lattice.

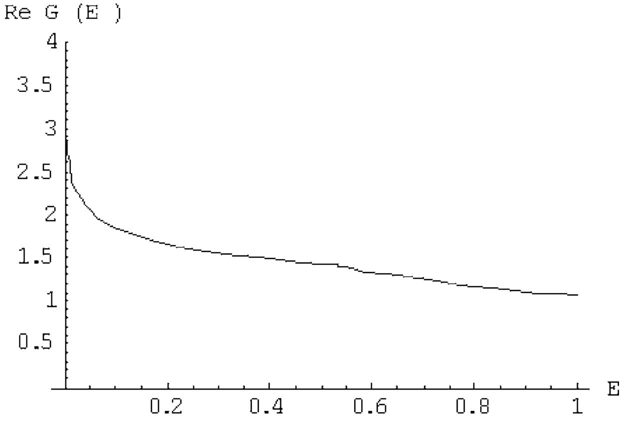

Fig. 2. Real part of Green's function for the perfect diamond lattice.

noted previously. Figure 4 shows the density of states for the diamond 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 diverges as E goes to zero. The peak value varies with the potential strengths and reaches its maximum at $\varepsilon' = 0.3$. The divergence of the density of states is removed by adding such impurities. Figure 5 shows the density of states for the diamond 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 0 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 diamond with

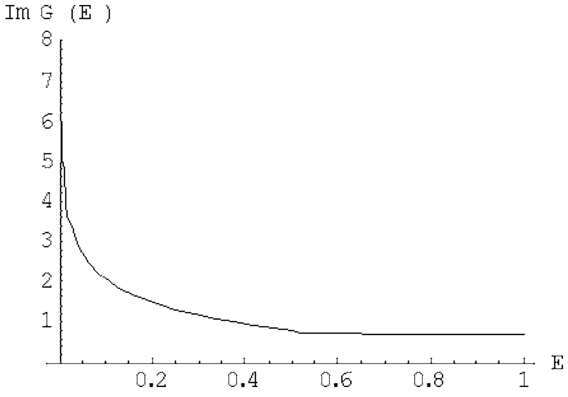

Fig. 3. Imaginary part of Green's function for the perfect diamond lattice.

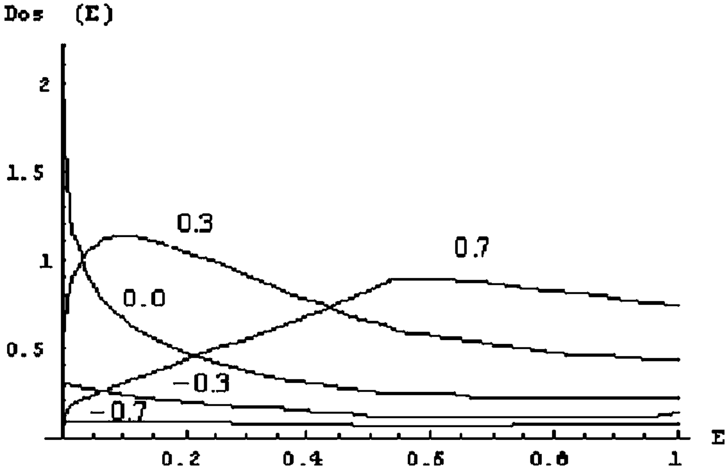

Fig. 4. The density of states (DOS) for the diamond lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

single impurity for different potential strengths ε'. For $\varepsilon' = 0.0$, δ_0, vanishes as the potential is turned off (perfect lattice); this behavior is clear from the definition of δ_0. 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 0.35, δ_0, is positive. In the range ε' between 0.35 and 0.94 we have discontinuity as shown

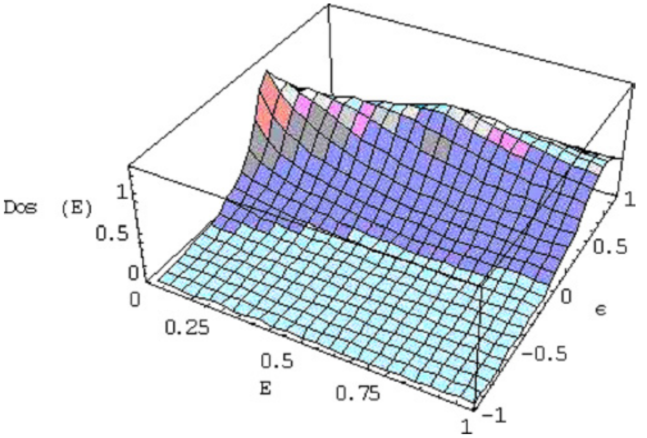

Fig. 5. Three-dimensional density of states (DOS) for the diamond lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

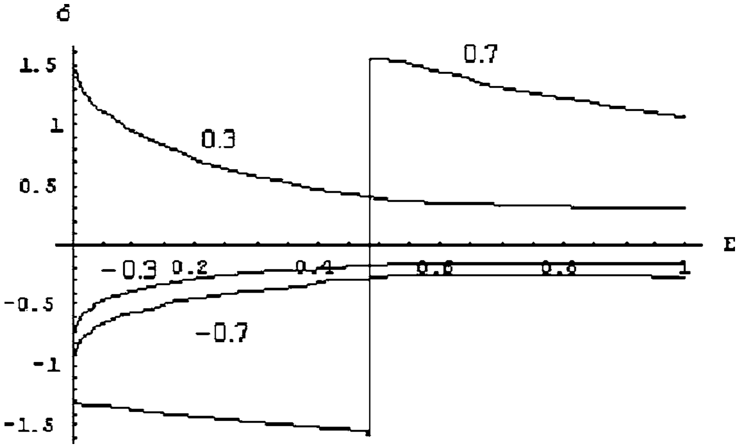

Fig. 6. The phase shift, δ_0, for the diamond lattice with single impurity for different potential strengths ε' (−0.7, −0.3, 0.0, 0.3, and 0.7).

in Fig. 6. The phase shift is separated into two regions around the discontinuity point: a positive right-hand region, which decreases as E increases, and a negative left-hand region, which increases as E increases. The discontinuity point moves to the right by increasing the values of ε'. In Fig. 7 the phase shift, δ_0, for the

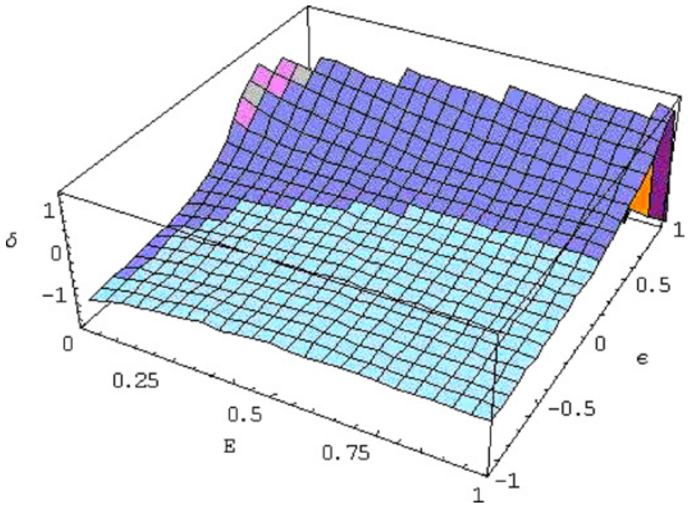

Fig. 7. The phase shift, δ_0, in three dimensions for the diamond lattice with single impurity for different potential strengths ε' varying between −1 and 1 (arbitrary units).

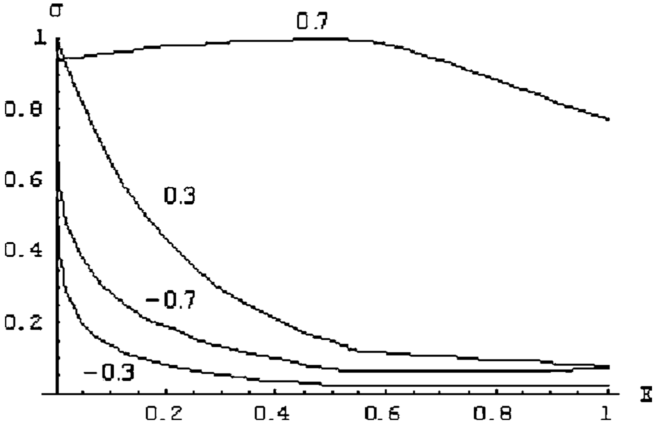

Fig. 8. The cross-section, σ, for the diamond lattice with single impurity for different potential strengths ε' (−0.7, −0.3,0.0,0.3, and 0.7).

diamond lattice with single impurity is shown for 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. It is related to some physical quantities such as the conductivity in metals. Figure 8 shows the cross-section, σ, for the diamond lattice with single

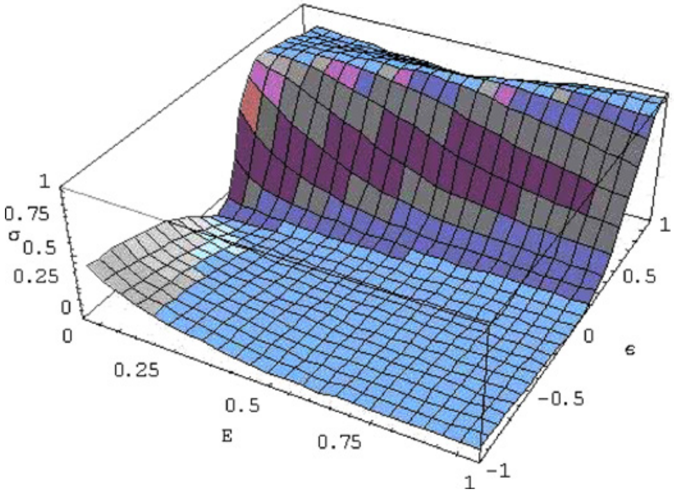

Fig. 9. The cross-section, σ, in three dimensions for the diamond lattice with single impurity for different potential strengths ε' varying between −1 and 1 (arbitrary units).

impurity for different potential strengths, ε'. The values are all positive since σ can be viewed as a sort of probability. For $\varepsilon' = 0.00$, the cross-section vanishes as the potential is turned off (perfect lattice). Peak value varies with the potential strength, it increases as ε' increases in range between $0.0 < \varepsilon' < 1.0$ and increases as ε' decreases in range between $-1.0 < \varepsilon' < 0.0$. Figure 9 displays the cross-section, σ, in three dimensions for the diamond lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

ACKNOWLEDGEMENT

R. S. Hijjawi would like to thank J. H. Asad, A. J. Sakaji, and J. M. khalifeh for helpful discussions.

APPENDIX A

Derivation of Green's function for the diamond lattice inside the band in this appendix we derive an expression for Green's function inside the band in terms of complete elliptic integral of the first kind. Green's function for the diamond lattice outside the band is given by (Guttmann and Prellberg, 1993; Ishioka and Koiwa, 1978; Joyce, 1973; Koiwa and Ishioka, 1979):

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

where

$$k_\pm^2 = \frac{1}{2}(1 + Z_\pm), \tag{A.2}$$

and

$$Z_\pm = \mp \frac{4\sqrt{E-1}}{E^{3/2}} - \frac{(E-2)\sqrt{(E-4)}}{E^{3/2}}, \tag{A.3}$$

or in the range E enclosed between 0 and 1

$$k_\pm^2 = \frac{1}{2}(1 + iX_\mp), \tag{A.4}$$

where

$$X_\mp = \pm \frac{4\sqrt{1-E}}{E^{3/2}} - \frac{(E-2)\sqrt{(4-E)}}{E^{3/2}}, \tag{A.5}$$

The complete elliptic integral of the first kind is expressed as (Bateman Manuscript Project, 1963; Gradshteyn and Ryzhik, 1965; Slater, 1966)

$$K(k) = \frac{\pi}{2} {}_2F_1\left(\frac{1}{2}, \frac{1}{2}, 1, k^2\right) \tag{A.6}$$

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

Kummer's identity is defined as (Gradshteyn and Ryzhik, 1965):

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4},1,\beta_\pm^{-1}\right) = {}_2F_1\left(\frac{1}{2},\frac{1}{2},1,\frac{1}{2}\left(1-\sqrt{1-\beta_\pm^{-1}}\right)\right) \tag{A.7} $$

Substituting (A.7) in (A.1) we have

$$ G^0(E) = \frac{{}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta_+^{-1}\right){}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta_-^{-1}\right)}{E} \tag{A.8} $$

where

$$ \beta_\pm^{-1} = 1 + X_\mp^2 \tag{A.9} $$

Using the following transformations (Bateman Manuscript Project, 1963; Slater, 1966):

$$ \begin{aligned} {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta_\pm^{-1}\right) = \beta_\pm^{1/4}\Bigg[&\frac{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}{2\sqrt{\pi^3}}{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta_\pm\right) \\ &+\sqrt{\beta_\pm-1}\,\frac{2\sqrt{\pi}}{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta_\pm\right)\Bigg], \end{aligned} \tag{A.10} $$

with

$$ \begin{aligned} &\frac{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}{\sqrt{\pi^3}}{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta_\pm\right) \\ &\quad = {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1+\sqrt{1-\beta_\pm}}{2}\right) + {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1-\sqrt{1-\beta_\pm}}{2}\right), \end{aligned} \tag{A.11} $$

and

$$ \begin{aligned} &\frac{4\sqrt{\pi}}{\left(\Gamma\left(\frac{1}{4}\right)\right)^2}\sqrt{1-\beta_\pm}\,{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta_\pm\right) \\ &\quad = {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta_\pm})\right) - {}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{1-\beta_\pm}\right)\right), \end{aligned} \tag{A.12} $$

Substituting (A.11) and (A.12) in (A.10) we obtain

$$ \begin{aligned} {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta_\pm^{-1}\right) = \frac{1}{2}\beta_\pm^{1/4}\Bigg[&(1+i){}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1+\sqrt{1-\beta_\pm}\right)\right) \\ &+(1-i){}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}\left(1-\sqrt{1-\beta_\pm}\right)\right)\Bigg], \end{aligned} \tag{A.13} $$

Or in terms of the complete elliptic integral of the first kind

$$
\begin{aligned}
&{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; 1; \beta_\pm^{-1}\right)\\
&= \frac{\beta_\pm^{1/4}}{\pi}\left[(1+i)K\left(\sqrt{\frac{1+\sqrt{1-\beta_\pm}}{2}}\right) + (1-i)K\left(\sqrt{\frac{1-\sqrt{1-\beta_\pm}}{2}}\right)\right],
\end{aligned}
\tag{A.14}
$$

Substituting (A.14) in (A.8) then we obtain

$$
\begin{aligned}
G^0(L, L, E) = \frac{\beta_-^{1/4}\beta_+^{1/4}}{\pi^2 E}&\left[(1+i)K\left(\sqrt{\frac{1+\sqrt{1-\beta_-}}{2}}\right)\right.\\
&\left.+(1-i)K\left(\sqrt{\frac{1-\sqrt{1-\beta_-}}{2}}\right)\right]\left[(1+i)K\left(\sqrt{\frac{1+\sqrt{1-\beta_+}}{2}}\right)\right.\\
&\left.+(1-i)K\left(\sqrt{\frac{1-\sqrt{1-\beta_+}}{2}}\right)\right],
\end{aligned}
\tag{A.15}
$$

then

$$
\begin{aligned}
G^0(L, L, E) = \frac{2}{\pi^2 E}&[(Z_+^2+1)(Z_-^2+1)]^{-1/4}(K(v_+)K(u_-)\\
&+K(v_-)K(u_+) + i(K(v_+)K(u_+) - K(v_-)K(u_-))),
\end{aligned}
\tag{A.16}
$$

where

$$
v_\pm^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{X_-^2}{X_-^2+1}}\right)
\tag{A.17}
$$

$$
u_\pm^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{X_+^2}{X_+^2+1}}\right)
\tag{A.18}
$$

If we have a single impurity then Green's function is defined as (Economou, 1983):

$$
G(L, L, E) = \frac{G^0(L, L, E)}{1 - \varepsilon' G^0(L, L, E)}
\tag{A.19}
$$

After some mathematical manipulation, Eq. (A.19) becomes.

$$\begin{aligned} G(L,L,E) = {} & \frac{\pi^2}{2}(E+1)[(Z_+^2+1)(Z_-^2+1)]^{1/4}[K(v_+)K(u_-)+K(v_-)K(u_+) \\ & + i(K(v_+)K(u_+)-K(v_-)K(u_-))] - 2\varepsilon'[K^2(v_+)+K^2(v_-)] \\ & \times [K^2(u_+)+K^2(u_-)] \Big/ \Big[\frac{\pi^2}{2}(E+1)((Z_+^2+1)(Z_-^2+1))^{1/4} \\ & - \varepsilon'(K(v_+)K(u_-)+K(v_-)K(u_+))\Big]^2 \\ & + \varepsilon^2[K(v_+)K(u_+)-K(v_-)K(u_-)]^2. \end{aligned} \tag{A.20}$$

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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