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On the Green function of the almost-Mathieu operator

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Abstract

The square tight-binding model in a magnetic field leads to the almost-Mathieu operator, which, for rational fields, reduces to a $q \times q$ matrix depending on the components μ , ν of the wavevector in the magnetic Brillouin zone. We calculate the corresponding Green function without explicit knowledge of eigenvalues and eigenfunctions and obtain analytical expressions for the diagonal and the first off-diagonal elements; the results which are consistent with the zero-magnetic-field case can be used to calculate several quantities of physical interest (e.g. the density of states over the entire spectrum, impurity levels in a magnetic field).

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1. Introduction

Different approaches to the problem of an electron in a two-dimensional periodic potential with an applied perpendicular magnetic field (see e.g. [1] or [2]) allow the reduction of the two-dimensional eigenvalue equation to a one-dimensional difference equation of the form

$$g_{m+1} + g_{m-1} + 2\gamma \cos(2\pi\alpha m - \nu)g_m = \epsilon g_m \quad (1)$$

known as the almost-Mathieu or Azbel–Harper equation, where ϵ is the energy of the electron scaled in units of the bandwidth at zero magnetic field.

Equation (1) corresponds to an effective Hamiltonian

$$\mathbf{H}_{eff} = 2 \cos(\hat{p}_x) + 2\gamma \cos(2\pi\alpha\hat{x} - \nu).$$

It has been studied extensively ever since Hofstadter's pioneering work [1], both for the fascinating Cantor-set properties and self-similarities of its eigenvalue spectrum $\text{spec} = \{\epsilon | g_m \text{ non diverging}\}$ (see e.g. [3–5] and references therein) and for its significance for periodically structured two-dimensional-electron systems (e.g. [6] and [7]).

In the following we restrict ourselves to the symmetric case $\gamma = 1$ corresponding to square symmetry of the two-dimensional periodic potential.

The phase $\nu \in [0, 2\pi[$ in (1) represents the component of the wavevector in the y -direction, α is the number of magnetic flux quanta per unit cell or—depending on the chosen ansatz—the number of unit cells per flux quantum.

As in most other work on this problem, we restrict α to the dense set of rational values

$$\alpha = \frac{p}{q} \quad (p \in \mathbb{Z}, q \in \mathbb{N}).$$

With this restriction (1) becomes periodic, i.e. it remains invariant under the substitution $m \mapsto m + q$. Therefore we may assume $m \in \{0, 1, \dots, q - 1\}$. According to Floquet's theorem (1) then has at least one solution of the form

$$g_{m+q} = e^{iq\mu} g_m. \quad (2)$$

The phase μ can be identified with the wavevector in the x -direction. With (2) the solution of the almost-Mathieu equation (1) can be reduced to the eigenvalue problem

$$\mathbf{H}\psi = \epsilon\psi \quad (3)$$

of the q -dimensional matrix corresponding to the almost-Mathieu operator \mathbf{H} for rational α :

$$\mathbf{H}(\mu, \nu) = \mathbf{H} := \begin{pmatrix} c_1 & 1 & 0 & \cdots & 0 & e^{iq\mu} \\ 1 & c_2 & 1 & & & 0 \\ 0 & 1 & \ddots & & & \vdots \\ \vdots & 0 & & & \ddots & 0 \\ 0 & \vdots & & \ddots & \ddots & 1 \\ e^{-iq\mu} & 0 & \cdots & 0 & 1 & c_q \end{pmatrix} \quad (4)$$

where $c_j := 2 \cos(2\pi j\alpha - \nu)$.

As has first been shown in [2], the eigenvalues of (4) can be obtained as the roots ϵ of the equation

$$\det(\epsilon - \mathbf{H}) = P(\epsilon) - 2 \cos(q\mu) - 2 \cos(q\nu) = 0. \quad (5)$$

Here $P(\lambda)$ is defined as the polynomial of degree q in λ for any $\lambda \in \mathbb{C}$:

$$P(\lambda) := \det \left(\lambda - \mathbf{H} \left(\frac{\pi}{2q}, \frac{\pi}{2q} \right) \right) = \det(\lambda - \mathbf{H}(0, 0)) - 4.$$

It depends only on λ and on α , and not on the phases μ and ν .

According to (5) the spectrum $\text{spec}(\mathbf{H})$ is given by the real solutions of

$$P(\epsilon) = P(\epsilon(\mu, \nu)) = 2 \cos(q\mu) + 2 \cos(q\nu). \quad (6)$$

Evidently for each fixed pair of values (μ, ν) (i.e. one point in the magnetic Brillouin zone) (6) yields q real eigenvalues. Varying $\nu \in [-\pi, \pi[$ and $\mu \in [-\pi, \pi[$, the eigenvalues are broadened into q magnetic subbands $\epsilon(\mu, \nu)$ [1]: each eigenvalue ϵ is a function of the momenta ν and μ and of the subband-index k , with $1 \leq k \leq q$. Except for some special cases where two subbands share one common point, e.g. for even q at $\epsilon = 0$, these subbands are disjoint. The graph of this subband structure in dependence on α is known as *Hofstadter's butterfly* [1].

According to (4), the eigenvectors ψ_k in (3) are vectors in \mathbb{C}^q with the elements g_1^k, \dots, g_q^k . Each g_j^k is a solution of (1) for $\epsilon = \epsilon_k(\mu, \nu)$; it depends on ν , μ , on the subband-index k and on its lattice site j .

In the next section we are going to develop a method to evaluate the resolvent or Green function \mathbf{G} of \mathbf{H} without explicit knowledge of the eigenvalues and eigenvectors of \mathbf{H} . This approach allows us to calculate an analytical expression for the diagonal elements of the resolvent in section 3, results that go beyond those obtained by Ueta in [8]. In section 4 we show how to calculate the off-diagonal elements of \mathbf{G} . A conclusion is given in section 5.

2. The Green function

The Green function $\mathbf{G}(\lambda, \mu, \nu)$ corresponding to $\mathbf{H}(\mu, \nu)$ is defined as

$$\mathbf{G}(\lambda, \mu, \nu) = (\lambda - \mathbf{H}(\mu, \nu))^{-1}$$

for all λ that are not in the spectrum of \mathbf{H} .

If the eigenvalues $\epsilon_k(\mu, \nu)$ and the eigenvectors $\psi_k(\mu, \nu)$ of \mathbf{H} were already known, $\mathbf{G}(\mu_0, \nu_0)$ could be evaluated through [9]

$$\mathbf{G}(\lambda, \mu_0, \nu_0) = \sum_{k=1}^q \frac{\psi_k(\mu_0, \nu_0) \psi_k^*(\mu_0, \nu_0)}{\lambda - \epsilon_k(\mu_0, \nu_0)}. \quad (7)$$

For most purposes (e.g. the calculation of impurity states) it is not sufficient to know \mathbf{G} at only one point (μ_0, ν_0) in the magnetic Brillouin zone; instead the Green function of the original two-dimensional tight-binding Hamiltonian, i.e. over the whole spectrum of \mathbf{H} , with $\mu \in [-\pi, \pi[$ and $\nu \in [-\pi, \pi[$, is needed. This is equivalent to a summation over the entire spectrum $\{\epsilon_k(\mu, \nu)\}$, i.e. by integrating over μ and ν :

$$\mathbf{G}(\lambda) = \frac{1}{4\pi^2} \sum_{k=1}^q \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{\psi_k(\mu, \nu) \psi_k^*(\mu, \nu)}{\lambda - \epsilon_k(\mu, \nu)} d\nu d\mu. \quad (8)$$

Alternatively the $(q \times q)$ matrix $\mathbf{G}(\mu, \nu)$ can be evaluated applying Cramer's rule for the inverse of a matrix:

$$\begin{aligned} (\mathbf{G}(\lambda, \mu_0, \nu_0))_{m,n} &= ((\lambda - \mathbf{H})^{-1})_{m,n} \\ &= \frac{A_{m,n}}{\det(\lambda - \mathbf{H})} \\ &= \frac{A_{m,n}}{P(\lambda) - 2 \cos(q\nu_0) - 2 \cos(q\mu_0)} \end{aligned} \quad (9)$$

for fixed values μ_0, ν_0 . $A_{m,n}$ in (9) represents the classical adjoint of $\lambda - \mathbf{H}$, i.e. the determinant of the matrix that we obtain when we delete the m th row and the n th column of $\lambda - \mathbf{H}$, multiplied by $(-1)^{m+n}$.

As in equation (8) we obtain the Green function of the original Hamiltonian, that is for all possible values of μ and ν through integration

$$(\mathbf{G}(\lambda))_{m,n} = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{A_{m,n}}{P(\lambda) - 2 \cos(q\nu) - 2 \cos(q\mu)} d\nu d\mu. \quad (10)$$

In this representation \mathbf{G} depends only on \mathbf{H} itself and not explicitly on the eigenvalues or eigenvectors of \mathbf{H} .

The Green function (10) has some really surprising features.

(i) An inspection of (4) shows that

$$\mathbf{G}(\lambda) \in \mathbb{R}^{(q \times q)} \quad (11)$$

for all $\lambda \in \mathbb{R}$, $\lambda \notin \text{spec}(\mathbf{H})$, because the imaginary part of $A_{m,n}$, if nonzero, always has a factor $\sin(q\mu)$, so it vanishes under the integral (10).

(ii) Due to the hermiticity of \mathbf{H} and (11):

$$(\mathbf{G}(\lambda))_{m,n} = (\mathbf{G}(\lambda))_{n,m} \quad (12)$$

for $\lambda \in \mathbb{R}$.

(iii) The elements in every (off-)diagonal are equal to each other:

$$(\mathbf{G}(\lambda))_{n,n+j} = (\mathbf{G}(\lambda))_{1,1+j} \tag{13}$$

for all $1 \leq n \leq q$ and $0 \leq j < q - n$. The proof of this property uses that

$$A_{n,n+j}(v) = A_{1,1+j}(v - 2\pi\alpha n)$$

which is easy to accept but rather lengthy to prove [10]; with this result the substitution $v \mapsto v' := v - 2\pi\alpha n$ leaves the integral (10) invariant.

3. The diagonal elements

Using equations (10)–(13) we are able to calculate the diagonal elements of \mathbf{G} . At first we take advantage of (13):

$$(\mathbf{G}(\lambda))_{n,n} = \frac{1}{q} \sum_{j=1}^q (\mathbf{G}(\lambda))_{j,j}.$$

From

$$\frac{d \det(\lambda - \mathbf{H}(\mu, v))}{d\lambda} = \frac{dP(\lambda) - 2 \cos(q\mu) - 2 \cos(qv)}{d\lambda} = \frac{dP(\lambda)}{d\lambda} = \sum_{j=1}^q A_{j,j}$$

the elements of (10) with $m = n$ can now be transformed to

$$(\mathbf{G}(\lambda))_{n,n} = \frac{1}{4\pi^2} \frac{1}{q} \frac{dP(\lambda)}{d\lambda} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} \frac{1}{P(\lambda) - 2 \cos(q\mu) - 2 \cos(qv)} dv d\mu. \tag{14}$$

The double integral in (14) is well known (see e.g. [11]), and $(\mathbf{G}(\lambda))_{n,n}$ evaluates to

$$(\mathbf{G}(\lambda))_{n,n} = \frac{2}{\pi q} \frac{1}{P(\lambda)} \frac{dP(\lambda)}{d\lambda} \mathbf{K} \left(\frac{4}{P(\lambda)} \right) \tag{15}$$

for all λ not in the spectrum of \mathbf{H} , hence, according to (6), for $|P(\lambda)| > 4$. \mathbf{K} denotes the complete elliptic integral of the first kind, cf [12].

In order to calculate the density of states (and other useful quantities) we need the well known extension of \mathbf{G} to complex λ and we define

$$\mathbf{G}^{\pm}(\lambda) = \lim_{s \rightarrow 0^+} \mathbf{G}(\lambda \pm is)$$

which is relevant for $\lambda \in \mathbb{R}$ in the continuous parts of $\text{spec}(\mathbf{H})$.

The diagonal elements of $\mathbf{G}^{\pm}(\lambda)$ are calculated with the analytic continuation of the elliptic integral [11]. For the real and the imaginary part we obtain

$$\begin{aligned} \text{Re}(\mathbf{G}^{\pm}(\lambda))_{n,n} &= \text{sign}(P(\lambda)) \frac{1}{2\pi q} \frac{dP(\lambda)}{d\lambda} \mathbf{K} \left(\frac{P(\lambda)}{4} \right) \\ \text{Im}(\mathbf{G}^{\pm}(\lambda))_{n,n} &= \mp \frac{1}{2\pi q} \frac{dP(\lambda)}{d\lambda} \mathbf{K}' \left(\frac{|P(\lambda)|}{4} \right). \end{aligned} \tag{16}$$

The density of states ρ is given by the imaginary part of \mathbf{G}^+ :

$$\rho(\lambda) = -\frac{1}{\pi} \text{Im}(\mathbf{G}^+(\lambda))_{n,n} = \frac{1}{2\pi^2 q} \frac{dP(\lambda)}{d\lambda} \mathbf{K}' \left(\frac{|P(\lambda)|}{4} \right).$$

This is identical to the result of Wannier *et al* [2].

The diagonal elements of \mathbf{G} and \mathbf{G}^+ are shown in figure 1.

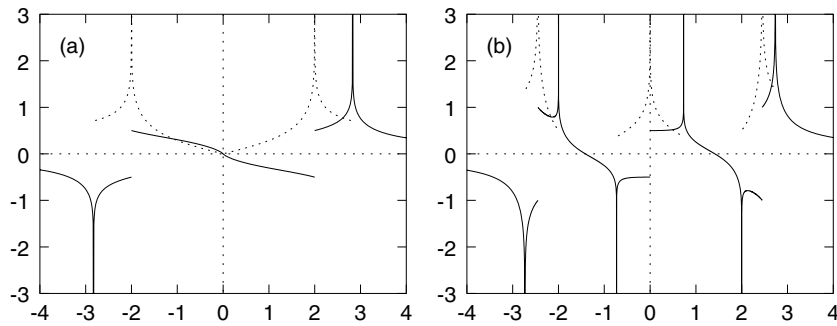


Figure 1. The diagonal elements of $G(\lambda)$ and $G^+(\lambda)$ versus λ : real (—) and imaginary part (- - -) for (a) $\alpha = \frac{1}{2}$ and (b) $\alpha = \frac{1}{3}$.

4. The off-diagonal elements

The off-diagonal elements of the Green function are required for many purposes, for example for the calculation of impurity states [13]. In the case of a vanishing magnetic field, where $P(\lambda) = \lambda$, it is possible to find a recurrence relation for all elements of the Green function [11]. In the presence of a magnetic field we were not able to find a general recurrence. Only the elements of the first off-diagonal $(G(\lambda))_{n,n\pm 1}$ may be evaluated in a similar way.

Using that

$$(\lambda - H)G(\lambda, \mu, \nu) = 1$$

and

$$G(\lambda, \mu, \nu)(\lambda - H) = 1$$

for every μ and ν , we obtain after integration

$$\begin{aligned} & (G(\lambda))_{i+1,j} + (G(\lambda))_{i-1,j} + (G(\lambda))_{i,j+1} + (G(\lambda))_{i,j-1} \\ &= \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} (2\lambda - c_i - c_j) \frac{A_{i,j}}{P(\lambda) - 2 \cos(q\mu) - 2 \cos(q\nu)} d\mu d\nu - 2\delta_{i,j}. \end{aligned}$$

With (12) we obtain an expression for the elements of the first off-diagonal:

$$(G(\lambda))_{i,i+1} = \frac{1}{2} \left(\frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} (\lambda - c_i) \frac{A_{i,i}}{P(\lambda) - 2 \cos(q\mu) - 2 \cos(q\nu)} d\mu d\nu - 1 \right). \quad (17)$$

The integral in (17) yields [10]

$$(G(\lambda))_{i,i+1} = \frac{1}{4}(\lambda(G(\lambda))_{i,i} - 1).$$

All the other elements of the Green function have to be calculated numerically by integrating (10); the result for $\alpha = \frac{1}{3}$ is shown in figure 2.

For some purposes it is necessary to extend the Green function over more than one magnetic period in the x -direction ($|m - n| > q$). For this case a continuation of G can be constructed by applying equations (2)–(7). The elements of this continuation are given by

$$(G(\lambda))_{m,n} = \frac{1}{4\pi^2} \int_{-\pi}^{\pi} \int_{-\pi}^{\pi} e^{iq\mu h} \frac{A_{m,n'}}{P(\lambda) - 2 \cos(q\nu) - 2 \cos(q\nu)} d\nu d\mu \quad (18)$$

where h is the integer part of $(m - n)/q$ and n' the remainder of n/q .

For each fixed $n' \in [0, q - 1]$ we see in figure 3, with $\alpha = \frac{1}{3}$ as an example, that $G(\lambda, m, n' + kq)$ decreases exponentially with growing $|m - n|$ (see figure 3).

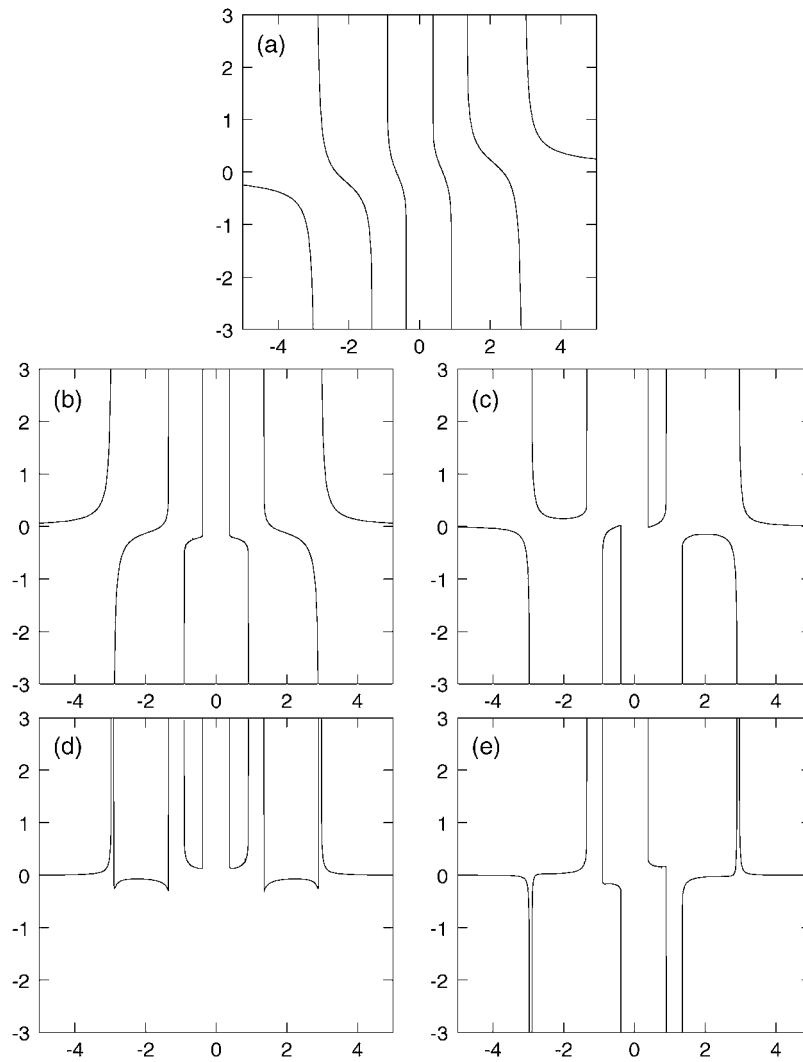


Figure 2. All different elements of G for $\alpha = \frac{1}{5}$: $(G(\lambda))_{n,n+l}$ versus λ with $l = 0$ (a), $l = 1$ (b), $l = 2$ (c), $l = 3$ (d) and $l = 4$ (e).

5. Conclusion

In the case of a vanishing magnetic field, $\alpha = 0$, $P(\lambda)$ reduces to

$$P(\lambda) = \lambda.$$

If we put this into the equations (15) and (16), we obtain the diagonal elements of the Green function of the tight-binding Hamiltonian as calculated in [11]. Thus our results are consistent in the limit $\alpha = 0$.

From another point of view, we could say that the minimal coupling to the vector potential

$$\hat{p} \mapsto \hat{p} + e\vec{A}$$

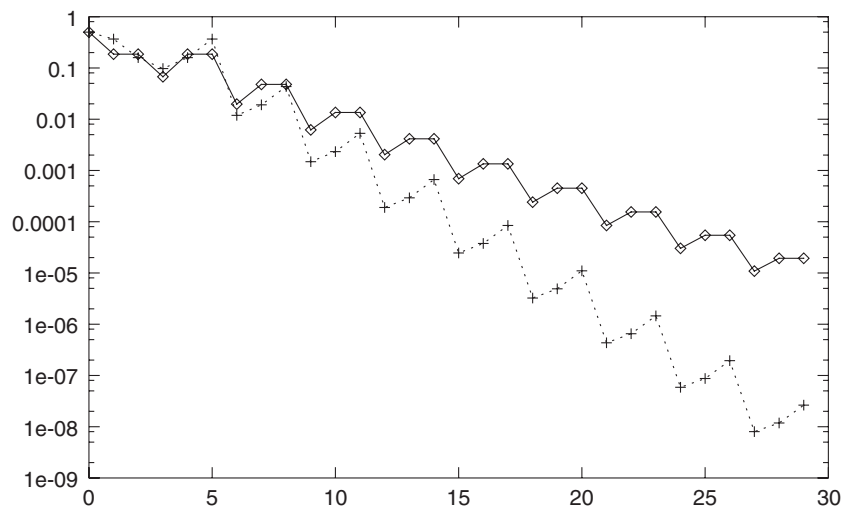


Figure 3. The extended Green function $(G(\lambda))_{m,n}$ (see equation (18)) for $\alpha = \frac{1}{3}$ versus $|m - n|$: $\lambda = 1.9$ (\diamond) and $\lambda = -3.4$ ($+$), scaled logarithmically. The lines only serve as a guide to the eye.

that is used to obtain the almost-Mathieu equation for electrons in the one-band model, is, within this model, equivalent to the transformation

$$\lambda \mapsto P(\lambda).$$

In a forthcoming paper [13] the results will be used to solve Dyson's equation for a model with isolated impurities, i.e. to calculate impurity states superimposed on Hofstadter's butterfly.

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