

## Lattice Green function for electrons in magnetic field

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The energy spectrum of electrons on a square lattice in an applied magnetic field composes the famous Hofstadter butterfly with a recursive internal subband structure. An effective method for calculating the Green function for such a system is proposed. The standard approach requires an explicit knowledge of the eigenstates and eigenenergies of the system; here we derive a Harper-like equation, that allows us to calculate the Green function for the lattice electrons in the field directly. The method is particularly useful in the weak-field regime, where the standard calculations are cumbersome.

**Introduction** The problem of two-dimensional Bloch electrons in an applied magnetic field has been intensively studied for several decades. Besides exhibiting an extremely rich energy band structure, it can be related to various phenomena such as the quantum Hall effect or superconductivity in the presence of magnetic field [1]. The energy spectrum of a system of tightly bound electrons on a square lattice in a perpendicular uniform magnetic field exhibits interesting, multifractal properties. It is described by a model commonly referred as the Hofstadter or Azbel–Hofstadter model [2, 3]. The band spectrum for rational values of the magnetic flux through an elementary plaquette  $\Phi$  is known as the “Hofstadter butterfly” [2]. In spite of the academic character of the model, experiments have been performed to uncover the multifractal structure [4]. This paper provides explicit expressions for the lattice Green functions in the presence of a magnetic field, that are convenient for both analytical and numerical calculations.

Following Hofstadter, we start from the Schrödinger equation, where the tight-binding Hamiltonian is given by

$$H = \sum_{\langle ij \rangle \sigma} t_{ij} e^{i\theta_{ij}} c_{i\sigma}^\dagger c_{j\sigma}. \quad (1)$$

Here,  $t_{ij}$  is the hopping integral between the nearest sites  $i$  and  $j$ ,  $c_{i\sigma}^\dagger$  ( $c_{i\sigma}$ ) creates (annihilates) an electron at the site  $i$  with the spin  $\sigma$ , and

$$\theta_{ij} = \frac{2\pi}{\Phi_0} \int_i^j \mathbf{A} \cdot d\mathbf{l} \quad (2)$$

is the magnetic phase factor.

For a constant magnetic field, perpendicular to the lattice, the Landau gauge can be chosen for the vector potential, i.e.,  $\mathbf{A} = (0, Bx, 0)$ . In general, the invariance of the Hamiltonian under a lattice trans-

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lation in the  $x$ -direction is lost, so the Bloch's theory holds only in the  $y$ -direction, and the eigenstates can be written in the following form:

$$\Psi(x, y) = \psi_{k_y}(x) e^{ik_y y},$$

where  $\psi(x)$  is given by the one-dimensional difference equation

$$-t[\psi(n-1) + \psi(n+1) + 2 \cos(2\pi\alpha - k_y)\psi(n)] = E\psi(n), \tag{3}$$

known as Harper's equation (or the almost Mathieu equation) [2, 5, 6]. Here,  $\alpha = \Phi/\Phi_0$  is the magnetic flux per unit cell in the units of the flux quantum  $\Phi_0 = hc/e$ , and the lattice constant  $a = 1$ . The index  $k_y$  has been dropped. It is interesting that the same equation describes eigenstates of nearly free electrons moving in a strong magnetic field (when the periodic lattice potential does not lead to a scattering between states from different Landau levels) [7]. It is also a model for a one-dimensional electronic system in two periodic potentials which are incommensurate.

For rational  $\alpha$ , such that  $\alpha = p/q$ , where  $p$  and  $q$  are coprime integers, the translational operator that moves  $q$  lattice spacing in the  $x$  direction leaves the Hamiltonian unchanged, as the total change in the hopping-integral phase is  $2\pi$ . In such a case the eigenstates can be labeled by wavevectors  $(k_x, k_y)$  from a reduced (magnetic) Brillouin zone:

$$-\frac{\pi}{q} \leq k_x \leq \frac{\pi}{q}, \quad -\pi \leq k_y \leq \pi.$$

Moreover, for rational  $\alpha$  the Hamiltonian can be written in the reciprocal space in the form:

$$H = -t \sum_{k,\sigma} [2 \cos(k_x a) c_{k,\sigma}^\dagger c_{k,\sigma} + e^{-ik_y} c_{k-g,\sigma}^\dagger c_{k,\sigma} + e^{ik_y} c_{k+g,\sigma}^\dagger c_{k,\sigma}], \tag{4}$$

where  $\mathbf{g} = (2\pi p/q, 0)$ . Note, that the Hamiltonian moves an electron from the point  $\mathbf{k}$  in the momentum space to  $\mathbf{k} + \mathbf{g}$ , then to  $\mathbf{k} + 2\mathbf{g}$ , and so on. After  $q$  hops the electron returns to the point  $\mathbf{k}$  (modulo  $2\pi$ ).

Starting with the Hamiltonian of Eq. (4) one can derive the equation of motion for the Green function  $\langle\langle c_{k,\sigma} | c_{k',\sigma'}^\dagger \rangle\rangle$ . Introducing  $\mathcal{G}_k^{(n)}(\omega) \equiv \langle\langle c_{k+ng,\sigma} | c_{k,\sigma}^\dagger \rangle\rangle_\omega$  we obtain the following hierarchy of Harper-like equations for the Green functions:

$$\begin{aligned} (\omega + 2 \cos k_x) \mathcal{G}_k^{(0)} &= 1 - e^{-ik_y} \mathcal{G}_k^{(1)} - e^{ik_y} \mathcal{G}_k^{(-1)}, \\ [\omega + 2 \cos(k_x + ng_x)] \mathcal{G}_k^{(n)} &= -e^{-ik_y} \mathcal{G}_k^{(n+1)} - e^{ik_y} \mathcal{G}_k^{(n-1)}, \quad n = 1, 2, \dots, q-1. \end{aligned} \tag{5}$$

Here, the system of equations is closed through the condition  $\mathcal{G}_k^{(0)} = \mathcal{G}_k^{(q)}$ . These equations can be written in the following matrix form:

$$\begin{pmatrix} A_k^{(0)} & e^{-ik_y} & 0 & \dots & e^{ik_y} \\ e^{ik_y} & A_k^{(1)} & e^{-ik_y} & \dots & 0 \\ 0 & e^{ik_y} & \ddots & & \vdots \\ \vdots & & & & e^{-ik_y} \\ e^{-ik_y} & 0 & \dots & e^{ik_y} & A_k^{(q-1)} \end{pmatrix} \begin{pmatrix} \mathcal{G}_k^{(0)} \\ \mathcal{G}_k^{(1)} \\ \vdots \\ \mathcal{G}_k^{(q-1)} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \tag{6}$$

where  $A_k^{(n)} \equiv \omega + 2 \cos(k_x + ng_x)$ .

**Equation for  $\mathcal{G}_k^{(0)}$**  If one is interested in  $\mathcal{G}_k^{(0)}$  only, i.e., the Green function for the momentum from the first magnetic Brillouin zone, the equations can be evaluated directly. Equation (6) can be written as a transfer matrix equation:

$$e^{-ik_y} \begin{pmatrix} \mathcal{G}_k^{(n+1)} \\ \mathcal{G}_k^{(n)} \end{pmatrix} = \begin{pmatrix} -\omega - 2 \cos(k_x + ng_x) & -e^{ik_y} \\ e^{-ik_y} & 0 \end{pmatrix} \begin{pmatrix} \mathcal{G}_k^{(n)} \\ \mathcal{G}_k^{(n-1)} \end{pmatrix}. \tag{7}$$

Starting with  $(\mathcal{G}_k^{(1)}, \mathcal{G}_k^{(0)})$ , and applying Eq. (7)  $q - 1$  times, one ends up with the following equation:

$$\begin{pmatrix} \mathcal{G}_k^{(q)} \\ \mathcal{G}_k^{(q-1)} \end{pmatrix} = e^{i(q-1)k_y} \prod_{n=1}^{q-1} \begin{pmatrix} -\omega - 2 \cos(k_x + ng_x) & -e^{ik_y} \\ e^{-ik_y} & 0 \end{pmatrix} \begin{pmatrix} \mathcal{G}_k^{(1)} \\ \mathcal{G}_k^{(0)} \end{pmatrix}. \quad (8)$$

On the other hand, Eq. (5) can be written in a matrix form as:

$$\begin{pmatrix} \mathcal{G}_k^{(1)} \\ \mathcal{G}_k^{(0)} \end{pmatrix} = e^{ik_y} \begin{pmatrix} -\omega - 2 \cos k_x + \frac{1}{\mathcal{G}_k^{(0)}} & -e^{ik_y} \\ e^{-ik_y} & 0 \end{pmatrix} \begin{pmatrix} \mathcal{G}_k^{(0)} \\ \mathcal{G}_k^{(-1)} \end{pmatrix}. \quad (9)$$

Combining Eqs. (8) and (9) one obtains

$$\begin{pmatrix} \mathcal{G}_k^{(q)} \\ \mathcal{G}_k^{(q-1)} \end{pmatrix} = e^{iqk_y} \mathcal{P}_k^q(\omega) \mathcal{R}_k(\omega) \begin{pmatrix} \mathcal{G}_k^{(0)} \\ \mathcal{G}_k^{(-1)} \end{pmatrix}, \quad (10)$$

where the two transfer matrices,  $\mathcal{P}_k^q$  and  $\mathcal{R}_k$ , have the following explicit form:

$$\mathcal{P}_k^q(\omega) \equiv \prod_{n=1}^{q-1} \begin{pmatrix} -\omega - 2 \cos(k_x + ng_x) & -e^{ik_y} \\ e^{-ik_y} & 0 \end{pmatrix}, \quad (11)$$

and

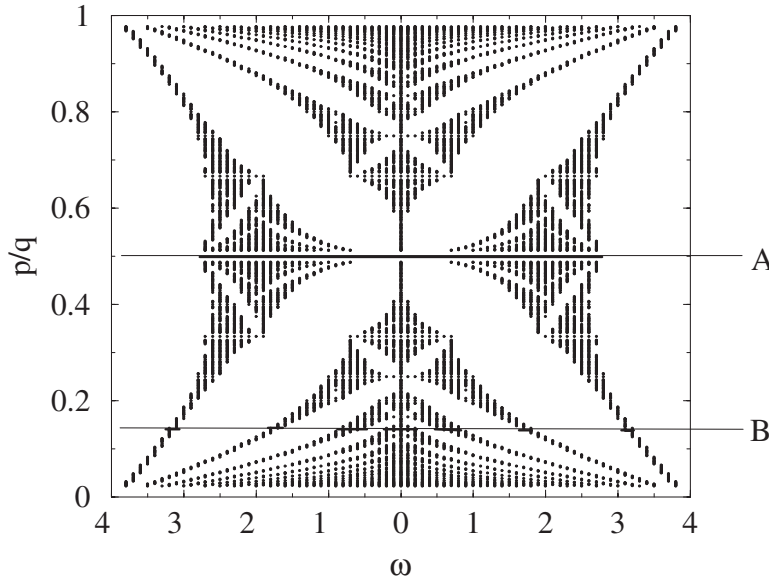
$$\mathcal{R}_k(\omega) \equiv \begin{pmatrix} -\omega - 2 \cos k_x + \frac{1}{\mathcal{G}_k^{(0)}} & -e^{ik_y} \\ e^{-ik_y} & 0 \end{pmatrix}. \quad (12)$$

Taking into account the properties of the Green functions  $\mathcal{G}_k^{(q)} = \mathcal{G}_k^{(0)}$  and  $\mathcal{G}_k^{(q-1)} = \mathcal{G}_k^{(-1)}$ , we get the equation for  $\mathcal{G}_k^{(0)}$  in the following form:

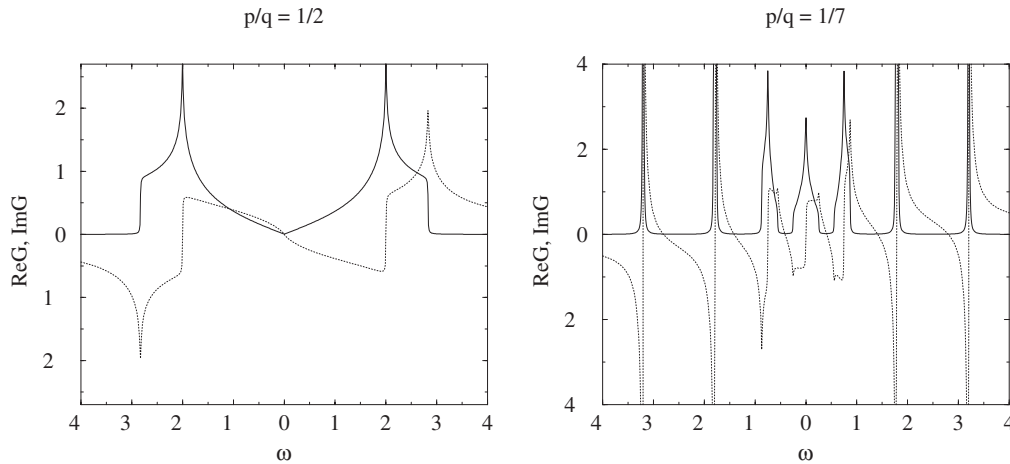
$$\det [\mathcal{P}_k^q(\omega) \mathcal{R}_k(\omega) - e^{-iqk_y} \mathbf{I}] = 0. \quad (13)$$

Then,  $\mathcal{G}_k^{(0)}(\omega)$  can be expressed as:

$$\begin{aligned} \mathcal{G}_k^{(0)}(\omega) = & [\mathcal{P}_k^q(\omega)]_{11} \{ \det \mathcal{P}_k^q(\omega) e^{iqk_y} + e^{-iqk_y} - [\mathcal{P}_k^q(\omega)]_{12} e^{-ik_y} + [\mathcal{P}_k^q(\omega)]_{21} e^{ik_y} \\ & + [\mathcal{P}_k^q(\omega)]_{11} (\omega + 2 \cos k_x) \}^{-1}. \end{aligned} \quad (14)$$



**Fig. 1** Magnetic subband structure for lattice electrons in a uniform magnetic field ("Hofstadter butterfly"). The horizontal lines "A" and "B" correspond to  $p/q = 1/2$  and  $p/q = 1/7$ , respectively.



**Fig. 2** Real (dotted line) and imaginary (solid line) part of the Green function determined for different values of the applied field. The left panel corresponds to  $p/q = 1/2$  (along line “A” in Fig. 1), the right to the value  $p/q = 1/7$  (along line “B” in Fig. 1).

**Discussion** For small  $q$  this quantity can be evaluated analytically, whereas for larger  $q$  Eqs. (11) and (14) allow us for determining the Green function numerically. Note, that for an arbitrary but rational  $p/q$  the Green function can be effectively calculated without finding the eigenstates of the original Hamiltonian.

The derived Eq. (14) for the Green function can be used to determine e.g., the density of states for lattice electrons in an applied magnetic field from the relation:

$$\rho(\omega) = -\frac{2}{\pi} \text{Im} G(\omega + i\eta)_{\eta \rightarrow 0^+}, \quad (15)$$

where  $G(\omega) \equiv \frac{1}{N} \sum_k \mathcal{G}_k^{(0)}(\omega)$ . The corresponding energy spectrum, known as the Hofstadter butterfly (cf. Fig. 1), was found to depend critically on the value of  $\alpha$ . Namely, if  $\alpha$  is a rational number,  $\alpha = p/q$ , each energy band is split into  $q$  subbands by the magnetic field. Otherwise, for any irrational number of  $\alpha$ , the spectrum forms a Cantor set. The calculated densities of states for two selected values of  $p/q = 1/2$  and  $1/7$ , as well as the real parts of  $G(\omega)$ , are presented in Fig. 2.

Recently, the Green function obtained for the tight-binding model on a square lattice in the applied magnetic field has been expressed by means of continued fractions by Ueta [8]. However, the derived expressions are more complicated, and therefore, as stated by the author, for large values of  $q$  ( $q > 5$ ) are difficult to solve.

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