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Lattice Green function in uniform magnetic fields

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Abstract. The Green function of a square tight-binding model in magnetic fields is expressed by means of continued fractions. For rational fields, the expression is reduced to a more useful one. The Green function expressing the out-going wave is numerically computed at arbitrary sites for the first time. It is found that the absolute value of the Green function takes maximum values on the reciprocal lattice of the magnetic Brillouin zone.

1. Introduction

Physics of two-dimensional (2D) electrons in a periodic lattice has been of special interest, since the microfabrication technology of the semi-conductor became available to prepare electron systems with large period in superlattices. In these systems, the band width is narrow and the effects of magnetic fields and periodic potentials are emphasized. The magnetoresistance has been measured in the samples with artificial periodicity and many interesting phenomena have been discovered. The realization of the Hofstadter-type energy spectrum is one of the typical examples [1–3].

Such systems are frequently modelled by means of tight-binding approximation. We consider tight-binding electrons with an isotropic nearest-neighbour hopping in a square lattice subjected to a uniform magnetic field applied perpendicularly. In the Landau gauge with the lattice constant chosen as the unit of length, the wavefunction $\varphi(\boldsymbol{n})$ at a lattice point $\boldsymbol{n} = (n_x, n_y)$ satisfies [4]

$$\begin{aligned} 2\varepsilon\varphi(\boldsymbol{n}) &= \sum_{i=1}^{4} T_{\boldsymbol{n}+\boldsymbol{a}_i,\boldsymbol{n}}\varphi(\boldsymbol{n}+\boldsymbol{a}_i) \\ T_{\boldsymbol{n}+\boldsymbol{a}_i,\boldsymbol{n}} &= \exp[-\mathrm{i}2\pi\alpha\ (0, n_x)\cdot\boldsymbol{a}_i]. \end{aligned} \tag{1}$$

Here $\boldsymbol{a}_i$ $(i = 1 \sim 4)$ represents a translation vector to the nearest-neighbour lattice points:

$$\boldsymbol{a}_1 = (1, 0) = -\boldsymbol{a}_3 \qquad \boldsymbol{a}_2 = (0, 1) = -\boldsymbol{a}_4$$

and $\alpha = \Phi/\Phi_0$ is the ratio of the magnetic flux through a unit cell $\Phi = B$ to the magnetic flux quantum $\Phi_0 = h/\mathrm{e}$.

Equation (1) has been investigated extensively since the pioneering works of Peierls [5]. A number of theoretical studies have been carried out in many different physical contexts, ranging from the quantum Hall effect [6] to quasiperiodic systems (for a review, see, for example, [7]). Its topological character has been revealed both for periodic boundary

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conditions [6] and for systems with edges [8]. Recently, Hatsugai *et al* [9] derived several analytical results for the weak-field limit and for the incommensurate golden-mean flux, by following the highly innovative Bethe ansatz approach proposed by Wiegmann and Zabrodin [10] using quantum group techniques. In the transport problems, the numerical technique with Green functions, which is conventionally called the recursive Green function method, has been widely used by many authors as a practical tool to simulate quantum transport in a variety of structures [11, 12]. The key of the method is to calculate the Green functions in a given system. Once the one-electron Green functions are known, it is possible to use them for a variety of purposes. One may compute the amplitudes for scattering, the density of states, electric current and conductivity [13]. The Green function, however, is proper to the given finite system. The retarded and advanced Green functions in infinite 2D space in perpendicular uniform magnetic fields have never been obtained except the diagonal element, that is, the density of states [14, 15].

One method of computing the Green function $G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)$ for equation (1) in 2D infinite system is the straightforward expansion in eigenfunctions which was used by Takahashi *et al* [16], for example, in order to obtain the Hall and longitudinal conductivities, that is, current–current correlation functions. It requires the normalized eigenfunctions belonging to all subbands as functions of the coordinates and a wavevector. When α is rational, i.e. $\alpha = p/q$ with mutual prime integers p and q, q kinds of the eigenfunctions can be obtained analytically, but that is not trivial and is inconvenient. When α is irrational, the eigenfunctions in infinite space cannot be calculated even numerically.

The purpose of the present paper is to derive a convenient expression of the Green function $G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)$ in a 2D infinite system and to numerically compute the one expressing the out-going wave at arbitrary sites for the first time. This, in principle, allows us to obtain the Green function numerically for any values of α.

The results obtained here propose the further interest of analytical and numerical study of themselves, and the Green function enables us to investigate the behaviour of tight-binding electrons in infinite 2D space in perpendicular uniform magnetic fields as well. For example, we can treat the scattering problems of tight-binding electrons in uniform magnetic fields by means of the Lippmann–Schwinger equation [17]. Further, the Kirchhoff–Helmholtz formula which were modified for tight-binding electrons in magnetic fields by Kawamura *et al* [18] becomes applicable exactly, although in [18] the semiclassical Green function was employed. Such a method corresponds to the boundary element method for continuous systems [19]. By using it, we can evaluate wavefunctions of tight-binding electrons confined with an arbitrary-shaped boundary [20].

In the next section, we will examine symmetry properties of the Green function, which will be helpful to save a numerical task greatly in obtaining the Green function. Especially, the translational symmetry of the Schrödinger equation (1) is broken by the presence of the vector potential, so that $G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)$ depends on $\boldsymbol{n}$ and $\boldsymbol{n}'$ separately. This feature is very serious, making it necessary to calculate the Green function for all combinations of $\boldsymbol{n}$ and $\boldsymbol{n}'$, not simply of $\boldsymbol{n} - \boldsymbol{n}'$ as in the usual case. Therefore, we will transform the Green function to a convenient form in which translational symmetry can be used. The transformed Green function will be expressed in terms of continued fractions in section 3. For rational magnetic fields, the expression will be further reduced analytically. The condition of the out-going wave will be derived. Numerical calculation of the Green function will be presented in section 4. The final section will be devoted to a summary and discussion.

2. Definition and symmetries of the Green function

The Green function $G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)$ for (1) is defined by the equation

$$\sum_{i=1}^{4} T_{\boldsymbol{n}+\boldsymbol{a}_i,\boldsymbol{n}} G(\boldsymbol{n}+\boldsymbol{a}_i, \boldsymbol{n}'; \varepsilon, \alpha) = 2\varepsilon G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha) - \delta_{\boldsymbol{n},\boldsymbol{n}'}. \tag{2}$$

From this equation, several kinds of symmetries with respect to the energy ε, the coordinate $\boldsymbol{n}$ and the magnetic field α are clarified. As for the energy, we can show that the following relation, analogous to the case in the absence of magnetic fields, holds;

$$G(\boldsymbol{n}, \boldsymbol{n}'; -\varepsilon + \mathrm{i}\delta, \alpha) = (-1)^{\xi+\eta+1} G^*(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon + \mathrm{i}\delta, -\alpha) \tag{3}$$

where we define $\xi \equiv n_x - n'_x$ and $\eta \equiv n_y - n'_y$ and an infinitely small imaginary part of energy $\delta(>0)$ is introduced in order to consider the out-going wave.

From the geometrical symmetry, we find

$$G(\pm(n_x, -n_y), \pm(n'_x, -n'_y); \varepsilon, -\alpha) = G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha) \tag{4}$$

and

$$G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha) = G(-\boldsymbol{n}, -\boldsymbol{n}'; \varepsilon, \alpha). \tag{5}$$

Although a kind of geometrical symmetry is held in the classical sense, the presence of a phase factor breaks it quantum mechanically as

$$\begin{aligned} G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha) &= \exp[\mathrm{i}2\pi\alpha(n_x n_y - n'_x n'_y)] G((n_y, n_x), (n'_y, n'_x); \varepsilon, -\alpha) \\ &= \exp[\mathrm{i}2\pi\alpha(n_x n_y - n'_x n'_y)] G((-n_y, n_x), (-n'_y, n'_x); \varepsilon, \alpha). \end{aligned} \tag{6}$$

In our system, in addition, the magnetic field spoils the translational symmetry. However, it is known that the Green function can be expressed exactly by the product between an exponential factor which breaks the translational symmetry and the translationally symmetric function [21] as

$$G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha) = \exp[\mathrm{i}2\pi\alpha n'_x(n_y - n'_y)] G_0(\xi, \eta; \varepsilon, \alpha). \tag{7}$$

Substituting (7) into (2), we see that $G_0(\xi, \eta; \varepsilon, \alpha)$ obeys the translationally invariant equation:

$$\begin{aligned} &G_0(\xi+1, \eta) + G_0(\xi-1, \eta) + \mathrm{e}^{-\mathrm{i}2\pi\alpha\xi} G_0(\xi, \eta+1) + \mathrm{e}^{\mathrm{i}2\pi\alpha\xi} G_0(\xi, \eta-1) \\ &\quad = 2\varepsilon G_0(\xi, \eta) - \delta_{\xi,0}\delta_{\eta,0} \end{aligned} \tag{8}$$

where the arguments, ε and α in G_0 are dropped for brevity. Also in the following sections, unessential arguments in the quantities frequently used will be suitably dropped.

Equations (3)–(6) show that if the Green function is calculated only for the restricted region of $\varepsilon \geqslant 0$, $\alpha \geqslant 0$, $\xi \geqslant 0$ and $\eta \geqslant 0$, it can be obtained for the whole region of ε, α and (ξ, η).

3. Analytical expressions

When $g(\xi, k_y)$ is defined by

$$G_0(\xi, \eta; \varepsilon, \alpha) = \frac{1}{2\pi} \int_{-\pi}^{\pi} \mathrm{e}^{\mathrm{i}k_y\eta} g(\xi, k_y)\, \mathrm{d}k_y \tag{9}$$

substitution of (9) into (8) yields the one-dimensional (1D) difference equations;

$$g(\xi+1, k_y) + g(\xi-1, k_y) - 2\beta_\xi(k_y, \varepsilon) g(\xi, k_y) = -\delta_{\xi,0} \tag{10}$$

with $\beta_\xi(k_y, \varepsilon) \equiv \varepsilon - \cos(k_y - 2\pi\alpha\xi)$.

If we introduce the quantity

$$B_\xi(k_y, \varepsilon) = \frac{g(\xi + 1, k_y)}{g(\xi, k_y)} \tag{11}$$

it can be written by a continued fraction as [22, 23]

$$B_\xi(k_y, \varepsilon) = \begin{cases} 2\beta_\xi(k_y, \varepsilon) - \dfrac{1}{B_{\xi-1}(k_y, \varepsilon)} & (\xi < 0) \\ \dfrac{1}{2\beta_{\xi+1}(k_y, \varepsilon) - B_{\xi+1}(k_y, \varepsilon)} & (\xi \geqslant 0). \end{cases} \tag{12}$$

Using B_ξ, we can express $g(\xi, k_y)$ for an arbitrary value of ξ by continued fractions. The result is

$$\text{for } \xi = 0 \qquad g(0, k_y) = \frac{1}{2\beta_0(k_y, \varepsilon) - B_0(k_y, \varepsilon) - \frac{1}{B_{-1}(k_y, \varepsilon)}} \tag{13}$$

$$\begin{aligned} \text{for } \xi > 0 \qquad g(\xi, k_y) &= \frac{g(\xi)}{g(\xi - 1)} \frac{g(\xi - 1)}{g(\xi - 2)} \cdots \frac{g(2)}{g(1)} \frac{g(1)}{g(0)} g(0, k_y) \\ &= \left(\prod_{i=0}^{\xi-1} B_i(k_y, \varepsilon) \right) g(0, k_y) \end{aligned} \tag{14}$$

$$\text{for } \xi < 0 \qquad g(\xi, k_y) = \left(\prod_{i=\xi}^{-1} \frac{1}{B_i(k_y, \varepsilon)} \right) g(0, k_y). \tag{15}$$

Substituting these equations into (9) and (7), we obtain the continued fraction expansion of the Green function. It is well known that a continued fraction expansion is a powerful method of obtaining density of states [24].

It is too difficult to analytically discuss the Green function for arbitrary α, so hereafter we confine ourselves to the case of rational α.

We can write $\alpha = p/q$, where p and q are relative prime integers. Using the periodicity $\beta_{\xi+q}(k_y, \varepsilon) = \varepsilon - \cos[k_y - 2\pi(\xi + q)p/q] = \beta_\xi(k_y, \varepsilon)$, we have

$$B_{\xi+q}(k_y, \varepsilon) = B_\xi(k_y, \varepsilon). \tag{16}$$

Then, equations (14) and (15) are reduced to

$$g(\xi, k_y) = r_q^{[\xi/q]}(k_y, \varepsilon) \left(\prod_{i=0}^{\mathrm{mod}(\xi,q)-1} B_i(k_y, \varepsilon) \right) g(0, k_y) \tag{17}$$

$$r_q(k_y, \varepsilon) \equiv \prod_{i=0}^{q-1} B_i(k_y, \varepsilon) \tag{18}$$

where the operator $[\xi/q]$ means Gauss symbol, that is, the maximum integer not more than the value of ξ/q and $\mathrm{mod}(\xi, q)$ is defined as $\xi - q[\xi/q]$. The second factor on the right-hand side of (17) is taken as unity when the upper limit of the product $\mathrm{mod}(\xi, q) - 1$ is negative.

Here, let us derive a useful expression of $r_q(k_y, \varepsilon)$. Equation (10) can be written in a matrix form as

$$\begin{pmatrix} g(\xi + 1, k_y) \\ g(\xi, k_y) \end{pmatrix} = \begin{pmatrix} 2\beta_\xi(k_y, \varepsilon) & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} g(\xi, k_y) \\ g(\xi - 1, k_y) \end{pmatrix} \tag{19}$$

except for $\xi = 0$. By defining

$$T_q(\xi) \equiv \prod_{i=0}^{q-1} \begin{pmatrix} 2\beta_{\xi+i}(k_y, \varepsilon) & -1 \\ 1 & 0 \end{pmatrix} \tag{20}$$

we have

$$\begin{pmatrix} g(\xi+q, k_y) \\ g(\xi+q-1, k_y) \end{pmatrix} = T_q(\xi) \begin{pmatrix} g(\xi, k_y) \\ g(\xi-1, k_y) \end{pmatrix}. \tag{21}$$

On the other hand, equation (17) leads to

$$g(\xi+q, k_y) = r_q(k_y, \varepsilon) g(\xi, k_y). \tag{22}$$

The combination of (21) and (22) then yields

$$T_q(\xi) \begin{pmatrix} g(\xi) \\ g(\xi-1) \end{pmatrix} = r_q(k_y, \varepsilon) \begin{pmatrix} g(\xi) \\ g(\xi-1) \end{pmatrix} \tag{23}$$

that is, $r_q(k_y, \varepsilon)$ is given as eigenvalues of the matrix $T_q(\xi)$. Since $r_q(k_y, \varepsilon)$ is independent of ξ, it is sufficient to consider $T_q(1)$.

Let us introduce the four quantities a_q, b_q, c_q and d_q for the matrix elements of $T_q(1)$;

$$\begin{pmatrix} a_q & b_q \\ c_q & d_q \end{pmatrix} \equiv T_q(1) = \prod_{i=1}^{q} \begin{pmatrix} 2\beta_i(k_y, \varepsilon) & -1 \\ 1 & 0 \end{pmatrix}. \tag{24}$$

Because of the relation

$$a_q d_q - b_q c_q = \det T_q(1) = 1 \tag{25}$$

the eigenvalues of $T_q(1)$ are written as

$$r_q^{\pm}(k_y, \varepsilon) = \Delta_q(k_y, \varepsilon) \pm \sqrt{\Delta_q^2(k_y, \varepsilon) - 1} \tag{26}$$

$$= \exp(\pm \mathrm{i} \cos^{-1} \Delta_q(k_y, \varepsilon)) \tag{27}$$

with $\Delta_q(k_y, \varepsilon)$ defined as

$$\Delta_q(k_y, \varepsilon) = (a_q + d_q)/2 = \tfrac{1}{2} \operatorname{Tr} T_q(1). \tag{28}$$

The problem is thus reduced to the calculation of a_q, b_q, c_q and d_q.

From (24), we have

$$\begin{aligned} T_n(1) &= \begin{pmatrix} 2\beta_n(k_y, \varepsilon) & -1 \\ 1 & 0 \end{pmatrix} T_{n-1}(1) \\ &= \begin{pmatrix} 2\beta_n a_{n-1} - c_{n-1} & 2\beta_n b_{n-1} - d_{n-1} \\ a_{n-1} & b_{n-1} \end{pmatrix} \\ &= \begin{pmatrix} a_n & b_n \\ c_n & d_n \end{pmatrix} \end{aligned}$$

and

$$T_1(1) = \begin{pmatrix} 2\beta_1(k_y, \varepsilon) & -1 \\ 1 & 0 \end{pmatrix} = \begin{pmatrix} a_1 & b_1 \\ c_1 & d_1 \end{pmatrix}.$$

Therefore, a_q, b_q, c_q and d_q are given by the following recursion relations;

$$a_n = 2\beta_n(k_y, \varepsilon) a_{n-1} - a_{n-2} (n \geqslant 2) \qquad a_1 = 2\beta_1(k_y, \varepsilon) \qquad a_0 = 1 \tag{29}$$

$$b_n = 2\beta_n(k_y, \varepsilon) b_{n-1} - b_{n-2} (n \geqslant 2) \qquad b_1 = -1 \qquad b_0 = 0 \tag{30}$$

$$c_n = a_{n-1} \tag{31}$$

$$d_n = b_{n-1}. \tag{32}$$

The quantity $g(\xi, k_y)$ can also be expressed in terms of the sequences $\{a_n\}$ and $\{b_n\}$ as shown in the following.

From the definition of $r_q(k_y, \varepsilon)$;

$$\begin{pmatrix} a_q - r_q^{\pm} & b_q \\ c_q & d_q - r_q^{\pm} \end{pmatrix} \begin{pmatrix} g(1, k_y) \\ g(0, k_y) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and the definition of $B_0(k_y, \varepsilon)$, (11), we obtain

$$B_0^{\pm}(k_y, \varepsilon) = \frac{g(1, k_y)}{g(0, k_y)} = \frac{b_q}{r_q^{\pm} - a_q}.$$

Equations (28), (25), (31) and (32) yield

$$\begin{aligned} B_0^{\pm}(k_y, \varepsilon) &= \frac{b_q(r_q^{\mp} - a_q)}{-a_q b_{q-1} + a_q b_{q-1} - b_q a_{q-1}} \\ &= \frac{a_q - r_q^{\mp}}{a_{q-1}} \\ &= \frac{a_q - r_q^{\mp} a_0}{a_{q-1} - r_q^{\mp} a_{-1}} \end{aligned} \tag{33}$$

where we define $a_{-1} \equiv 0$.

Using the relation $B_0(k_y, \varepsilon) = 2\beta_0(k_y, \varepsilon) - 1/B_{-1}(k_y, \varepsilon)$ given by (12), the physically meaningful solution $g^{\pm}(0, k_y)$ defined by (13) is transformed as follows

$$\begin{aligned} g^{\pm}(0, k_y) &= \frac{1}{2\beta_q(k_y, \varepsilon) - B_0(k_y, \varepsilon) - \frac{1}{B_{-1}(k_y, \varepsilon)}} \\ &= \frac{1}{B_0^{\pm}(k_y, \varepsilon) - B_0^{\mp}(k_y, \varepsilon)} \\ &= \mp \frac{a_{q-1} - r_q^{\mp} a_{-1}}{2\sqrt{\Delta_q^2 - 1}} \\ &= \mp \frac{a_{q-1} - r_q^{\mp} a_{-1}}{2\mathrm{i} \sin(\cos^{-1} \Delta_q)}. \end{aligned} \tag{34}$$

Further, by means of induction, we obtain from equations (12), (16) and (29)

$$B_{\xi}^{\pm}(k_y, \varepsilon) = \frac{a_{q+\xi} - r_q^{\mp} a_{\xi}}{a_{q+\xi-1} - r_q^{\mp} a_{\xi-1}}. \tag{35}$$

So that equation (14) can be written as

$$g^{\pm}(\xi, k_y) = \mp \frac{a_{q+\mathrm{mod}(\xi,q)-1} - \exp(\mp \mathrm{i} \cos^{-1} \Delta_q) a_{\mathrm{mod}(\xi,q)-1}}{2\mathrm{i} \sin(\cos^{-1} \Delta_q)} \mathrm{e}^{\pm \mathrm{i}[\xi/q] \cos^{-1} \Delta_q}. \tag{36}$$

Therefore, equations (9) and (17) are combined to give

$$\begin{aligned} G_0(\xi, \eta; \varepsilon, \alpha) = \mp \int_{-\pi}^{\pi} \frac{\mathrm{d}k_y}{2\pi} \mathrm{e}^{\mathrm{i}k_y \eta} \exp(\pm \mathrm{i}[\xi/q] \cos^{-1} \Delta_q) \\ \times \frac{a_{q+\mathrm{mod}(\xi,q)-1} - \exp(\mp \mathrm{i} \cos^{-1} \Delta_q) a_{\mathrm{mod}(\xi,q)-1}}{2\mathrm{i} \sin(\cos^{-1} \Delta_q)}. \end{aligned} \tag{37}$$

It can be rewritten by means of 2D Fourier transform as

$$G_0(\xi, \eta; \varepsilon + \mathrm{i}\delta, \alpha) = \frac{q}{2} \int\int_{-\pi}^{\pi} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^2} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{\xi}} \frac{a_{q+\mathrm{mod}(\xi,q)-1} - \mathrm{e}^{-\mathrm{i}k_x q} a_{\mathrm{mod}(\xi,q)-1}}{\Delta_q(k_y, \varepsilon) - \cos k_x q \pm \mathrm{i}\delta \frac{\partial \Delta_q}{\partial \varepsilon}} \mathrm{e}^{-\mathrm{i}k_x \,\mathrm{mod}(\xi,q)} \tag{38}$$

Table 1. $\Delta_q(k_y,\varepsilon)$ and $\partial\Delta_q/\partial\varepsilon$ for several values of α.

α	$\Delta_q(k_y,\varepsilon)$	$\frac{\partial\Delta_q}{\partial\varepsilon}$
0	$-\cos k_y+\varepsilon$	1
$\frac{1}{2}$	$-\cos 2k_y+2\varepsilon^2-2$	4ε
$\frac{1}{3}$	$-\cos 3k_y+4\varepsilon^3-6\varepsilon$	$6(2\varepsilon^2-1)$
$\frac{1}{4}$	$-\cos 4k_y+8\varepsilon^4-16\varepsilon^2+2$	$32\varepsilon(\varepsilon^2-1)$
$\frac{1}{5}$	$-\cos 5k_y+16\varepsilon^5-40\varepsilon^3+\frac{5(7-\sqrt{5})}{2}\varepsilon$	$5\left(16\varepsilon^4-24\varepsilon^2+\frac{7-\sqrt{5}}{2}\right)$
$\frac{2}{5}$	$-\cos 5k_y+16\varepsilon^5-40\varepsilon^3+\frac{5(7+\sqrt{5})}{2}\varepsilon$	$5\left(16\varepsilon^4-24\varepsilon^2+\frac{7+\sqrt{5}}{2}\right)$

where in order to obtain the out-going wave the sign of the integrand is selected as

$$\begin{cases} \Delta_q(k_y,\varepsilon)>1 & -\text{ sign} \\ \Delta_q(k_y,\varepsilon)<-1 & +\text{ sign} \\ |\Delta_q(k_y,\varepsilon)|\leqslant 1 & \begin{cases} \dfrac{\partial\Delta_q}{\partial\varepsilon}\geqslant 0 & -\text{sign} \\ \dfrac{\partial\Delta_q}{\partial\varepsilon}<0 & +\text{sign.} \end{cases} \end{cases} \tag{39}$$

Here, $\boldsymbol{k}=(k_x,k_y)$ and $\boldsymbol{\xi}=(\xi,\eta)$ are defined. It is confirmed that (37) is reduced to (38) by performing a contour integral along a unit circle $|z|=1$ with $z=\exp(\mathrm{i}k_xq)$.

For several values of α, the explicit expressions for Δ_q and $\partial\Delta_q/\partial\varepsilon$ are given in table 1. It shows that $\Delta_q(k_y,\varepsilon)$ is written as

$$\Delta_q(k_y,\varepsilon)=-\cos k_yq+1+\Delta_q(k_y=0,\varepsilon). \tag{40}$$

The derivative $\partial\Delta_q/\partial\varepsilon$ is, then, a function of only ε. A different branch to be chosen according to the value of $\partial\Delta_q/\partial\varepsilon$ is a characteristic feature in the presence of a magnetic field, because $\partial\Delta_q/\partial\varepsilon=1$ when $\alpha=0$. This peculiarity is caused by the fact that the band structure consists of q subbands. Note that if there is a single band, $\partial\Delta_q/\partial\varepsilon$ is a constant independent of ε.

The equation

$$\Delta_q(k_y,\varepsilon)-\cos k_xq=0 \tag{41}$$

which determines the poles of the integrand, just gives the dispersion relation derived by Chambers [25]. With (40), the dispersion relation (41) now reads

$$\Delta_q(0,\varepsilon)+1=\cos k_xq+\cos k_yq. \tag{42}$$

The unit cell in $\boldsymbol{k}$-space, the magnetic first Brillouin zone, is smaller than the Brillouin zone by a factor of q in each direction normal to the field. Because $\Delta_q(0,\varepsilon)$ is a polynomial of degree q of the energy ε, equation (41) is expressed as

$$\Delta_q(k_y,\varepsilon)-\cos k_xq=\prod_{m=1}^{q}[\varepsilon-\varepsilon_m(k_x,k_y)]=0 \tag{43}$$

where $\varepsilon_m(k_x,k_y)$ is a dispersion of the mth Landau subband. Thus, the band structure consists of q subbands. The centres of the subbands are given by $\cos k_xq+\cos k_yq=0$, that is, $\Delta_q(0,\varepsilon)+1=0$, while the edges of subbands are determined by $|\cos k_xq+\cos k_yq|=2$ or $|\Delta_q(0,\varepsilon)+1|=2$.

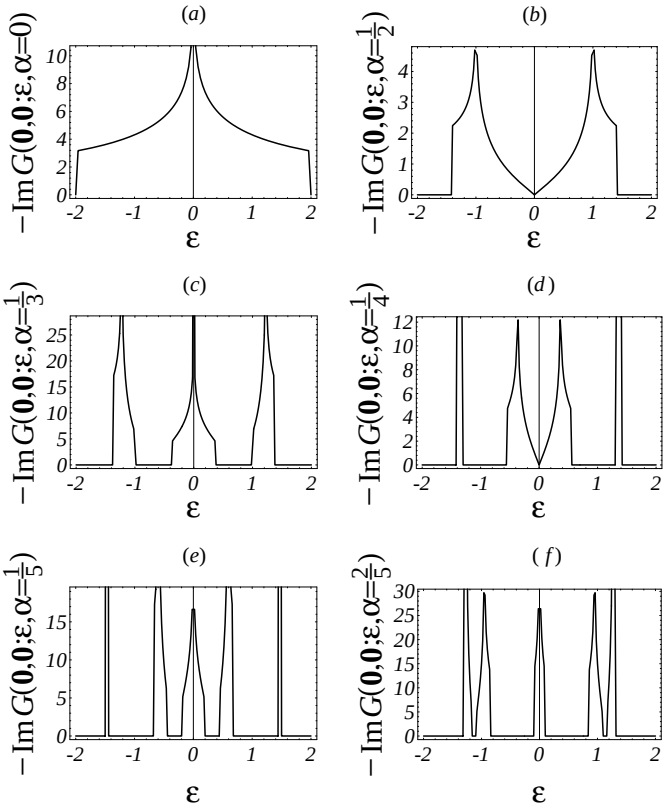

Figure 1. Demonstration of the density of states. The values of α in (*a*) are 0, (*b*) $\frac{1}{2}$, (*c*) $\frac{1}{3}$, (*d*) $\frac{1}{4}$, (*e*) $\frac{1}{5}$ and (*f*) $\frac{2}{5}$.

4. Numerical calculation

4.1. Density of states

When α is rational, the density of states (DOS) $\rho(\varepsilon)$ in infinite 2D space can be computed exactly, since the imaginary part of $G(\mathbf{0},\mathbf{0};\varepsilon,\alpha)$ is related to DOS as follows

$$\begin{aligned}-\mathrm{Im}\,G(\mathbf{0},\mathbf{0};\varepsilon,\alpha) &= \frac{q}{2}\pi\int\!\!\int_{-\pi}^{\pi}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^2}\delta(\Delta_q(k_y,\varepsilon)-\cos qk_x)\\ &= \frac{q}{2}\pi\int\!\!\int_{-\pi}^{\pi}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^2}\sum_m\frac{\delta(\varepsilon-\varepsilon_m(k_x,k_y))}{\left|\frac{\partial\Delta_q}{\partial\varepsilon}\right|}\\ &= \frac{q\pi}{2\left|\frac{\partial\Delta_q}{\partial\varepsilon}\right|}\rho(\varepsilon). \qquad (44)\end{aligned}$$

The imaginary part of the Green function for several values of α is plotted in figure 1. They correspond to the DOS of the energy spectrum obtained by Hofstadter [4].

His statement that bands form hierarchically organized cluster-like fractal structures is clearly demonstrated in the calculated DOS. Namely, DOS of the subband located at the centre of figures 1(*a*), (*c*) and (*e*) are similar, DOS of the two centre subbands in figure 1(*d*)

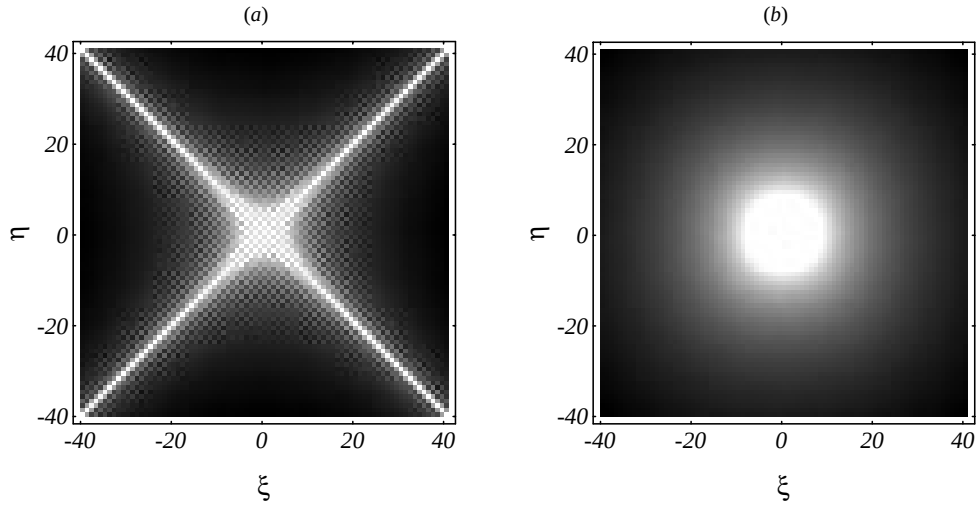

Figure 2. The density plot of the Green function in the absence of a magnetic field for energy (*a*) $\varepsilon = 0.01$ and (*b*) $\varepsilon = 1.9$, where black and white represents minimum and maximum values, respectively.

are similar to that of figure 1(*b*) and so are the central three subbands in figures 1(*e*) and (*c*). He conjectured that only $q-1$ bands occurred for even q, because the two central bands touch in the middle point $\varepsilon = 0$. We can indeed confirm this phenomenon, since the DOS vanished just at $\varepsilon = 0$ for both figures 1(*b*) and (*d*).

The divergence of DOS in the centre of subbands reflects 1D motion as DOS of free electrons in 1D space diverges in the limit $\varepsilon \to 0$ like $1/\sqrt{\varepsilon}$.

4.2. Space variation of the Green function

The density plot of $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = 0)|$ is presented in figure 2, near the band centre $\varepsilon = 0.01$ in (*a*) and near a band edge $\varepsilon = 1.99$ in (*b*). Near the band edge, $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = 0)|$ is smooth, while near the band centre it shows a checkered pattern as it takes maximum value when $\xi + \eta$ is even and minimum when $\xi + \eta$ is odd. Also the anisotropy of group velocity is well reflected in the profile of $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = 0)|$. We can expect such properties in the presence of a magnetic field as discussed below.

In contrast to the Green function $G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)$, the quantity $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)|$ can be written as a function of the relative coordinate (ξ, η). The density plots of $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)|$ for $\alpha = \frac{1}{2}$ are presented in figure 3 for (*a*) $\varepsilon = 0.5$, (*b*) 0.9999 and (*c*) 1.4. The Green function near an edge of a subband (figure 3(*c*)) is isotropic as well as figure 2(*b*) for $\alpha = 0$, $\varepsilon = 1.9$, whereas figures 3(*a*) and (*b*) show anisotropy. In particular, the wave favourably propagates in the diagonal directions of the lattice near the centre of subbands even for $\alpha = \frac{1}{2}$ due to anisotropy of the group velocity. That reflects the anisotropy of the group velocity. In fact, by differentiating both sides of (42) by $\boldsymbol{k}$, the group velocity is obtained as

$$\boldsymbol{v} = -q \left. \frac{(\sin k_x q, \sin k_y q)}{\frac{\partial \Delta_q(0,\varepsilon)}{\partial \varepsilon}} \right|_{\Delta_q(0,\varepsilon)+1=\cos k_x q+\cos k_y q.} \tag{45}$$

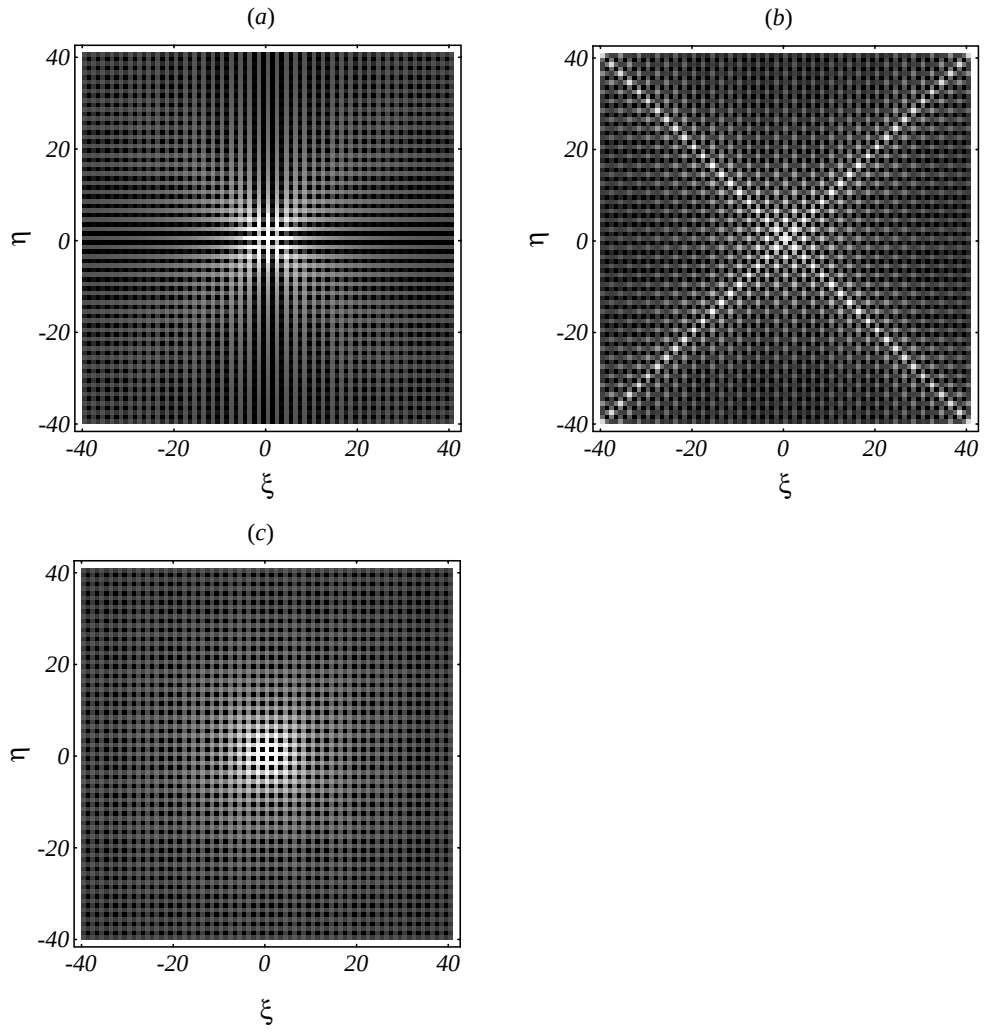

Figure 3. The density plot of $|G_0(\xi, \eta; \alpha = \frac{1}{2})|$ for energy (*a*) $\varepsilon = 0.5$, (*b*) $\varepsilon = 0.9999$ and (*c*) $\varepsilon = 1.4$.

When energy of electrons lies at the centre of subbands, equation (45) becomes

$$\boldsymbol{v} = -q \frac{\sin k_x q (1, \pm 1)}{\frac{\partial \Delta_q(0,\varepsilon)}{\partial \varepsilon}}. \tag{46}$$

It shows that electrons only propagate in four diagonal directions of the square lattice. This fact reflects in the divergence of DOS in the centre of subbands. On the other hand, when energy lies near an edge of subbands with $k_x, k_y \sim 0$, equation (45) yields

$$|\boldsymbol{v}|^2 = 2q^2 \frac{1 - \Delta_q(0, \varepsilon)}{\left(\frac{\partial \Delta_q(0,\varepsilon)}{\partial \varepsilon}\right)^2}. \tag{47}$$

Since the right-hand side of (47) is independent of $\boldsymbol{k}$, isotropic propagation is realized.

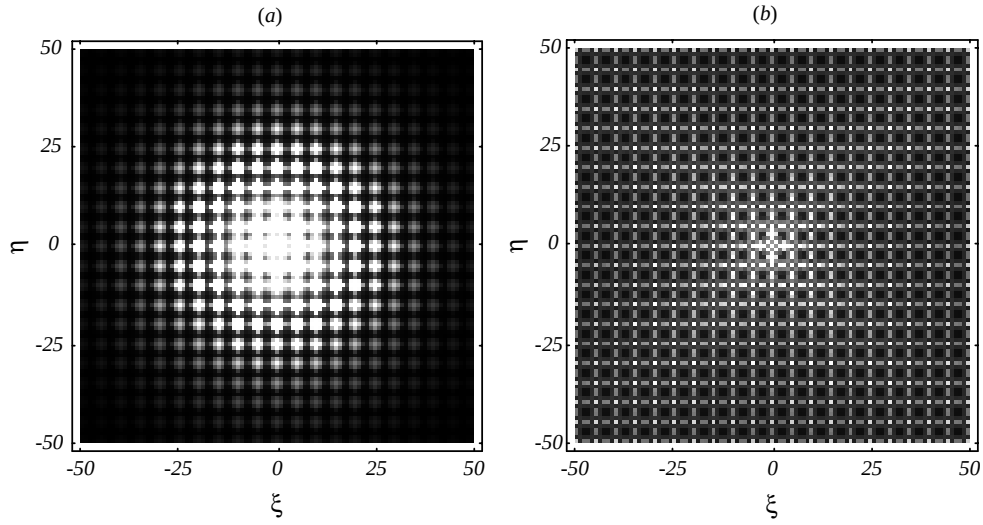

Figure 4. The density plot of $|G_0(\xi, \eta; \alpha)|$ for (*a*) $\alpha = \frac{1}{5}$, $\varepsilon = 1.45$ and (*b*) $\alpha = \frac{2}{5}$, $\varepsilon = 0.05$.

Although $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = 0)|$ is smooth near the subband edge, as shown in figure 2(*b*), $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = \frac{1}{2})|$ is not smooth even near the subband edges. From figures 3(*a*) and (*c*), we can see that $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha = \frac{1}{2})|$ has maximum values at the lattice points where ξ and η are even simultaneously. In figure 3(*b*), it has maximum values when $(\xi + \eta)/2$ is even. The oscillation observed in figure 3(*b*) seems superposition of two kinds of oscillation. The one appears near the centre of subbands as appeared in figure 2(*a*). The other is characteristic for $\alpha = \frac{1}{2}$ as appeared in figures 3(*a*) and (*c*). In figure 4, $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)|$ is plotted in (*a*) for $\alpha = \frac{1}{5}$, $\varepsilon = 1.45$ and in (*b*) for $\alpha = \frac{2}{5}$, $\varepsilon = 0.05$. Both figures 4(*a*) and (*b*) show complicated behaviours and have maximum values when both ξ and η are simultaneously multiples of 5. From these facts, we guess that the maximum of $|G(\boldsymbol{n}, \boldsymbol{n}'; \varepsilon, \alpha)|$ occurs on the lattice points of a square 'magnetic superlattice' [4] of q lattice spacing on a side for $\alpha = p/q$. The 'magnetic superlattice' is the reciprocal lattice of the magnetic Brillouin zone which is $(1/q)^2$ of the Brillouin zone. The unit cell of the magnetic superlattice is the smallest square cell that intercepts an integral number of flux quanta.

5. Summary and discussion

The square lattice Green function in magnetic fields has been expressed in terms of continued fractions. For rational magnetic fields ($\alpha = p/q$), the expression has been analytically reduced to a tractable form in terms of the two sequences and the out-going boundary condition has been applied for it. Its numerical calculation has been performed for several values of α. It is found that the Green function is isotropic near the subband edges, while near the centres of subbands it shows a marked anisotropy reflecting that of the group velocity. It has maximum value on the reciprocal lattice of the magnetic Brillouin zone.

However, some problems remain to be conquered. Although the Green function has been calculated for $q \leqslant 5$ numerically in this paper, the calculation for large values of q is very difficult. One of the reasons is that the out-going condition is too complicated to solve. Another is that it is difficult to perform Fourier transform of $g(\xi, k_y)$ numerically

since $g(\xi, k_y)$ has at most $2q$ singular points in k_y space when $\alpha = p/q$. Of course, the time consuming but steady calculations for each value of α gives us values of the Green function at arbitrary lattice points, but from a practical point of view, it is crucial to find a more convenient method. The eigenfunction expansion method never improves such a situation, since after analytical calculations, we will finally obtain an expression essentially equivalent to (38).

In this paper, we have derived the condition of the out-going wave for the commensurate cases. The reason is that the integrand of (37), that is $g^{\pm}(\xi, k_y)$, essentially depends on ξ as $\exp(\pm \mathrm{i}[\xi/q]\cos^{-1}\Delta_q)$. For the incommensurate cases, however, the condition cannot be determined, since we cannot know the dependence of the integrand on ξ. This is a very interesting and important problem. The results obtained here indicate an interesting possibility in the further study of the square tight-binding Green function.

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References

[1] Grehardts R R, Weiss D and von Klitzing K 1989 *Phys. Rev. Lett.* **62** 1173
[2] Winkler R W, Kotthaus J P and Ploog K 1989 *Phys. Rev. Lett.* **62** 1177
[3] Weiss D, Roukes M L, Menschig A, Grambow P, von Klitzing K and Weimann G 1991 *Phys. Rev. Lett.* **66** 2790
[4] Hofstadter D R 1976 *Phys. Rev.* B **14** 2239
[5] Peierls R E 1933 *Z. Phys.* **80** 763
[6] Thouless D J, Kohmoto M, Nightingale P and den Nijs M 1982 *Phys. Rev. Lett.* **49** 405
[7] Hiramoto H and Kohmoto M 1992 *Int. J. Mod. Phys.* B **6** 281
[8] Hatsugai Y 1993 *Phys. Rev.* B **48** 11 851
[9] Hatsugai Y, Kohmoto M and Wu Y S 1994 *Phys. Rev. Lett.* **73** 1134
[10] Wiegmann P B and Zabrodin A V 1994 *Phys. Rev. Lett.* **72** 1890
[11] Thouless D J and Kirkpatrick S 1981 *J. Phys. C: Solid State Phys.* **14** 235
[12] MacKinnon A 1985 *Z. Phys.* B **59** 385
[13] Ando T 1991 *Phys. Rev.* B **44** 8017
[14] Wannier G H, Obermair G M and Ray R 1979 *Phys. Status Solidi* **93** 337
[15] Schweitzer L, Kramer B and MacKinnon A 1984 *J. Phys. C: Solid State Phys.* **17** 4111
[16] Takahashi M, Hatsugai Y and Kohmoto M 1996 *J. Phys. Soc. Japan* **65** 529
[17] Schiff L I 1968 *Quantum Mechanics* (Auckland: McGraw-Hill) p 319
[18] Kawamura K, Ueta T and Sawano H 1992 *Japan. J. Appl. Phys.* **31** 317
[19] Ueta T 1996 *Engineering Analysis with Boundary Elements* **17** 69
[20] Ueta T *Engineering Analysis with Boundary Elements* submitted
[21] Ueta T 1992 *J. Phys. Soc. Japan* **61** 4314
[22] Czycholl G and Kramer B 1980 *Z. Phys.* B **39** 193
[23] MacKinnon A 1980 *J. Phys. C: Solid State Phys.* **13** L1031
[24] Pettifor D G and Weaire D L (ed) 1985 *The Recursion Method and Its Applications* (Berlin: Springer)
[25] Chambers W G 1965 *Phys. Rev.* A **140** 135