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THE INFLUENCE OF ANISOTROPY ON THE GREEN'S FUNCTION OF A MODEL CRYSTAL*

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Abstract. We consider the model of an electron moving on a 2D square lattice in a constant transversal magnetic field taking into account the anisotropy parameter. After the determination of a suitable generalized energy polynomial the diagonal elements of the Green's function mediated over the whole Brillouin zone were determined without the explicit knowledge the eigenvalues or eigenvectors. The consistence of our results with the previously obtained isotropic ones is pointed out. Further more the density of states for the anisotropic case is reobtained together with the derivative of the Lyapunov exponent with regard to the energy.

Key words: anisotropic Harper equation, characteristic polynomial, Green's function, density of states, Lyapunov exponent.

1. INTRODUCTION

The study of the physical properties of a tight binding electron moving in a 2D lattice subjected to a constant transversal magnetic field is of particular interest of both theoretical and practical point of view due to the rich properties displayed by such structures and many practical applications. The magnetic flux ϕ through a plaquette is usually measured in units of flux quanta $\phi_0 = hc/e$ and it can be expressed by a rational number p/q, where p and q are mutually prime integers. In such cases, butterfly-shaped energy spectra were obtained for square lattices with nearest-neighbor hopping [1, 2], hexagonal [3], triangular [4] and rhombic [5] lattices. The energy spectrum was obtained mainly by direct diagonalization of the Hamiltonian, while the energy eigenvalue polynomial was determined only for a few models [6]. Closed forms for the density of states functions (DOS) were also

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determined [3, 7, 8]. The DOS can be applied to deduce the thermodynamic properties while the number of electrons or chemical potential remains fixed [9]. An important parameter describing the motion of electrons in 2D square lattices is the one characterizing the anisotropy of the hopping. The conclusion of [10] was that electronic states are extended if the anisotropy parameter is smaller than the unity, exponentially localized in the supra-unitary domain and the isotropic hopping represents metal-insulator phase transition. The localization properties were deduced by the means of the asymptotic behavior of the mean of the Lyapunov exponent as a function of the anisotropy parameter [10, 11]. Both DOS and the derivative of the Lyapunov exponent with respect to the energy can be determined, up to a scaling factor, from the imaginary and real parts of the mediated diagonal elements of the Green's function. Such computations were previously made mostly by numerical means, for isotropic hopping in the case the 2D square lattice [12] or graphene [13]. Analytic computations which led to a closed form for the diagonal elements of the Green's function were done for isotropic hopping of an electron on a 2D square lattice in a constant transversal magnetic field [14].

In the present article we consider the case of anisotropic movement of an electron on 2D square lattice subjected to a constant transversal magnetic field. A brief review of the general form of the energy eigenvalue polynomial is presented, as it is needed for further derivation of the Green's function. The recurrence relation for the coefficients of the polynomial is given and the general form of the coefficients is deduced. This leads to the eigenvalue polynomial for any rational magnetic field taking into account the anisotropy. The diagonal elements of the Green's function mediated over the Brillouin zone $[-\pi, \pi]\times[-\pi, \pi]$ are obtained by analytic means in an enclosed form. For the considered Hamiltonian all computations are made without explicit knowledge of its eigenvalues and eigenvectors. The consistence of our results with the isotropic ones is pointed out and the significance of the computed real and imaginary parts of the Green's function is underlined.

2. MODEL AND FORMULATION

To describe the anisotropic movement of an electron on a 2D square lattice with nearest-neighbour hopping in the presence of a constant transversal magnetic field one can consider the magnetic flux Φ through a plaquette measured in units of flux quanta and equal with a rational number $\beta = p/q$, where p and q are mutually prime integers. If the Landau-gauge is taken into account with the vector potential $\vec{A} = B(0, x, 0)$, we obtain the one dimensional difference equation known as the Harper-equation [1]:

$$u_{n+1}\mathrm{e}^{\mathrm{i}\gamma_1} + 2\Delta\cos\left(2\pi\beta + \gamma_2\right)u_n + u_{n-1}\mathrm{e}^{-\mathrm{i}\gamma_1} = Eu_n, \tag{1}$$

where γ_1 and γ_2 are the Brillouin phase factors multiplied by the lattice constant a. The parameter which describes the hopping-anisotropy through the lattice is denoted Δ and it discriminates between metallic and insulator states. The spectrum with the fine structure of q sub-bands known as the Hofstadter-butterfly can be obtained by direct diagonalization of the complex hermitic $q \times q$ eigenvalue matrix, or by the transfer matrix approach. Many important properties for this model crystal can be obtained without explicit knowledge of the eigenvalues or eigenvectors. The general form of the energy eigenvalue polynomial is needed in the subsequent computations.

To determine the eigenvalue polynomial we have to resort to a symmetric gauge [15]:

$$\vec{A} = \left((-1)\frac{B}{2}\left(x + y - \frac{a}{2}\right),\ \frac{B}{2}\left(x + y + \frac{a}{2}\right),\ 0\right), \tag{2}$$

leading to the q-symmetrized Harper equation with anisotropy [16]:

$$\mathrm{i}\left(\frac{1}{z} + \Delta\tilde{q}z\right)\tilde{u}\left(\tilde{q}z\right) - \mathrm{i}\left(\frac{z}{\tilde{q}} + \Delta\frac{1}{z}\right)\tilde{u}\left(\frac{z}{\tilde{q}}\right) = E\tilde{u}\left(z\right). \tag{3}$$

Taking the wave function in the form of a Laurent sum:

$$\tilde{u}\left(z\right) = \sum_{n=-q}^{q} C_n z^n, \tag{4}$$

with the conditions $C_{-1} = 0$ and $C_0 = 1$ the three term recurrence relation for the coefficients C_n is obtained:

$$\mathrm{i}\left(\tilde{q}^{\,n+1} - \Delta\tilde{q}^{\,-(n+1)}\right)C_{n+1} + \mathrm{i}\left(\tilde{q}^{\,n} - \Delta\tilde{q}^{\,-n}\right)C_{n-1} = EC_n. \tag{5}$$

After a few iterations the general form of the coefficients can be deduced and the general formulae can be proven by mathematical induction. These coefficients can be found explicitly in [16], and they will be omitted here. The generalized eigenvalue polynomial, after rescaling the coefficients to $\tilde{C}_n$, has the following form:

$$P\left(\beta, \Delta, E\right) = \tilde{C}_q - \left(1 - \Delta\right)^2 \tilde{C}_{-q}. \tag{6}$$

Using the eigenvalue polynomial one can deduce the influence of the anisotropy parameter Δ on the energy bands [15, 16]. This polynomial was also used for the determination of the DOS [8].

3. THE GREEN'S FUNCTION

If we denote with $D(\gamma_1,\gamma_2)$ the secular matrix describing the difference equation (1), where ***I*** is the unit matrix, then Green's function is defined as the inverse of the operator $E\mathbf{I}-D(\gamma_1,\gamma_2)$ [14]:

$$G(E,\gamma_1,\gamma_2)=\left[E\mathbf{I}-D(\gamma_1,\gamma_2)\right]^{-1}. \tag{7}$$

It verifies the following relationship:

$$\left[E\mathbf{I}-D(\gamma_1,\gamma_2)\right]^{-1}G(E,\gamma_1,\gamma_2)=G(E,\gamma_1,\gamma_2)\left[E\mathbf{I}-D(\gamma_1,\gamma_2)\right]^{-1}=\mathbf{I}. \tag{8}$$

We can make the notation $\Delta^q=b$. Knowing that [6]:

$$\det\left(E\mathbf{I}-D(\gamma_1,\gamma_2)\right)=P(\beta,\Delta,E)-2\cos(\gamma_1)-2b\cos(\gamma_2) \tag{9}$$

and the operator $E\mathbf{I}-D(\gamma_1,\gamma_2)$ is a $q\times q$ matrix, in the subsequent computations we have to assume that $E\notin\mathrm{Spec}\left(D(\gamma_1,\gamma_2)\right)$ not to have a vanishing denominator. The matrix elements of $G(E,\gamma_1,\gamma_2)$ can be written now as:

$$G_{m,n}(E,\gamma_1,\gamma_2)=\frac{A_{m,n}}{\det\left(E\mathbf{I}-D(\gamma_1,\gamma_2)\right)}=\frac{A_{m,n}}{P(\beta,\Delta,E)-2\cos(\gamma_1)-2b\cos(\gamma_2)}. \tag{10}$$

Here $A_{m,n}$ are the cofactors of $E\mathbf{I}-D(\gamma_1,\gamma_2)$. These are the determinants of the matrices that result from deleting the n^{th} row and m^{th} column from the original matrix and multiplying the result by $(-1)^{m+n}$.

We will compute only the diagonal elements of the Green's function mediated over all energy bands and the whole Brillouin zone $[-\pi,\pi]\times[-\pi,\pi]$ for $E\notin\mathrm{Spec}\left(D(\gamma_1,\gamma_2)\right)$, then we will consider the analytical continuation of the result over the spectrum of the Harper equation.

$$G_{q,q}(E)=\frac{1}{4\pi^2}\frac{1}{q}\sum_{i=1}^{q}\int_{-\pi}^{\pi}\int_{-\pi}^{\pi}\frac{A_{i,i}}{P(\beta,\Delta,E)-2\cos(\gamma_1)-2b\cos(\gamma_2)}\mathrm{d}\gamma_1\mathrm{d}\gamma_2. \tag{11}$$

Analytical computations for under and above the diagonal matrix elements were also made, but only in the isotropic case, and they were used to describe the Harper equation with impurities [14].

One must observe that after interchanging the integration with the summation we have:

$$\sum_{i=1}^{q}A_{i,i}=\frac{\mathrm{d}}{\mathrm{d}E}P(\gamma_1,\gamma_2). \tag{12}$$

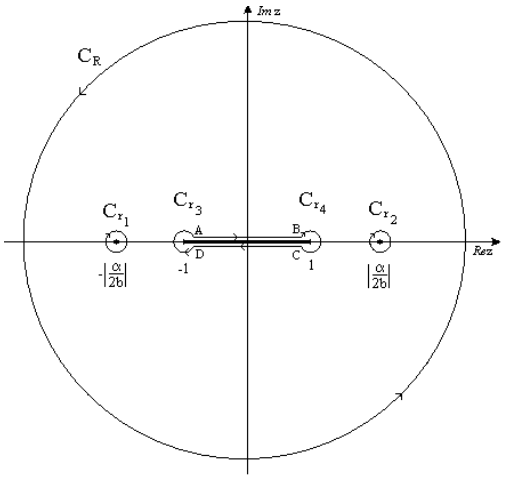

Fig. 1 – The contour in the complex plane used for evaluation of the integral from equation (11).

To proceed with the integration over γ_2 one must be split integral in equation (11) over two symmetric intervals from 0 to $\pm\ \pi$. After a suitable change of variable one can integrate in the complex plane over the contour shown in Fig. 1, and make use of the residue theory, stating that during the computations E is not an eigenvalue.

We obtain the following form of the Green's function:

$$G_{q,\,q}\left(E\right)=\frac{1}{2\pi}\frac{1}{q}\frac{\mathrm{d}P}{\mathrm{d}E}\int_{-\pi}^{\pi}\frac{1}{\sqrt{\left(P\left(\beta,\Delta,E\right)-2\cos\left(\gamma_1\right)\right)^2-4b^2}}\mathrm{d}\gamma_1. \tag{13}$$

The integral over γ_1 can be split once again over the symmetric intervals from 0 to $\pm\ \pi$. After a suitable change of variable the one can apply formula 252.00 from [17], obtaining:

$$G_{q,\,q}\left(E\right)=\frac{1}{2\pi q\sqrt{b}}\frac{\mathrm{d}P}{\mathrm{d}E}\sqrt{\frac{16b}{P^2-\left(2-2b\right)^2}}K\left(\sqrt{\frac{16b}{P^2-\left(2-2b\right)^2}}\right), \tag{14}$$

where *K(x)* denotes the complete elliptic integral of the first kind. For $b = 1$ the result is consistent with the one found in [14].

One can define the following analytical continuations of *G(E)*:

$$G^{\pm}\left(E\right)=\lim_{\xi\to 0^+}G\left(E\pm i\xi\right). \tag{15}$$

The real and imaginary part of $G_{q,q}{}^{\pm}\left(E\right)$ can be seen in Fig. 2.

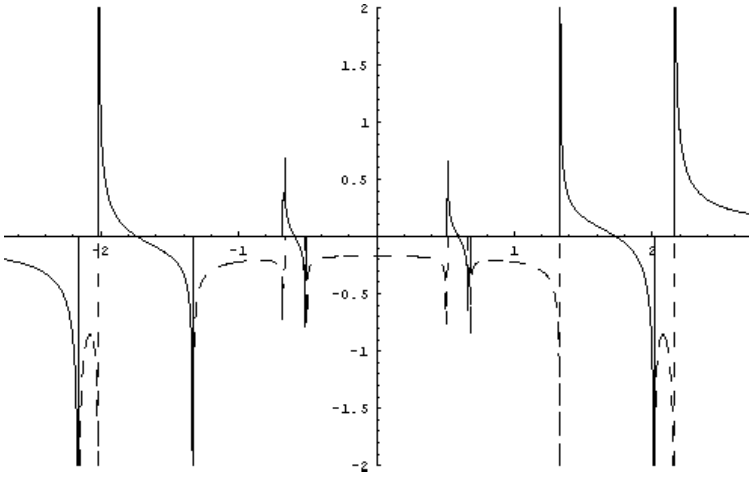

Fig. 2 – The real (continuous line) and imaginary part (dashed line) of the diagonal elements of the Green's function with p/q = 1/6 and Δ = 0,35**.**

Dividing the imaginary part by π one can obtain once again the density of states (DOS) computed previously by a different method [8]:

$$g^{(q)}\left(E,\ \Delta\right)=\mp\frac{1}{\pi}\operatorname{Im}\left(G_{q,\,q}{}^{\pm}\left(E\right)\right). \tag{16}$$

It is important to note that the Heaviside distribution used in formulae obtained for DOS not to cover the gaps is not necessary in the case of the Green's function. It automatically selects only the eigenvalues. In applications, for example the thermodynamic properties, one can use the Green's function instead of the DOS and complex calculus. At the end of computations the imaginary part of the result should be selected and divided by π to obtain the results.

The real part of the diagonal elements of $G^{\pm}\left(E\right)$ is written as:

$$\operatorname{Re}\left(G_{q,\,q}{}^{\pm}\left(E\right)\right)=\begin{cases}\dfrac{1}{2\pi q\sqrt{b}}\dfrac{\mathrm{d}P}{\mathrm{d}E}\sqrt{\dfrac{16b}{P^2-\left(2-2b\right)^2}}K\left(\sqrt{\dfrac{16b}{P^2-\left(2-2b\right)^2}}\right)\operatorname{sign}\left(P\right), \\ \qquad\text{if}\quad P\notin\left[-2-2b,\ \ 2+2b\right] \\ \dfrac{1}{2\pi q\sqrt{b}}\dfrac{\mathrm{d}P}{\mathrm{d}E}K\left(\sqrt{\dfrac{P^2-\left(2-2b\right)^2}{16b}}\right)\operatorname{sign}\left(P\right), \\ \text{if}\quad P\in\left[-2-2b,-2+2b\right]\cup\left[2-2b,\ \ 2+2b\right] \\ 0,\quad\text{if}\quad P\in\left(-2+2b,\ \ 2-2b\right).\end{cases} \tag{17}$$

Formula (17) represents the derivative of the Lyapunov exponent with respect to the energy [11]. It was previously deduced using the Thouless formula written for chaotic systems [18]. The Lyapunov exponent is used to describe the localization properties of the charge carrier in the lattice. Using the Green's function in such computations and taking the real part of the results can help proving the Aubry-André conjecture [10] which states that the electronic states for our model are extended for $\Delta<1$, exponentially localized for $\Delta>1$, and critical for $\Delta=1$.

4. CONCLUSIONS

In the present paper we succeeded to deduce a closed form of the diagonal elements of the Green's function mediated over all energy bands and the whole Brillouin zone $[\pi, \pi]\times[\pi, \pi]$ for a 2D square lattice with constant transversal magnetic field taking into account the hopping anisotropy. To achieve this goal a suitable generalized eigenvalue polynomial was used, resulting from the q-symmetrized Harper equation. For the derivation of the Green's function we resorted to integration in the complex plane and residue theory while the variable E was not an eigenvalue. The analytical continuation over the eigenvalues determined the real and imaginary parts of the diagonal elements for the Green's function. The real part was indentified as the derivative of the Lyapunov exponent with respect to the energy, and the imaginary part is equal with the density of states. The consistence of our results whit the isotropic hopping results was pointed out.

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