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Applications of the lattice Green's Functions for Triangular Lattice

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Abstract: An expression for the Green's Function for triangular lattice is evaluated analytically and numerically for single impurity lattices of zero range potential. Also the S-phase shift, and scattering cross section are expressed in terms of complete elliptic integrals.

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1. Introduction

Lattice Green's function plays an important role in many areas of mathematics and physics, for example Random Walks (Polya walks)[2-5], statistical model of ferromagnetism such as Ising model [6], Heisenberg model [7], spherical model [8], lattice dynamics [1,9,10], disordered system such as anistropic systems for localization [11] , Andersion localization in anisotropic systems, such are high T_c superconductors of anistropic [11,12], and recently on perturbation of infinite networks of resistors [17].

The theoretical studies of lattice vibrations of graphite need the LGF. For the graphite structure. In that structure, the distance between layers is greater than the distance between the nearest atoms in the same layer, then the LGF for honeycomb lattice is needed for the studies on the lattice vibration of the graphite. And the honeycomb lattice Green's function can be written in terms of triangular lattice Green's function[13,16,18].

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The Hamiltonian of the problem can be written as:

$$H = H_0 + H_1 \tag{1}$$

Where H_0 is the unperturbed part (perfect lattice), we restrict our attention to a system which can be described with a tight-binding Hamiltonian with

$$H_0 = \sum_n |n\rangle \, \varepsilon_0 \, \langle n| + \sum_{n,m} t_{nm} \, |n\rangle \, \langle m| \tag{2}$$

where the sites {n} form a regular lattice. The off-diagonal matrix elements $t_{nm} \neq 0$ only for nearest neighbor sites [13] , and H_1 is the perturbation arising from the substitutional impurity .

$$H_1 = |l\rangle \, \varepsilon' \, \langle l| \tag{3}$$

Now Green's function can be expressed as (Dyson Equation) [4]

$$G(m,n;\varepsilon) = G_0(m,n;\varepsilon) + \varepsilon' \frac{G_(m,l;\varepsilon) G_0(l,n;\varepsilon)}{1 - \varepsilon' G(l,n;\varepsilon)} \tag{4}$$

where G_0 is unperturbed part and G is the total Green's function so that, the density of states $n(\varepsilon)$ is defined as [13].

$$n(\varepsilon) = (-1/\pi) Im G(l,l;\varepsilon) \tag{5}$$

The scattering of a single particle from a potential V(x) is described by S-wave shift as [16, 20]

$$\tan(\delta_0) = \frac{\pi n_0(\varepsilon)}{\frac{1}{\varepsilon} - G_0^{Re}(l,l;\varepsilon)} \tag{6}$$

where G_0^{Re} is the real part of the Green's function, and the cross section σ is [16]

$$\sigma = \frac{4\pi}{p^2} \left[\frac{\pi^2 n_0(\varepsilon)}{\frac{1}{\varepsilon'} - \{G_0^{Re}(l,l;\varepsilon)^2 + \pi^2 n_0^2(\varepsilon)} \right] \tag{7}$$

For certain special cases Lattice Green's Function (LGF) has the form:

$$G(E) = \frac{\Omega}{(2\pi)^d} \int\limits_{1BZ} \frac{F(\vec{k})}{E - E(\vec{k})} d\vec{k} \tag{8}$$

where E(k) represents a dispersion relation, F(k) ia an appropriate function, Ω denotes the volume of the first Brillouin zone . The above Green's Function is called scalar Green's Function (SGF),[5,13,19,21].

2. Green's Function for Triangular Lattice.

The Green's function for Triangular lattice with nearest neighbors interaction has the form [13,16,18].

$$G^0(l,m;E) = \frac{1}{\pi^2}\int_0^\pi \int_0^\pi \frac{Cos(my)Cos(lx)}{E-(Cos(2x)+2Cos(y)Cos(x))}dxdy \tag{9}$$

the value of the Green's function G^0(l,m;E) Eq. (9) at an arbitrary lattice site is calculated by using some recurrence formulas if the values of G^0(0,0;E) , G^0(2,0;E) and G^0(4,0;E) are known [16].

After Solving this integral, and using the analytic continuation , the pure Green's function at the origin is :

$$G^0(0,0;E) = \begin{cases} \frac{1}{2\pi}aK(k) \;\; for\; ImE \succ 0 \; and \, Imk \prec 0 \\ or \quad ImE \prec 0 \; and \, Imk \succ 0 \\ \frac{1}{2\pi}a(K(k)+2iK(\sqrt{1-k^2})) \;\; for\; ImE \succ 0 \; and \, Imk \succ 0 \\ \frac{1}{2\pi}a(K(k)-2iK(\sqrt{1-k^2})) \;\; for\; ImE \prec 0 \; and \, Imk \prec 0 \end{cases} \tag{10}$$

Where

$a = \frac{8}{(\sqrt{2E+3}-1)^{(\frac{3}{2})}(\sqrt{2E+3}+3)^{(\frac{1}{2})}}$

and

$k = \frac{4(2E+3)^{(\frac{1}{4})}}{(\sqrt{2E+3}-1)^{(\frac{3}{2})}(\sqrt{2E+3}+3)^{(\frac{1}{2})}}$

So that the density of states has the form:

$$DOS^0(E) = \begin{cases} \frac{1}{\pi^2}a(K(\sqrt{1-k^2})) \;\; for\; ImE \succ 0 \; and \, Imk \succ 0 \\ \frac{1}{\pi^2}a(-K(\sqrt{1-k^2})) \;\; for\; ImE \prec 0 \; and \, Imk \prec 0 \end{cases} \tag{11}$$

Solving Dyson equation (4) for a single substitutional impurity with a potential strength V, at site l, the defect Green's function for the Triangular lattice is:

$$G(0,0;E) = \begin{cases} \frac{\frac{1}{2\pi}aK(k)}{1-V\frac{1}{2\pi}aK(k)} \;\; for\; ImE \succ 0 \; and \, Imk \prec 0 \\ or \quad ImE \prec 0 \; and \, Imk \succ 0 \\ \frac{\frac{1}{2\pi}a(K(k)+2iK(\sqrt{1-k^2}))}{1-V\frac{1}{2\pi}a(K(k)+2iK(\sqrt{1-k^2}))} \;\; for\; ImE \succ 0 \; and \, Imk \succ 0 \\ \frac{\frac{1}{2\pi}a(K(k)-2iK(\sqrt{1-k^2}))}{1-V\frac{1}{2\pi}a(K(k)-2iK(\sqrt{1-k^2}))} \;\; for\; ImE \prec 0 \; and \, Imk \prec 0 \end{cases} \tag{12}$$

And the density of states is

$$DOS(E) = \frac{1}{\pi} \begin{cases} \frac{1}{2\pi} aK(k) \frac{\frac{1}{2\pi} aK(k) - V \frac{1}{2\pi} aK(k)}{(1 - V \frac{1}{2\pi} aK(k))^2} & for\ ImE \succ 0\ and\ Imk \prec 0 \\ or \quad ImE \prec 0\ and\ Imk \succ 0 & \\ \frac{\frac{1}{2\pi} aK(k) - V(\frac{1}{2\pi} aK(k) + 2K(\sqrt{1-k^2}))}{(1 - V \frac{1}{2\pi} aK(k))^2 + V(2K(\sqrt{1-k^2})))^2} & for\ ImE \succ 0\ and\ Imk \succ 0 \\ \frac{\frac{1}{2\pi} aK(k) - V(\frac{1}{2\pi} aK(k) - 2K(\sqrt{1-k^2}))}{(1 - V \frac{1}{2\pi} aK(k))^2 + V(2K(\sqrt{1-k^2})))^2} & for\ ImE \prec 0\ and\ Imk \prec 0 \end{cases} \tag{13}$$

If we have a potential strength V of zero range (localized potential) the S-wave shift (which defined as the shift in the phase of the wave function due to the presence of the impurity potential)can be written as :

$$\tan(\delta_o) = \begin{cases} \frac{2K(\sqrt{1-k^2})}{1/V - \frac{1}{2\pi} a(K(k)} & for\ ImE \succ 0\ and\ Imk \succ 0 \\ \frac{-2K(\sqrt{1-k^2})}{1/V - \frac{1}{2\pi} a(K(k)} & for\ ImE \prec 0\ and\ Imk \prec 0 \end{cases} \tag{14}$$

The cross section σ, is defined as the area in impurity atom presents to the incident electron, it is related to some physical quantities such as conductivity in metals, using Eq. (7) one can write ,the cross section σ as:

$$\sigma = \frac{4\pi}{p^2} \left(\frac{2\pi K(\sqrt{1-k^2})}{1/V - (\frac{1}{2\pi} a(K(k))^2 + \pi^2 (2K(\sqrt{1-k^2}))^2} \right) \tag{15}$$

3. Results

The results for lattice Green's function for triangular lattice are shown in figures (1-9), these figures shows the real (RG) and imaginary (IG) parts of the Green's functions for pure and defect lattices with different potential strength , density of states, phase shift, and the cross section as a function of energy and potential strength. The singularities (logarithmic singularities) are found at the singular points which are determined by the critical points $\frac{\partial E}{\partial \vec{k}} = 0$, the Van Hove singularities of the density of states are shown in figure(3). Figure(1) shows the real part of LGF for a perfect triangular lattice, figure(2) shows the imaginary part of LGF for a perfect triangular lattice, figure(3) shows the density of states of LGF for a perfect triangular lattice, figure (4) shows the density of states of LGF for a perturbed triangular lattice with potential strength v=0.1 at arbitrary units , figure (5) shows the scattering cross section of LGF for perturbed triangular lattice with potential strength v=0.1 at arbitrary unit, figure(6) shows the phase shift of LGF for a perturbed triangular lattice with potential strength v=0.1 at arbitrary unit ,and figures(7-9) show three dimensional graphs of density of states, scattering cross section and the phase shift for the perturbed triangular lattice respectively.

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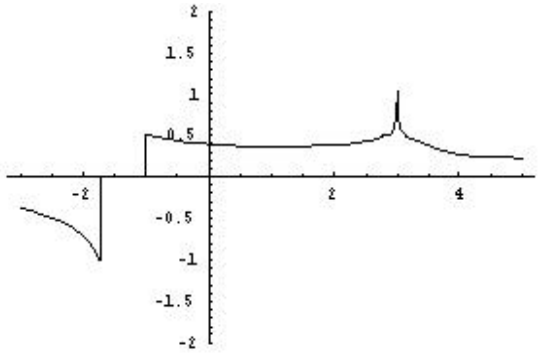

Fig. 1 Real Part of LGF for perfect Triangular Lattice

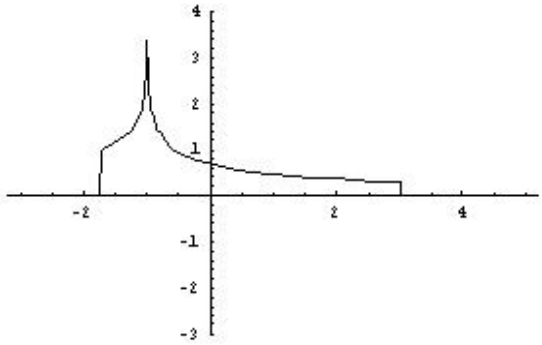

Fig. 2 Imaginary Part of LGF for perfect Triangular Lattice

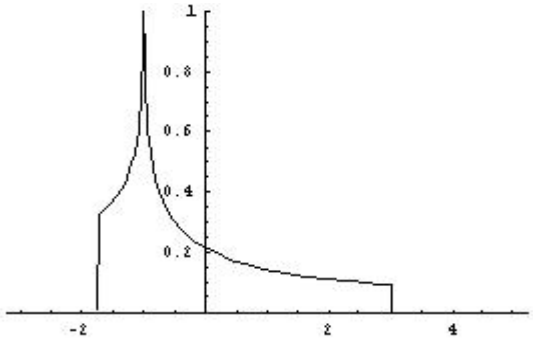

Fig. 3 Density of Statesof LGF for perfect Triangular Lattice

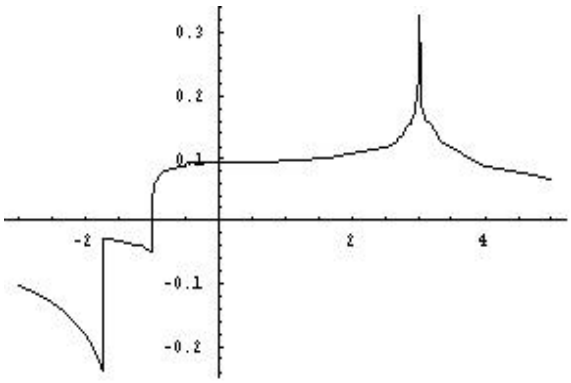

Fig. 4 Density of States of LGF for Perturbed Triangular Lattice with potential strength v=0.1 (arbitrary unit)

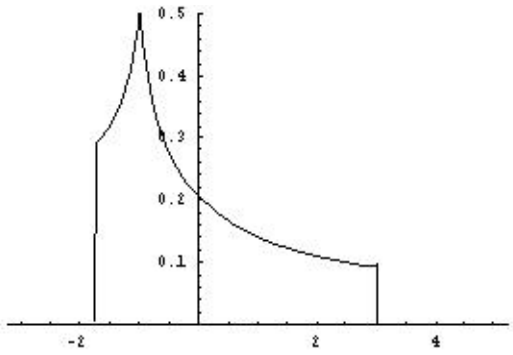

Fig. 5 Scattering Cross Section of LGF for Perturbed Triangular Lattice with potential strength v=0.1 (arbitrary unit)

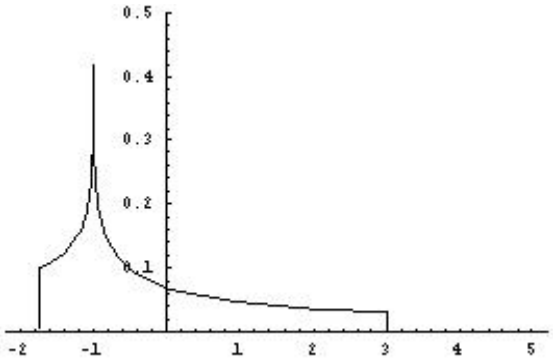

Fig. 6 Phase Shift of LGF for Perturbed Triangular Lattice with potential strength v=0.1 (arbitrary unit)

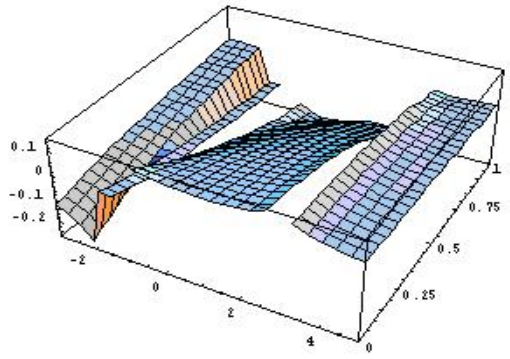

Fig. 7 Density of States of LGF for Perturbed Triangular Lattice

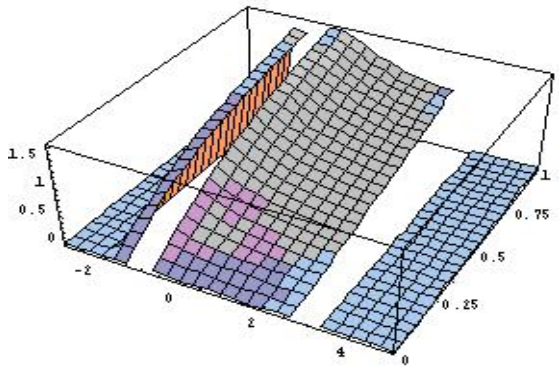

Fig. 8 Scattering Cross Section of LGF for Perturbed Triangular Lattice

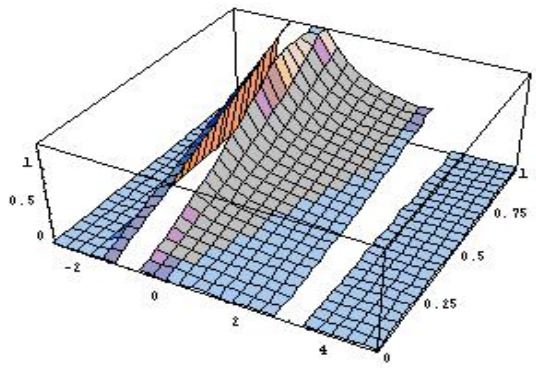

Fig. 9 Phase shift of LGF for Perturbed Triangular Lattice