

Applications of the lattice Green's Functions for One and Two Dimensional Lattices

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Abstract:

An expression for the Green's Function for one and two-dimensional lattices is evaluated analytically and analytically for a single impurity lattices of zero range potential. Also the S-phase shift, and scattering cross section are expressed in terms of Chebyshev polynomials and elliptic integrals.

1- Introduction

Lattice Green's function play 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 [9,10], disordered system such as anistropic systems for localization [11] , Anderson 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 Hamiltonian of the problem can be written as:

$$H=H_0+H_1 \quad 1.1$$

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

$$H_0 = \sum_n |n\rangle \varepsilon_0 \langle n| + \sum_{n,m} t_{nm} |n\rangle \langle m| \quad 1.2$$

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.

$$H_1 = |l\rangle \varepsilon' \langle l| \quad 1.3$$

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

$$G(m, n; \varepsilon) = G_0(m, n; \varepsilon) + \varepsilon' \frac{G(m, l; \varepsilon) G_0(l, n; \varepsilon)}{1 - \varepsilon' G(l, n; \varepsilon)} \quad 1.4$$

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].

$$n(\varepsilon) = (-1/\pi) \text{Im } G(l, l; \varepsilon) \quad 1.5$$

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

$$\tan(\delta_0) = \frac{\pi n_0(\varepsilon)}{\frac{1}{\varepsilon} - G_0^{\text{Re}}(l, l; \varepsilon)} \quad 1.6$$

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

$$\sigma = \frac{4\pi}{p^2} \left[\frac{\pi^2 n_0(\varepsilon)}{\frac{1}{\varepsilon'} - \{G_0^{\text{Re}}(l, l; \varepsilon)\}^2 + \pi^2 n_0^2(\varepsilon)} \right] \quad 1.7$$

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

$$G(E) = \frac{\Omega}{(2\pi)^d} \int_{1BZ} \frac{F(\vec{k})}{E - E(\vec{k})} d\vec{k} \quad 1.8$$

where $E(k)$ represents a dispersion relation, $F(k)$ is 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].

2- Green's Function for One Dimensional Lattice.

2.1 Periodic Boundary Conditions

The Green's function for one-dimensional lattice with nearest neighbors interaction can be written as [4]:

$$G^0(l, m; z) = \frac{a}{2\pi} \int_{-\frac{\pi}{a}}^{\frac{\pi}{a}} \frac{e^{ika(l-m)}}{z - \varepsilon_0 - 2V \cos(ka)} dk \quad 2.1.1$$

or

$$G^0(l, m; E) = \frac{1}{\pi} \int_0^\pi \frac{\cos(n\varphi)}{E_0 - \cos(\varphi)} d\varphi \quad 2.1.2$$

where G^0 is Green's function for pure lattice, a is the lattice constant; hence $\varphi = ka$, $n = l - m$, with $B = 2V$ where V is the potential strength and

$E = \frac{z - \varepsilon_0}{B}$ which is called the reduce energy.

Using the method of complex variable and the properties of Chebyshev polynomials [20], we can write Green's function inside and outside the band as :

$$G^0(l, m; E) = \left\{ \begin{array}{ll} \frac{U_{|l-m|}(E) + iT_{|l-m|}(E)}{\sqrt{1-E^2}} & |E| < 1 \\ \frac{[E - \sqrt{E^2 - 1}]^{|l-m|}}{\sqrt{E^2 - 1}} & |E| > 1 \end{array} \right\} \quad 2.1.3$$

So that the density of states of the unperturbed system has the form:

$$DOS^0(E) = \frac{1}{\pi} \left\{ \begin{array}{ll} \frac{1}{\sqrt{1-E^2}} & |E| < 1 \\ 0 & |E| > 1 \end{array} \right\} \quad 2.1.4$$

For a single substitutional impurity atom at site l and energy ε' [13], using equation (1.4) and after some mathematical manipulation the single impurity Green's function can be written as:

$$G(l, l; E) = \left\{ \begin{array}{ll} \frac{1}{\sqrt{E^2 - 1} - \varepsilon'} & |E| > 1 \\ \frac{-\varepsilon' + i\sqrt{1-E^2}}{1-E^2 + \varepsilon'} & |E| < 1 \end{array} \right\} \quad 2.1.5$$

Therefore, the local density of states of the perturbed system , at site l has the form:

$$DOS(E) = \frac{\sqrt{1-E^2}}{\pi(1-E^2 - \varepsilon')} \quad 2.1.6$$

And the S-wave shift is:

$$\tan(\delta_0) = \frac{\varepsilon'}{\sqrt{1-E^2}} \quad 2.1.7$$

Where ε' is a constant (depends on the strength of the potential of the impurity), localized potential.

Using eq.(1.7) the cross section can be evaluated as:

$$\sigma = \frac{4\pi}{p^2} \frac{\pi\varepsilon'(1-E^2)}{\sqrt{1-E^2}(1-E^2+\varepsilon')} \quad 2.1.8$$

2.2- Both Ends Clamped

The Green's function for N atoms chain with clamped ends is [21,22]:

$$G^0(n, m; z) = \{T_{n-m}(z) - T_{n+m}(z)\} \frac{T_{N+1}(z)}{(z^2 - 1)U_N(z)} - U_{|n-m|-1}(z) + U_{n+m-1}(z) \quad 2.2.1$$

Using Dyson equation eq. (1.4) and after some mathematical manipulations the single impurity Green's function at site l can be written:

$$G(l, l; z) = \frac{(1 - T_{|2l|}(z)) \frac{T_{N+1}(z)}{(z^2 - 1)U_N(N)} + U_{2l-1}}{1 - \varepsilon'((1 - T_{|2l|}(z)) \frac{T_{N+1}(z)}{(z^2 - 1)U_N(N)} + U_{2l-1})} \quad 2.2.2$$

2.3 Both Ends Free

The boundary conditions when both ends are free are designed to ensure that the force on each end of the chain is zero, so that we find the Green's function to be [21,22]

$$G^0(n, m; z) = \{T_{n-m}(z) + T_{n+m}(z)\} \frac{T_{N+1}(z)}{(z^2 - 1)U_{N-1}(z)} - U_{|n-m|-1}(z) - U_{n+m-1}(z) \quad 2.3.1$$

Using eq.(1.4) the single impurity Green's function at site l is:

$$G(l, l; z) = \frac{(1 + T_{|2l|}(z)) \frac{T_{N+1}(z)}{(z^2 - 1)U_{N-1}(N)} + U_{2l-1}}{1 - \varepsilon' \left((1 + T_{|2l|}(z)) \frac{T_{N+1}(z)}{(z^2 - 1)U_{N-1}(N)} + U_{2l-1} \right)} \quad 2.3.2$$

3- Green's Function for Two Dimensional Lattice.

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

$$G^0(m, n; E) = \frac{1}{\pi^2} \int_0^\pi \int_0^\pi \frac{\cos(my)\cos(nx)}{E - (\cos(x) + \cos(y))} dx dy \quad 3.1$$

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

$$G^0(0,0;E) = \left\{ \begin{array}{ll} \frac{2}{\pi E} K\left(\frac{2}{E}\right) & |E| < 2 \\ \left(\frac{2}{\pi}\right) (\varepsilon(\chi) K\left(\frac{E}{2}\right) + iK\left(\sqrt{1-\frac{E^2}{4}}\right)) & |E| > 2 \end{array} \right\} \quad 3.2$$

Where

$$\varepsilon(\chi) = \left\{ \begin{array}{ll} 1 & E > 0 \\ -1 & E < 0 \end{array} \right\}$$

and the density of states is:

$$DOS^0(E) = \frac{2}{\pi^2} K\left(\sqrt{1-\frac{E^2}{4}}\right) \quad 3.3$$

Solving Dyson equation (1.4) for a single substitutional impurity, at site 1, the defect Green's function for the square lattice is:

$$G(0,0;E) = \left\{ \begin{array}{ll} \frac{2K\left(\frac{2}{E}\right)}{\pi E - 2\varepsilon' K\left(\frac{2}{E}\right)} & |E| > 2 \\ \frac{\frac{\pi}{2} \varepsilon(\chi) K\left(\frac{E}{2}\right) - \varepsilon \left(K^2\left(\frac{E}{2}\right) + K^2\left(\sqrt{1-\frac{E^2}{4}}\right) \right) + i\frac{\pi}{2} K\left(\sqrt{1-\frac{E^2}{4}}\right)}{\left(\frac{\pi}{2} - \varepsilon' K\left(\frac{E}{2}\right)\right)^2 + \varepsilon'^2 K^2\left(\sqrt{1-\frac{E^2}{4}}\right)} & |E| < 2 \end{array} \right\} \quad 3.4$$

And the density of states is

$$DOS(E) = \frac{\frac{1}{2}K(\sqrt{1-\frac{E^2}{4}})}{\left(\frac{\pi}{2} - \varepsilon'K\left(\frac{E}{2}\right)\right)^2 + \varepsilon'^2 K^2(\sqrt{1-\frac{E^2}{4}})} \quad 3.5$$

If we have a potential of zero range (localized potential) the S-wave shift can be written as :

$$\tan(\delta_0) = \frac{2K(\sqrt{1-\frac{E^2}{4}})}{\frac{\pi}{\varepsilon'} - 2\varepsilon(\chi)K\left(\frac{E}{2}\right)} \quad 3.6$$

using eq.(1.7) we can write the cross section as:

$$\sigma = \frac{4\pi}{p^2} \frac{2\pi^3 K(\sqrt{1-\frac{E^2}{4}})}{-4K^2\left(\frac{E}{2}\right) + \frac{\pi^2}{\varepsilon'} + 4\pi^2 K^2(\sqrt{1-\frac{E^2}{4}})} \quad 3.7$$

4- Results:

The results for lattice Green's function for one and two dimensional lattices are shown in figures (1-12), 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. [20].

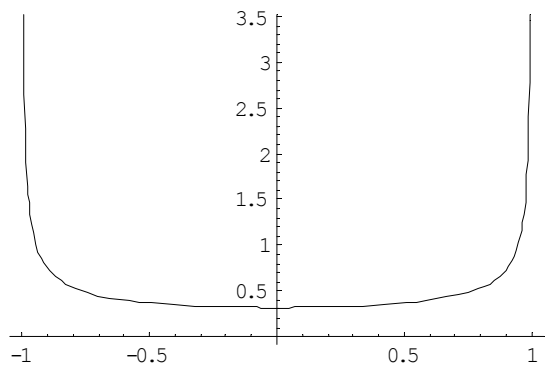


Fig.1 The density of states DOS for the 1D lattice

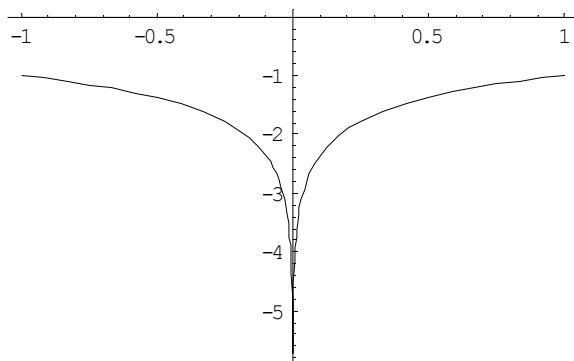


Fig.2 Real and imaginary parts of Green's function for the 1D lattice

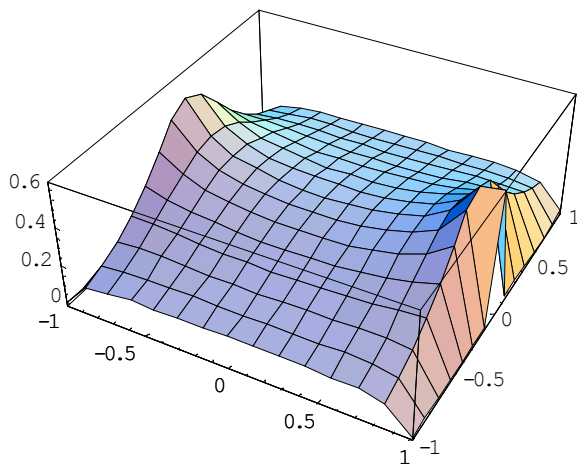


Fig.3 Three dimensional DOS for the 1D lattice with single impurity for potential strengths ε' varying between -1 and 1 (arbitrary units)

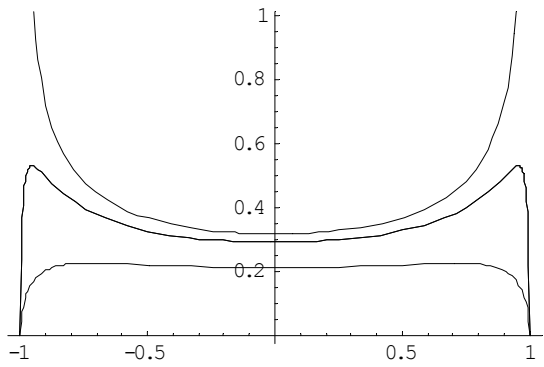


Fig.4 The DOS for the 1D lattice with single impurity for different potential strengths ϵ' (-0.7,-0.3,0.0,0.3,0.7)

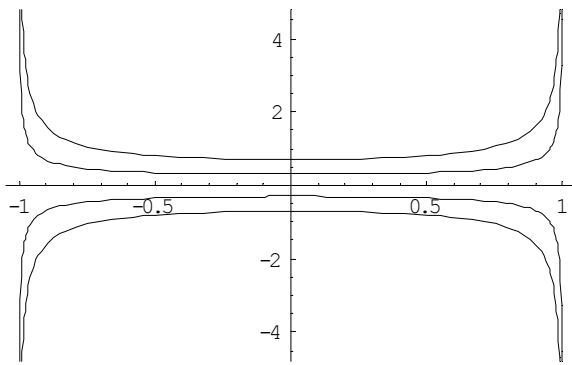


Fig.5 The phase shift for the 1D lattice with single impurity for different potential strengths ϵ' (-0.7,-0.3,0.0,0.3,0.7)

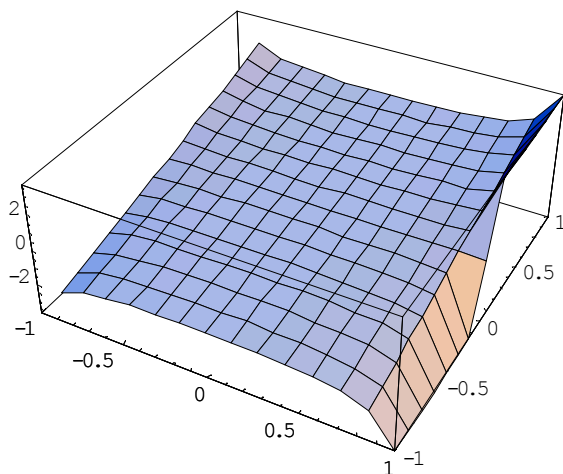


Fig.6 The phase shift for the 1D lattice with single impurity strengths ϵ' varying between -1 and 1 (arbitrary units)

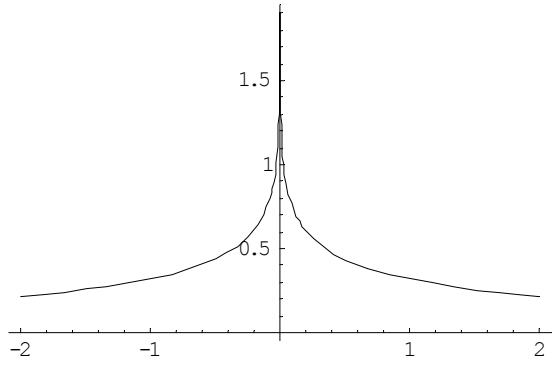


Fig.7 The density of states DOS for the 2D lattice

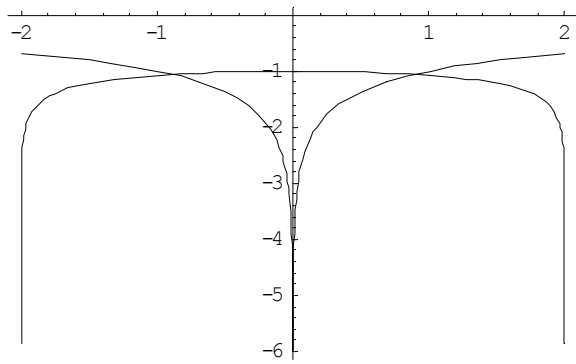


Fig.8 Real and imaginary parts of Green's function for the 2D lattice

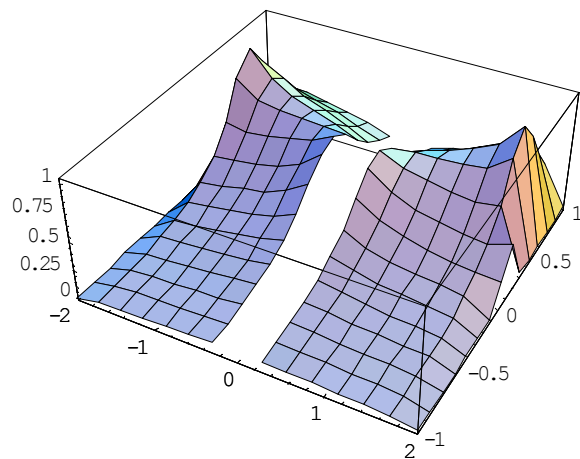


Fig.9 Three dimensional DOS for the 2D lattice with single impurity for potential strengths ϵ' varying between -1 and 1 (arbitrary units)

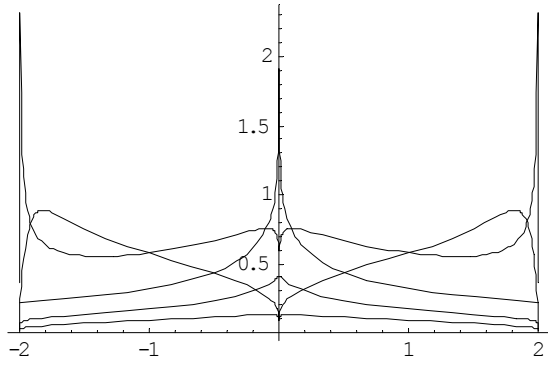


Fig.10 The DOS for the 2D lattice with single impurity for different potential strengths ε' (-0.7,-0.3,0.0,0.3,0.7)

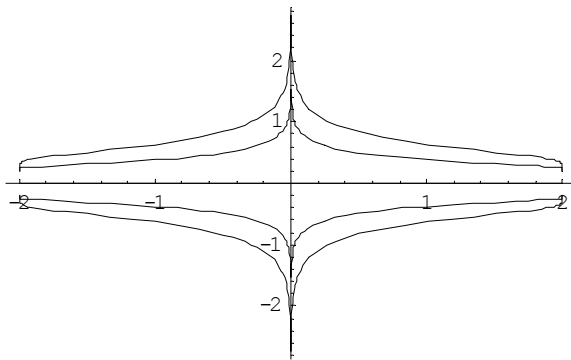


Fig.11 The phase shift for the 2D lattice with single impurity for different potential strengths ε' (-0.7,-0.3,0.0,0.3,0.7)

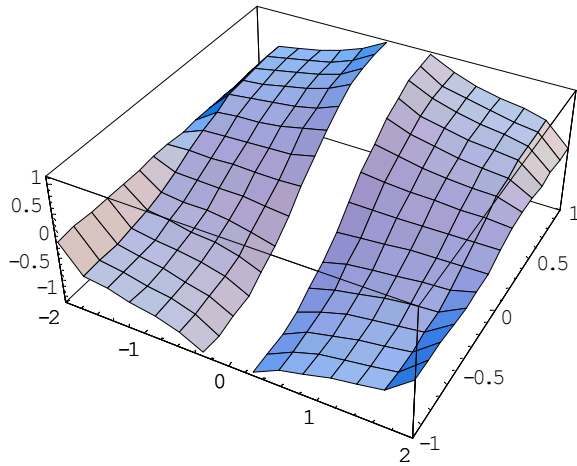


Fig.12 The phase shift for the 2D lattice with single impurity strengths ε' varying between -1 and 1 (arbitrary units)

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