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Lattice Green's Function in the General Glasser Case

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We have investigated the lattice Green's function for the general Glasser cubic lattice. Expressions for its density of states, phase shift, and scattering cross section in terms of complete elliptic integrals of the first kind are derived.

KEY WORDS: general Glasser lattice; Green's function.

1. INTRODUCTION

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

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

where $E(\vec{k})$ represents a dispersion relation, $F(\vec{k})$ is an appropriate function, Ω denotes the volume of the crystal in the real space, d is the dimension, and 1BZ indicates that the integration is carried over the first Brillouin zone.

In this paper we report on the lattice Green's function and 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 cubic lattice in terms of the first kind elliptic integrals. This section also contains the formulae for the density of states (DOS), the phase shift, and the cross section for a point defect case. In Section 3 we present the results and discussion for the special Glasser case. Finally, the details of the Green's function derivation inside the band are given in Appendix A.

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2. LATTICE GREEN'S FUNCTION

The Green's function for the Glasser cubic lattice is defined as (Economou, 1983; Glasser, 1972; Glasser and Zucker, 1977; Hioe, 1978; Montaldi, 1981; Sakaji *et al.*, in press)

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

where,

$$E(k_x, k_y, k_z) = a_1 \operatorname{Cos}k_x(1 + \operatorname{Cos}k_y + \operatorname{Cos}k_z + \operatorname{Cos}k_x \operatorname{Cos}k_y) + a_2 \operatorname{Cos}k_y + a_3 \operatorname{Cos}k_z + a_{23} \operatorname{Cos}k_y \operatorname{Cos}k_z$$

The special case $a_1 = a_2 = a_3 = a_{23} = 1$, refers to the Glasser case studied by us elsewhere (Sakaji *et al.*, in press). Integrating the above equation and using the method of analytic continuation, the diagonal Green's function outside the band has the form (Rashid, 1980)

$$G^0(L, L; E) = \frac{4}{\pi^2 C} K(k_+)K(k_-), \quad E > 4a_1 + a_2 + a_3 + a_{23} \tag{2.2}$$

where $K(k_\pm)$ is the complete elliptic integral of the first kind and

$$k_\pm^2 = \frac{1}{2}\left[1 \pm \sqrt{A^2 - B^2} - \sqrt{(1 - A)^2 - B^2}\right] \tag{2.3}$$

$$C = \sqrt{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})}$$

$$A = \frac{4(Ea_{23} + a_2 a_3)}{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})} \tag{2.4}$$

$$B = \frac{4a_1(E + a_2 + a_3 - a_{23})}{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})}$$

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

$$G^0(L, l; E) = \begin{cases} \frac{4}{\pi^2 C} K(k_+)K(k_-), & E > 4a_1 + a_2 + a_3 + a_{23} \\ \frac{K(v_+)K(u_-) + K(v_-)K(u_+) + i[K(v_+)K(u_+) - K(v_-)K(u_-)]}{D}, & \\ -(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} & \end{cases} \tag{2.5}$$

where

$$y_\pm = -\sqrt{[B^2 - (1 - A)^2]} \pm \sqrt{B^2 - A^2} \tag{2.6}$$

$$v_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{y_-^2}{y_-^2+1}}\right) \tag{2.7}$$

$$u_{\pm}^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{y_+^2}{y_+^2+1}}\right) \tag{2.8}$$

$$D = \frac{\pi^2 C}{2[(y_+^2+1)(y_-^2+1)]^{-1/4}} \tag{2.9}$$

Therefore, the DOS is

$$\mathrm{DOS}^0(E) = \frac{[K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]}{\pi D}, \quad -(a_2 - a_3 - a_{23}) \times (a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} \tag{2.10}$$

We consider the case where perfect periodicity is destroyed by modifying just one site (the L site). The situation can be thought of physically as arising by substituting the host atom at the L site by a foreign atom (Economou, 1983; Rickayzen, 1980) i.e., a localized zero-range potential of strength ε' is introduced. In the tight-binding model, ε' is proportional to the charge difference between the impurity other electrons and those of the host atom.

Thus our Green's function for this single impurity is

$$G(L, L; E) = \left\{ \begin{array}{l} \frac{K(k_+)K(k_-)}{(\pi^2 C/4 - \varepsilon' K(k_+)K(k_-)}, \quad |E| > 4a_1 + a_2 + a_3 + a_{23} \\ \frac{D[K(\nu_+)K(u_-)+K(\nu_-)K(u_+)+i(K(\nu_+)K(u_+)-K(\nu_-)K(u_-))]-\varepsilon'[K^2(\nu_+)+K^2(\nu_-)][K^2(u_+)+K^2(u_-)]}{[D-\varepsilon'(K(\nu_+)K(u_-)+K(\nu_-)K(u_+))]^2+\varepsilon'^2[K(\nu_+)K(u_+)-K(\nu_-)K(u_-)]^2}, \\ -(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} \end{array} \right\} \tag{2.11}$$

The DOS can be written as

$$\mathrm{DOS}(E) = \frac{1}{\pi} \frac{D[K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]}{[D - \varepsilon'(K(\nu_+)K(u_-) + K(\nu_-)K(u_+))]^2 + \varepsilon'^2[K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]^2} \tag{2.12}$$

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

$$\tan\delta_0 = \frac{\pi \mathrm{DOS}^0(E)}{1/\varepsilon' - \mathrm{Re}\, G^0(E)} \tag{2.13}$$

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

$$\tan\delta_0 \frac{K(\nu_+)K(u_+) - K(\nu_-)K(u_-)}{D/\varepsilon' - [K(\nu_+)K(u_-) + K(\nu_-)K(u_+)]} \tag{2.14}$$

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

$$\sigma = \frac{4\pi}{P^2} \frac{\pi^2[\mathrm{DOS}^0(E)]^2}{\left[\mathrm{Re}\, G^0(E) - 1/\varepsilon^2\right] + \pi^2[\mathrm{DOS}^0(E)]^2} \tag{2.15}$$

Here, P refers to the electron momentum. Therefore, the cross-section becomes

$$\sigma = \frac{4\pi}{P^2} \frac{[K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]^2}{[K(\nu_+)K(u_-) + K(\nu_-)K(u_+) - D/\varepsilon']^2 + [K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]^2} \tag{2.16}$$

If a special cases of interest is considered (special Glasser case), when $a_1 = a_3 = a_{23} = 1$ and $a_2 = 0$ or $a_1 = a_2 = a_{23} = 1$ and $a_3 = 0$, then we obtain the diagonal Green's function outside the band as

$$G^0(L, L; E) = \frac{4}{\pi^2\sqrt{E(E+2)}} K^2(k), \quad E > 6 \tag{2.2′}$$

where

$$k^2 = \frac{1}{2}\left[1 - \sqrt{\frac{E-6}{E+2}}\right], \tag{2.3′}$$

$$A = \frac{4}{(E+2)}, \qquad B = \frac{4}{(E+2)}, \qquad C = \sqrt{E(E+2)} \tag{2.4′}$$

Green's function outside and inside the band can be written as (all mathematical Manipulations are given in the Appendix)

$$G^0(L, L; E) = \begin{cases} \frac{4}{\pi^2\sqrt{E(E+2)}} K^2(k), & E > 6 \\ \frac{1}{\pi^2\sqrt{2E}}(2K(\nu_+)K(\nu_-) + i[K^2(\nu_+) - K^2(\nu_-)]), & 0 < E < 6 \end{cases} \tag{2.5′}$$

where

$$y_\pm = -\sqrt{\frac{6-E}{E+2}} \tag{2.6′}$$

and

$$u_\pm = \nu_\pm = \frac{1}{2}\left(1 \pm \sqrt{\frac{6-E}{8}}\right) \tag{2.7′–2.8′}$$

and

$$D = \pi^2\sqrt{2E} \tag{2.9'}$$

Therefore, the DOS is

$$\mathrm{DOS}^0(E) = \frac{[K^2(u_+) - K^2(u_-)]}{\pi^3\sqrt{2E}} \tag{2.10'}$$

Thus our diagonal Greens function for the single impurity case can be written as

$$G(L, L; E) = \begin{cases} \dfrac{K^2(k)}{\pi^2\sqrt{E(E+2)}/4 - \varepsilon' K^2(k)}, & E > 6 \\ \dfrac{2K(u_+)K(u_-) - (\varepsilon'/\pi^2\sqrt{2E})[K^2(u_+) + K^2(u_-)]^2 + i[K^2(u_+) - K^2(u_-)]}{1/\pi^2\sqrt{2E}([\pi^2\sqrt{2E} - 2\varepsilon' K(u_+)K(u_-)]^2 + \varepsilon'^2[K^2(u_+) - K^2(u_-)]^2)} & \\ 0 < E < 6 \end{cases} \tag{2.11'}$$

and the DOS can be written as

$$\mathrm{DOS}(E) = \frac{[K^2(u_+) - K^2(u_-)]}{1/\pi^2\sqrt{2E}([\pi^2\sqrt{2E} - 2\varepsilon' K(u_+)K(u_-)]^2 + \varepsilon'^2[K^2(u_+) - K^2(u_-)]^2)} \tag{2.12'}$$

The S-wave phase shift δ_0 is

$$\tan\delta_0 = \frac{K^2(u_+) - K^2(u_-)}{\pi^2\sqrt{2E}/\varepsilon' - 2K(u_+)K(u_-)} \tag{2.13'}$$

The cross-section is

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

3. RESULTS AND DISCUSSION

The results for the special Glasser cubic lattice are shown in Figs. 1–8. Figure 1 shows the DOS for the special perfect Glasser lattice case. It diverges as E goes to zero and falls off exponentially as expected from eq. (2.10′). The real part of Green's function for the perfect lattice is displayed in Fig. 2. It has the same behavior as above. Figure 3 gives the DOS for the special Glasser lattice case with a single impurity potential strength ε' (-0.8, -0.2, 0.0, 0.2, and 0.8). For the perfect lattice case ($\varepsilon' = 0.00$ in arbitrary units) the DOS diverges as E goes to zero and falls off exponentially as expected. The peak value varies with the potential strength and reaches its maximum at $\varepsilon' = 0.2$; the divergence of the DOS is removed by adding such impurities. Figure 4 shows the DOS in three dimensions, with one axis representing the potential strength ε' varying between-1 and 1 (arbitrary units), whereas the second axis is the energy scale varying between 0 and 6 as indicated in the formalism.

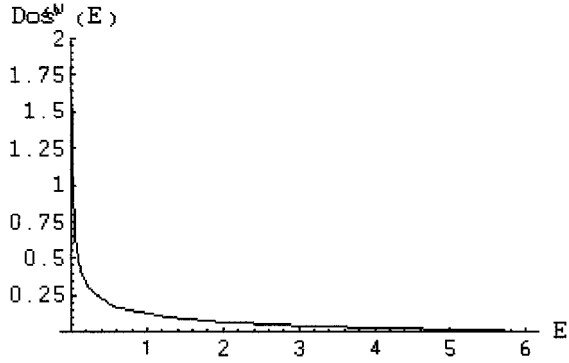

Fig. 1. The density of states (DOS) for the special perfect Glasser lattice case.

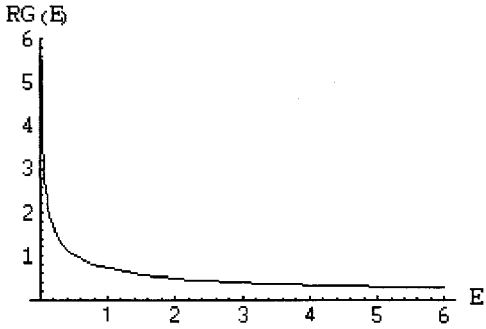

Fig. 2. Real part of Green's function for the special perfect Glasser lattice case.

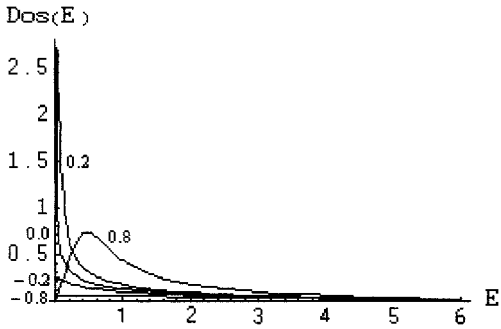

Fig. 3. The density of states (DOS) for the special Glasser lattice case with single impurity for different potential strengths ε' (-0.8, -0.2, 0.0, 0.2, and 0.8).

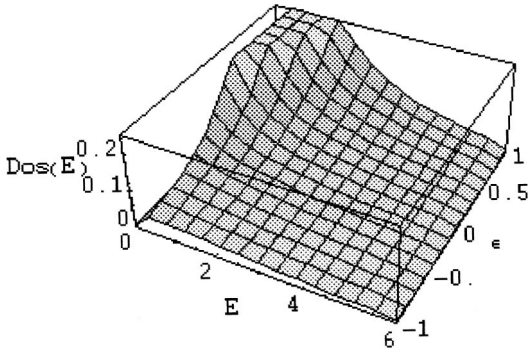

Fig. 4. Three-dimensional density of states (DOS) for the special Glasser lattice case with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

The phase shift δ_0 is defined as the shift in the phase of the wave function because of the presence of the impurity potential. Figure 5 displays δ_0 for the special Glasser lattice with single impurity for different potential strengths $\varepsilon'(-0.8, -0.2,$ 0.0, 0.2, and 0.8). For $\varepsilon' = 0.00$, δ_0 vanishes as 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'. In the range for ε' varying between 0.00 and 0.20, δ_0 is positive. For ε' varying between 0.2 and 1.0 we have a discontinuity occurring in the curve as shown in Fig. 5. The phase shift δ_0 is separated into two regions about 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. 6, the phase shift δ_0 for the special Glasser lattice with single impurity

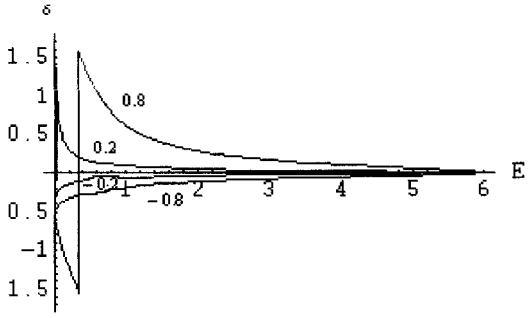

Fig. 5. The phase shift for the special Glasser lattice case with single impurity for different potential strengths ε' (-0.8, -0.2, 0.0, 0.2, and 0.8).

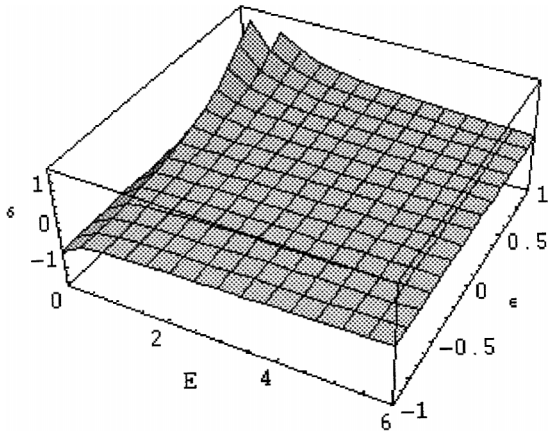

Fig. 6. The phase shift δ_0 for the special Glasser lattice case with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

is shown for potential strengths ε' varying between -1 and 1 (arbitrary units). The cross section σ can be defined as the area an impurity atom presents to the incident electron (total surface area of the sphere). Figure 7 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 value of one for all values of $\varepsilon' > 0.30$. The peak value increases in range between $0.14 < \varepsilon' < 0.19$ as ε' increases and decreases otherwise.

The values are all positive since σ can be viewed as a sort of probability. It is related to some physical quantities such as the resistivity in metals. Figure 8 shows the

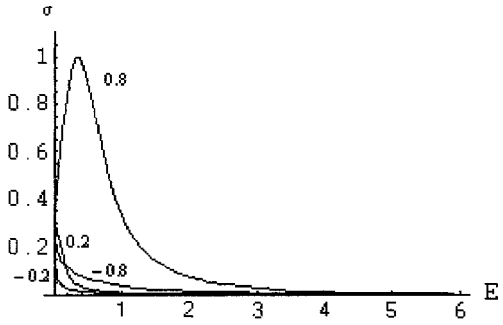

Fig. 7. The cross-section σ for the special Glasser lattice case with single impurity for different potential strengths ε' (-0.8, -0.2, 0.0, 0.2, and 0.8).

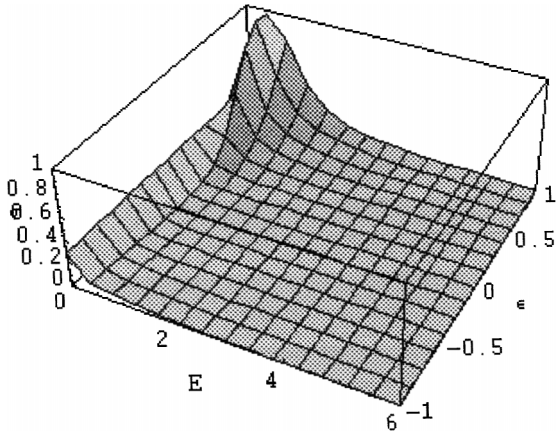

Fig. 8. The cross-section σ in three dimensions for the special Glasser lattice case with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

cross-section σ in three dimensions for the special Glasser lattice with single impurity for different potential strengths ε' varying between -1 and 1 (arbitrary units).

APPENDIX: DERIVATION OF GREEN'S FUNCTION FOR THE GENERAL GLASSER CUBIC 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 general Glasser lattice cubic lattice outside the band is given by (Rashid, 1980)

$$G^0(L, L; E) = \frac{4}{\pi^2 C} K(k_+) K(k_-), \quad E > 4a_1 + a_2 + a_3 + a_{23} \tag{A1}$$

where $K(k_\pm)$ is the complete elliptic integral of the first kind and

$$k_\pm^2 = \frac{1}{2}\left[1 \pm \sqrt{A^2 - B^2} - \sqrt{(1-A)^2 - B^2}\right] \tag{A2}$$

$$C = \sqrt{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})}$$

$$A = \frac{4(E a_{23} + a_2 a_3)}{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})} \tag{A3}$$

$$B = \frac{4a_1(E + a_2 + a_3 - a_{23})}{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})}$$

Or in the range E enclosed between $-(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23})$ and $4a_1 + a_2 + a_3 + a_{23}$

$$k_{\pm}^2 = \frac{1}{2}(1 + iy_{\mp}), \quad -(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} \tag{A4}$$

where

$$y_{\pm} = -\sqrt{[B^2 - (1 - A)^2]} \pm \sqrt{B^2 - A^2} \tag{A5}$$

The complete elliptic integral of the first kind is expressed as (Gradshteyn and Ryzhik, 1965)

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

where ${}_2F_1(1/2, 1/2; 1; k^2)$ is the Gauss hypergeometric function. Substituting (A6) in (A1) we have

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

Using the following transformations (Gradshteyn and Ryzhik, 1965; Bateman Manuscript Project, 1963)

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

with

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

$$\frac{2\Gamma(1/2)}{(\Gamma(3/4))^2}{}_2F_1\left(\frac{1}{4}, \frac{1}{4}; \frac{1}{2}; \frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}\right) = {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2}\left(1 + \sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}}\right)\right) + {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2}\left(1 - \sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}}\right)\right) \tag{A10}$$

$$\frac{2\Gamma(-1/2)}{(\Gamma(1/4))^2}\sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}}{}_2F_1\left(\frac{3}{4}, \frac{3}{4}; \frac{3}{2}; \frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}\right) = {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2} \times \left(1 - \sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}}\right)\right) - {}_2F_1\left(\frac{1}{2}, \frac{1}{2}; 1; \frac{1}{2}\left(1 + \sqrt{\frac{Z_{\mp}^2}{Z_{\mp}^2 - 1}}\right)\right) \tag{A11}$$

Substituting (A8)–(A11) in (A7) then we have

$$G^0(L, L; E) = \frac{(K(\nu_+)K(u_-) + K(\nu_-)K(u_+) + i(K(\nu_+)K(u_+) - K(\nu_-)K(u_-)))}{D},$$
$$-(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} \quad \text{(A12)}$$

where

$$\nu_\pm^2 = \frac{1}{2}\left(1 \pm \sqrt{\frac{Z_-^2}{Z_-^2 + 1}}\right) \quad \text{(A13)}$$

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

and

$$D = \frac{\pi^2\sqrt{(E - a_2 + a_3 + a_{23})(E + a_2 - a_3 + a_{23})}}{2\left[\left(y_+^2 + 1\right)\left(y_-^2 + 1\right)\right]^{-1/4}} \quad \text{(A15)}$$

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

$$G(L, L; E) = \frac{G^0(L, L; E)}{1 - \varepsilon' G^0(L, L; E)} \quad \text{(A16)}$$

After some mathematical manipulation Eq. (A16) becomes

$$G(L, L; E)$$
$$= \frac{D[K(\nu_+)K(u_-) + K(\nu_-)K(u_+) + i(K(\nu_+)K(u_+) - K(\nu_-)K(u_-))] - \varepsilon'[K^2(\nu_+) + K^2(\nu_-)][K^2(u_+) + K^2(u_-)]}{[D - \varepsilon'(K(\nu_+)K(u_-) + K(\nu_-)K(u_+))]^2 + \varepsilon'^2[K(\nu_+)K(u_+) - K(\nu_-)K(u_-)]^2},$$
$$-(a_2 - a_3 - a_{23})(a_3 - a_2 - a_{23}) < E < 4a_1 + a_2 + a_3 + a_{23} \quad \text{(A17)}$$

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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