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Remarks on the lattice Green's function: The Glasser case

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We have investigated the lattice Green's function for the 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. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1421063]

I. INTRODUCTION

The lattice Green's function is defined as

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

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 article is organized as follows. Section II 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 formulas for the density of states, the phase shift, and the cross section for a point defect case. In Sec. III we present the results and discussion. Finally, the details of the Green's function derivation inside the band are given in the Appendix.

II. LATTICE GREEN'S FUNCTION

The Green's function for the Glasser cubic lattice is defined as[1–5]

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

where

$$E(k_x,k_y,k_z)=\cos k_x+\cos k_y+\cos k_z+\cos k_x\cos k_y+\cos k_x\cos k_z$$
$$+\cos k_y\cos k_z+\cos k_x\cos k_y\cos k_z\,.$$

This case is of practical interest in studying the properties of a Heisenberg ferromagnet with axial anisotropy,[1,6]

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$$G^0(E)=\frac{4}{\pi^2(E+1)}K^2(k), \tag{2.2}$$

where

$$k^2=\frac{1}{2}\left[1-\frac{(E-7)^{1/2}}{(E+1)^{1/2}}\right], \tag{2.3}$$

and $K(k)$ is the complete elliptic integral of the first kind.

The Green's function inside and outside the band can be written as[7] (some mathematical manipulations are given in the appendix)

$$G^0(E)=\begin{cases}\dfrac{4}{\pi^2(E+1)}K^2(k), & |E|>7\\ \dfrac{\sqrt{2}}{\pi^2\sqrt{E+1}}K(k_+)K(k_-)+i\dfrac{1}{\sqrt{2}\pi^2\sqrt{E+1}}[K^2(k_+)-K^2(k_-)], & -1<E<7.\end{cases} \tag{2.4}$$

Therefore, the density of states is

$$\mathrm{DOS}^0(E)=\frac{1}{\sqrt{2}\pi^3\sqrt{E+1}}[K^2(k_+)-K^2(k_-)], \tag{2.5}$$

where

$$k_{\pm}^2=\tfrac{1}{2}(1\pm((7-E)/8)^{1/2}). \tag{2.6}$$

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,[8] 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 outer electrons and those of the host atom. Thus our Green's function for this single impurity is[7,9,10]

$$G(L,E)=\begin{cases}\dfrac{4K^2(k)}{(E+1)\pi^2-4\varepsilon' K^2(k)}, & |E|>7\\ \dfrac{2\sqrt{2}\pi^2(E+1)^{1/2}K(k_+)K(k_-)-2\varepsilon' K^2(k_+)K^2(k_-)-\varepsilon'[(K^4(k_+)+K^4(k_-))]+i\pi^2((E+1)2)^{1/2}[K^2(k_+)-K^2(k_-)]}{[\sqrt{2}\pi^2(E+1)^{1/2}-2\varepsilon' K(k_+)K(k_-)]^2+\varepsilon'^2[(K^2(k_+)-K^2(k_-))]^2}, & |E|<7\end{cases}. \tag{2.7}$$

The density of states can be written as[7,9,10]

$$\mathrm{DOS}^0(E)=\frac{\sqrt{2}\pi(E+1)^{1/2}[K^2(k_+)-K^2(k_-)]}{[\sqrt{2}\pi^2(E+1)^{1/2}-2\varepsilon' K(k_+)K(k_-)]^2+\varepsilon'^2[K^2(k_+)-K^2(k_-)]^2}. \tag{2.8}$$

The S-wave phase shift, δ_0, is defined as[7,9,10]

$$\tan\delta_0=\frac{\pi\mathrm{DOS}^0(E)}{\dfrac{1}{\varepsilon'}-\mathrm{Re}\,G^0(E)}. \tag{2.9}$$

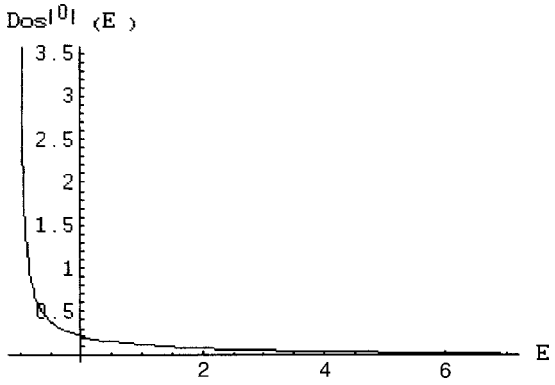

FIG. 1. The density of states (DOS) for the perfect Glasser lattice.

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

$$\tan \delta_0 = \frac{K^2(k_+) - K^2(k_-)}{\sqrt{2}(E+1)^{1/2}\pi^2/\varepsilon' - 2K(k_+)K(k_-)}. \tag{2.10}$$

The cross section, σ, is defined as[7,9,10]

$$\sigma = \frac{4\pi}{P^2} \frac{\pi^2[\mathrm{DOS}^0(E)]^2}{\left[\mathrm{Re}\, G^0(E) - \dfrac{1}{\varepsilon'}\right]^2 + \pi^2[\mathrm{DOS}^0(E)]^2}. \tag{2.11}$$

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

$$\sigma = \frac{4\pi}{P^2} \frac{(K^2(k_+) - K^2(k_-))^2}{2\pi^4\left(\dfrac{\sqrt{2}}{\pi^2}K(k_+)K(k_-) - \dfrac{\sqrt{E+1}}{\varepsilon'}\right)^2 + (K^2(k_+) - K^2(k_-))^2}. \tag{2.12}$$

III. RESULTS AND DISCUSSION

The results for the Glasser cubic lattice are shown in Figs. 1–8. Figure 1 shows the density of states for the perfect Glasser lattice. It diverges as E goes to minus one and falls off exponentially as expected from Eq. (2.5). The real and imaginary parts of Green's function for the perfect lattice are displayed in Fig. 2, they have the same behavior as noted previously. Figure 3 gives the density

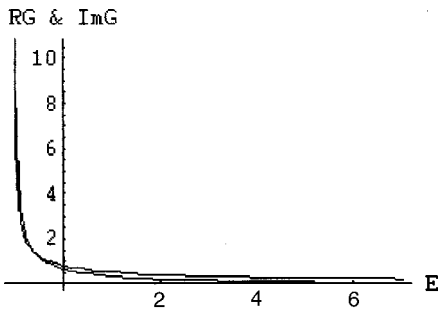

FIG. 2. Real and imaginary parts of Green's function for the perfect Glasser lattice.

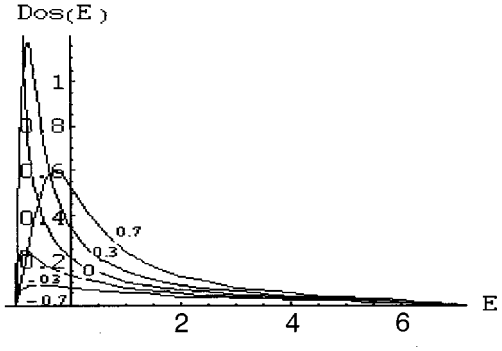

FIG. 3. The DOS for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

of states for the Glasser lattice with a single impurity potential with strength ε' (-0.7, -0.3, 0.0, 0.3, and 0.7). For $\varepsilon'=0.0$ and 0.3 (in arbitrary units), the density of states diverges as E goes to minus one (as previously) and falls off exponentially. The peak value varies with the potential strength and reaches its maximum at $\varepsilon'=0.7$. Figure 4 shows the density of states (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 -1 and 7 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 5 displays δ_0 for the Glasser lattice with single impurity for different potential strengths ε'. If an attractive potential is turned on, then it gives rise to a positive phase shift and vice versa. That is, a point defect just to the left of the host in the periodic table leads to positive δ_0. The curves are mirror images of each other. The phase shift vanishes as the potential is turned off (perfect lattice); this behavior is clear from the definition of δ_0. In Fig. 6 we have a more general case of the phase shift, δ_0, for the Glasser lattice with single impurity 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. It is related to some physical quantities such as the conductivity in metals. Figure 7 shows the cross section, σ, for the Glasser lattice with single impurity for different potential strengths ε'. The values are all positive since σ can be viewed as a sort of probability. The cross

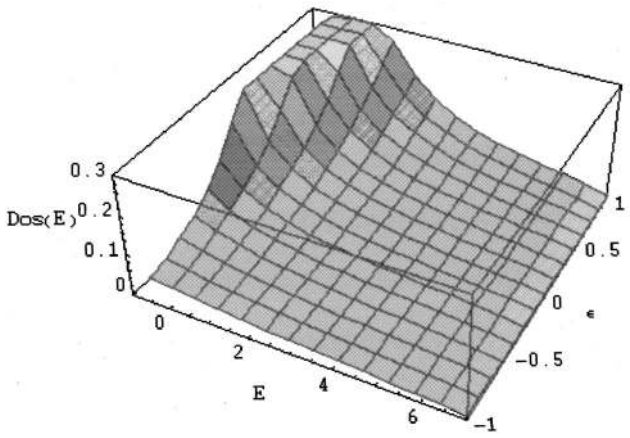

FIG. 4. Three-dimensional DOS for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

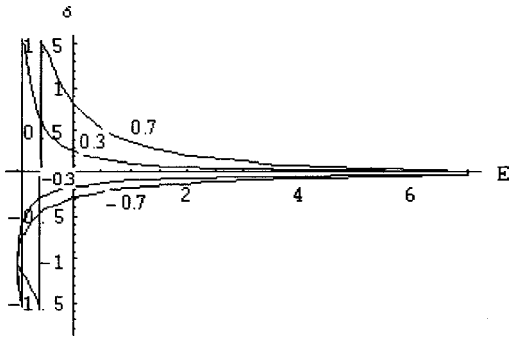

FIG. 5. The phase shift for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

section vanishes for a perfect lattice as expected. Figure 8 displays the cross section, σ, in three dimensions for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

APPENDIX: DERIVATION OF GREEN'S FUNCTION FOR THE GLASSER LATTICE

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 Glasser lattice outside the band is given by[3,4,7]

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

where

$$k=\sqrt{\frac{1}{2}[1-\sqrt{1-\beta^{-1}}]}, \quad \beta=\frac{E+1}{8}<1.$$

The complete elliptic integral of the first kind is expressed as

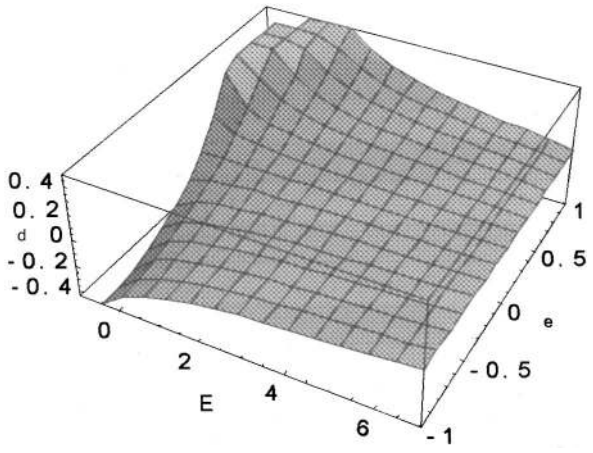

FIG. 6. The phase shift, δ_0, for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

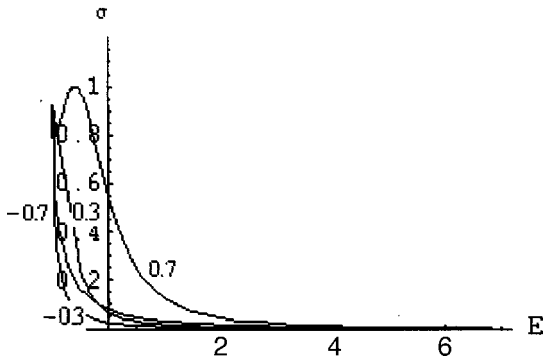

FIG. 7. The cross section, σ, for the Glasser lattice with single impurity for different potential strengths ε' (-0.7, -0.3, 0.0, 0.3, and 0.7).

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

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

Kummer's identity is[11]

$${}_2F_1(\tfrac{1}{4},\tfrac{1}{4};1;\beta^{-1})={}_2F_1(\tfrac{1}{2},\tfrac{1}{2};1;\tfrac{1}{2}(1-\sqrt{1-\beta^{-1}})). \tag{A3}$$

Substituting (A3) in (A1) we have

$$G^0(E)=\frac{({}_2F_1(\frac{1}{4},\frac{1}{4};1;\beta^{-1}))^2}{(E+1)}. \tag{A4}$$

Using the following transformations:[12]

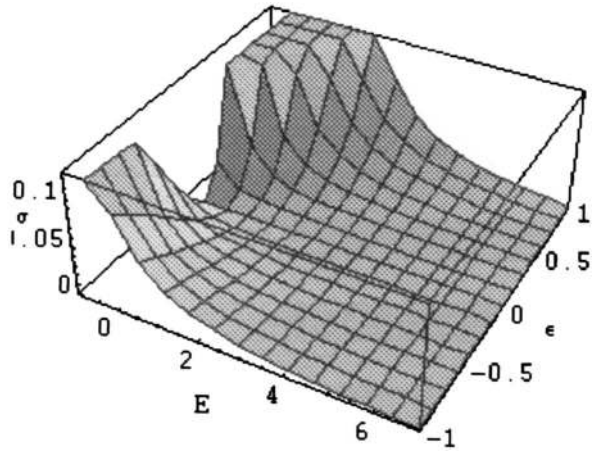

FIG. 8. The cross section, σ, in three dimensions for the Glasser lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units).

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\beta^{1/4}\left(\frac{(\Gamma(\frac{1}{4}))^2}{2\pi^{3/2}}{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta\right)+2\pi^{1/2}\frac{\sqrt{\beta-1}}{(\Gamma(\frac{1}{4}))^2}{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta\right)\right), \tag{A5} $$

with

$$ \frac{(\Gamma(\frac{1}{4}))^2}{\pi^{3/2}}{}_2F_1\left(\frac{1}{4},\frac{1}{4};\frac{1}{2};1-\beta\right)={}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right)+{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right), \tag{A6} $$

and

$$ \frac{4\pi^{1/2}\sqrt{1-\beta}}{(\Gamma(\frac{1}{4}))^2}{}_2F_1\left(\frac{3}{4},\frac{3}{4};\frac{3}{2};1-\beta\right)={}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right) $$
$$ -{}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right), \tag{A7} $$

in (A5) we obtain

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\frac{\beta^{1/4}}{2}\left((1+i){}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1+\sqrt{1-\beta})\right)\right. $$
$$ \left.+(1-i){}_2F_1\left(\frac{1}{2},\frac{1}{2};1;\frac{1}{2}(1-\sqrt{1-\beta})\right)\right), \tag{A8} $$

or in terms of complete elliptic integral of the first kind

$$ {}_2F_1\left(\frac{1}{4},\frac{1}{4};1;\beta^{-1}\right)=\frac{\beta^{1/4}}{\pi}((1+i)K(k_+)+(1-i)K(k_-)), \tag{A9} $$

where

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

Substituting (A9), in (A4) then we obtain

$$ G^0(E)=\frac{\beta^{1/2}}{\pi^2(E+1)}((1+i)K(k_+)+(1-i)K(k_-))^2, \tag{A10} $$

then

$$ G^0(E)=\frac{1}{\sqrt{2}\pi^2\sqrt{E+1}}(2K(k_+)K(k_-)+i(K^2(k_+)-K^2(k_-))). \tag{A11} $$

If a single impurity characterized by a localized potential is introduced in the perfect lattice, then according to Dyson's equation Green's function is defined as[8]

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

After some mathematical manipulation Eq. (A12) becomes.

$$G(L,E)$$

$$= \frac{2\pi^2\sqrt{2(E+1)}K(k_+)K(k_-) - 2\varepsilon' K^2(k_+)K^2(k_-) + i\pi^2\sqrt{2(E+1)}(K^2(k_+) - K^2(k_-)) - \varepsilon'[K^4(k_+) + K^4(k_-)]}{(\pi^2\sqrt{2(E+1)} - 2\varepsilon' K(k_+)K(k_-))^2 + \varepsilon'^2(K^2(k_+) - K^2(k_-))^2}. \tag{A13}$$

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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