HOFSTADTER’S BUTTERFLY

The quantum mechanical system of an electron moving in a two-dimensional periodic potential in a constant magnetic field transverse to the plane of motion has attracted a great deal of interest. In particular, it has interesting connections to the quantum Hall effect and to the mean-field theory of the Hubbard model.

The Hamiltonian of our interest is given by

$$H = \frac{1}{2m} \left[ -i\hbar \vec{\nabla} - \frac{e}{c} \vec{A} \right]^2 + V(\vec{x})$$

(1)

with $B = \partial_x A_y - \partial_y A_x$ constant. The potential $V(\vec{x})$ is periodic with

$$V(\vec{x} + \vec{l}) = V(\vec{x}) ,$$

(2)

where $\vec{l} = n\vec{e}_1 + m\vec{e}_2$ ($n, m \in \mathbb{Z}$) and $\vec{e}_{1,2}$ form a basis for the two-dimensional lattice. We will restrict ourselves to a square lattice determined by a simple potential

$$V(\vec{x}) = -V_0 \left[ \cos (2\pi x/a) + \cos (2\pi y/a) - 2 \right] \text{ with } V_0 \geq 0 .$$

(3)

[1] Since the system is invariant under finite translations by the basis vectors of the lattice, we expect that the spectrum consists of Bloch bands parameterized by the eigenvalues of translation operators. However, one can show that naive expressions of translation operators below

$$U_x^{(0)} = e^{ip_x a/\hbar}$$

$$U_y^{(0)} = e^{ip_y a/\hbar}$$

(4)

do not commute with the Hamiltonian (1).

(a) Choosing the Landau gauge $\vec{A} = (-By, 0)$, construct correct translation operators $U_x$ and $U_y$ commuting with the Hamiltonian (1).

(b) Show that $U_x$ and $U_y$ no longer commute with each other;

$$U_x U_y = e^{2\pi i \alpha} U_y U_x ,$$

(5)

where $2\pi \alpha = \frac{ea^2}{\hbar c}$. The phase factor $e^{2\pi i \alpha}$ can be understood as the Aharonov-Bohm phase.
(c) Since \( U_x \) and \( U_y \) do not commute with each other, one cannot find eigenstates diagonalizing two translation operators \( U_x \) and \( U_y \) simultaneously. However, when
\[
\alpha = \frac{p}{q}
\]
with \( p, q \) integers, one can show that
\[
\left[U_x^q, U_y\right] = 0.
\]
One can then construct Bloch wave-functions on the magnetic lattice, which are eigenstates of the Hamiltonian (1) as well as of the magnetic translation operators \( U_x^q \) and \( U_y \).

In the absence of tunneling, we have approximate possible ground states localized at minima of the potential (3), denoted by pairs of integers
\[
|\bar{n}\rangle \equiv |(n_x, n_y)\rangle.
\]
Using (8), construct \( q \) different approximate ground states,
\[
|\vec{\theta} = (\theta_x, \theta_y), j\rangle \quad (j = 0, 1, ..., q - 1),
\]
that are eigenvectors of \( U_x^q \) and \( U_y \) with eigenvalues \( e^{i\theta_x} \) and \( e^{i\theta_y} \).

Let us now consider the matrix element
\[
\langle \vec{\theta}, j | e^{-HT/\hbar} | \vec{\theta}', j' \rangle.
\]
Since \( H \) commute with \( U_x^q \) and \( U_y \), this matrix element will be diagonal in \( \vec{\theta} \), but we expect that there will be mixing between states labeled by different \( j \) due to tunneling. This implies that there exist \( q \) different lowest bands.

[2] In the present work, let us propose to use the dilute-instanton-gas sum to compute the energy of \( q \) different lowest bands in the semi-classical limit. We have learned that the transition amplitudes between two approximate ground states can be described as
\[
\langle (n_x, n_y) | e^{-HT/\hbar} | (0, 0) \rangle \propto \lim_{T \to \infty} \int D\vec{x} \langle \vec{x}(\tau) \rangle e^{-S_E[\vec{x}(\tau)]/\hbar},
\]
subject to the boundary conditions
\[
\vec{x}(-T/2) = (0, 0), \quad \vec{x}(+T/2) = (n_x, n_y).
\]
In the semi-classical limit, the above path-integral is dominated by the stationary points of the Euclidean action \( S_E \), called the instanton configurations.
(a) Show that the instanton equations of motion are given by
\[
\begin{align*}
\frac{d^2}{d\xi^2} \bar{x} &= g^2 \left[ -i \frac{d}{d\xi} \bar{y} + 2\pi \sin (2\pi \bar{x}) \right], \\
\frac{d^2}{d\xi^2} \bar{y} &= g^2 \left[ +i \frac{d}{d\xi} \bar{x} + 2\pi \sin (2\pi \bar{y}) \right],
\end{align*}
\]
where \( \bar{x} = x/a \), \( \bar{y} = y/a \), and \( \xi = \frac{tE}{\tau} \), with \( \tau = \frac{2\pi\alpha}{a} \sqrt{\frac{V_0}{m}} \). Note that \( g \) is the ratio of the cyclotron frequency, \( \omega_c = \frac{eB}{mc} \), to the frequency of oscillation about a minimum of the potential \( V \), \( \omega_o = \frac{2\pi}{a} \sqrt{\frac{V_0}{m}} \), i.e., \( g = \frac{2\pi\omega_c}{\omega_o} \).

(b) First, we are looking for solutions to (13) that start at the bottom of one well, \((x,y) = (n_x, n_y)\) and travel to the bottom of an adjacent well along the \(x\)-direction, \((x,y) = (n_x \pm 1, n_y)\).

Since the terms related to the magnetic field (13) are imaginary, we cannot find real solutions. Instead, we look for a complex solution that takes the following from
\[
\begin{align*}
\bar{x}(\xi) &= n_x + x_R(\xi) , & \bar{y}(\xi) &= n_y + iy_I(\xi) ,
\end{align*}
\]
with \( x_R(-\infty) = 0 \), \( x_R(+\infty) = \pm 1 \) and \( y_I(\pm\infty) = 0 \). Explain why the above ansatz is legitimate to choose.

Substituting (14) into (13), the instanton equations become purely real:
\[
\begin{align*}
\frac{d^2}{d\xi^2} x_R &= g^2 \left[ \frac{d}{d\xi} y_I + 2\pi \sin (2\pi x_R) \right], \\
\frac{d^2}{d\xi^2} y_I &= g^2 \left[ \frac{d}{d\xi} x_R + 2\pi \sinh (2\pi y_I) \right].
\end{align*}
\]
Show that the Euclidean action for such a complex instanton solution in the \(x\) direction (15) is given by
\[
S_{Ex}/\hbar = \Re\left[ S_{Ex}/\hbar \right] + i\Im\left[ S_{Ex}/\hbar \right]
\]
with
\[
\Re\left[ S_{Ex}/\hbar \right] = 2\pi\alpha \int_{-\infty}^{+\infty} d\xi \left[ \frac{1}{2g^2} \left( \frac{dx_R}{d\xi} \right)^2 - \left( \frac{dy_I}{d\xi} \right)^2 \right] - y_I \frac{dx_R}{d\xi} \left( \cos (2\pi x_R) + \cosh (2\pi y_I) - 2 \right),
\]
and
\[
\Im\left[ S_{Ex}/\hbar \right] = 2\pi\alpha n_y \Delta x_R \quad (\Delta x_R \equiv x_R(+\infty) - x_R(-\infty) = \pm 1).
\]
(c) It is also interesting to consider a regime where the magnetic field is large compared to the strength of the potential, i.e., $g^2 \to \infty$. This is the regime where one can compare the path-integral calculation we are pursuing with a perturbative calculation of the splitting of the lowest Landau level.

Show that, in this limit $g^2 \to \infty$,

$$\pm 2\pi x_R(\xi) \simeq 2\tan^{-1}(\sqrt{2}\sinh(4\pi^2 \xi)) + \pi,$$

$$2\pi y_I(\xi) \simeq -\cosh^{-1}(1 + 2\text{sech}(8\pi^2 \xi)).$$

and

$$\Re\left[\frac{S_{Ex}}{\hbar}\right] = \alpha \int_0^1 dx_R \cosh^{-1}[2 - \cos(2\pi x_R)] \simeq (7.32772)\frac{\alpha}{2\pi}. \quad (19)$$

(d) Next, let us consider solutions to (13) that start at the bottom of one well, $(x, y) = (n_x, n_y)$ and travel to the bottom of an adjacent well along the $y$-direction, $(x, y) = (n_x, n_y \pm 1)$.

Choosing a reasonable ansatz for such a complex instanton solution in $y$-direction, show that the corresponding Euclidean action $S_{Ey}$ has no imaginary part, and agrees with the real part of $S_{Ex}$ obtained above.

(e) One can show that the contribution to the path-integral from each instanton in the $\pm x$ direction is

$$\int dt \ K_x e^{-S_E/\hbar} e^{-2\pi i n_y \delta x_R},$$

while each instanton in the $\pm y$ direction contributes

$$\int dt \ K_y e^{-S_E/\hbar}, \quad (22)$$

where $S_E = \Re[S_{Ex}] = S_{Ey}$, and two factors $K_x$ and $K_y$ are due to the Gaussian integrals around the classical instanton solutions in the $x$ and $y$ directions respectively. More precisely, $K_x$ and $K_y$ are proportional to

$$K_x = K_y \propto \sqrt{\frac{\det[D + V''(\vec{l})]}{\det[D + V''(\vec{x}_{\text{inst}})]}}, \quad (23)$$

where the operators $D$ and $V''(\vec{x})$ are given by

$$D = m \begin{pmatrix} \frac{d^2}{dt^2} & -i\omega_c \frac{d}{dt} \\ +i\omega_c \frac{d}{dt} & -\frac{d^2}{dt^2} \end{pmatrix}, \quad (24)$$
and

$$V''(\vec{x}) = \begin{pmatrix} \frac{\partial^2 V}{\partial x^2} & \frac{\partial^2 V}{\partial x \partial y} \\ \frac{\partial^2 V}{\partial y \partial x} & \frac{\partial^2 V}{\partial y^2} \end{pmatrix}. \tag{25}$$

For later convenience, show that, for large $T$,

$$\det \left[ D + V''(\vec{l}) \right]^{-1/2} \propto e^{-\frac{1}{2} \sqrt{\omega^2 + 4\omega^2_0} T}, \tag{26}$$

where $\vec{l} = (n_x, n_y)$ denotes the each lattice site.

[3] We are ready to evaluate the path-integral for the transition amplitude in the dilute-gas approximation. This is accomplished by summing over all classical paths in which the particle travels from one minimum of the potential to another minimum along adjoining instanton paths. We assume that the only significant contribution is due to instantons traveling between two adjacent minima, discussed in [2].

Sprinkling instantons in the $\pm x$ and $\pm y$ directions, the dilute-gas sum then becomes

$$\langle (n_x, n_y) | e^{-HT/\hbar} | (0, 0) \rangle \propto e^{-\frac{1}{2} \sqrt{\omega^2 + 4\omega^2_0} T} \sum_{\text{all possible paths}} \int_{-T/2}^{T/2} dt_1 \int_{-T/2}^{t_1} dt_2 \cdots \int_{-T/2}^{t_{M+N-1}} dt_{M+N} \left( K e^{-S_{\tilde{x}}/\hbar} \right)^{M+N} \exp \left[ -2\pi i \alpha \sum_{k=1}^{M+N} \left( y_k \Delta x_k / a^2 \right) \right], \tag{27}$$

where the sum is performed over all instanton paths from $\vec{x}_i = (0, 0)$ to $\vec{x}_f = a(n_x, n_y)$. For each path, $M$ and $N$ are the total number of instantons in the $\pm x$ and $\pm y$ directions. $y_k$ denotes the initial $y$ coordinate of the $k$-th instanton and $\Delta x_k$ is the distance it travels in the $x$ direction.

To evaluate the dilute-gas sum, it is convenient to parameterize the paths as follows: Divide a given path into $N + 1$ intervals labeled from 0 to $N$. During the $i$th interval, except the first one, the particle first takes one step in the $y$ direction. We define a number $n_i = \pm 1$ to described the distance $an_i \hat{y}$ traveled in the $i$th interval. The particle then takes $M_i$ steps in the $x$ direction. To described each of these $M_i$ steps we require the set of numbers $(m_i1, m_i2, ..., m_iM_i)$ with $m_ia = \pm 1$ so that $am_ia \hat{x}$ is the total distance traveled on the $a$th step during the $i$th interval.

In terms of these parameters, one can write the total number of steps taken in the $x$ direction as

$$M = \sum_{i=0}^{N} M_i, \tag{28}$$
and the total distance traveled as

\[ \vec{x}_f - \vec{x}_i = a \left( \sum_{i=0}^{N} \sum_{a=1}^{M_i} m_{ia}, \sum_{i=1}^{N} n_{i} \right). \] (29)

(a) Show that, using the above parametrization, the dilute-gas sum can be expressed as

\[
e^{-\frac{1}{2}\sqrt{\omega_c^2 + 4\omega_0^2}T} \sum_{N=0}^{\infty} \prod_{i=0}^{N} \left\{ \sum_{M_i=0}^{\infty} \right\} \prod_{j=1}^{N} \left\{ \sum_{n_j=\pm 1} \right\} \prod_{k=0}^{M_k} \prod_{a=1}^{n_{ka}=\pm 1} \left[ \delta_{n_y-\sum_{r=1}^{N} n_r} \times \right.
\]

\[
\delta_{n_x-\sum_{s=0}^{N} \sum_{c=1}^{M_s} m_{sc}} \cdot \frac{1}{(M+N)!} (KTE^{-S_E/h})^{M+N} \cdot \exp \left( -2\pi i \alpha \sum_{l=0}^{N} \sum_{b=1}^{M_l} \sum_{l=1}^{l} n_{l} \right), \] (30)

where \( \sum_{i=1}^{0} n_{i} \) is defined to be 0.

(b) Verify that performing the sums over \( m_{ia} \) and \( M_i \) can reduce (30) down to a sum over one-dimensional random walks,

\[
\langle (n_x, n_y) | e^{-HT/h} | (0, 0) \rangle \propto e^{-\frac{1}{2}\sqrt{\omega_c^2 + 4\omega_0^2}T} \int_{0}^{2\pi} d\theta_1 \int_{0}^{2\pi} d\theta_2 \int_{0}^{2\pi} d\nu \int_{0}^{2\pi} d\nu \cdot e^{-i\theta_1 n_x} e^{-i\theta_2 n_y} \cdot e^{Te^{i\nu}} \cdot G(\theta_1, \theta_2, \nu). \] (31)

with

\[ G(\theta_1, \theta_2, \nu) = \sum_{N=0}^{\infty} \prod_{i=1}^{N} \left[ \sum_{n_i=\pm 1} \right] \left[ e^{-i\nu N} \cdot (KE^{-S_E/h})^{N} \cdot e^{i\theta_2 \sum_{j=1}^{N} n_j} \times \right. \]

\[
\prod_{k=0}^{N} \left\{ 1 - 2KE^{-S_E/h}e^{-i\nu \cos (2\pi \alpha \sum_{t=1}^{k} n_{t} - \theta_1) \right\}^{-1} \right]\]. (32)

(c) When \( \alpha = p/q \), (32) implies that the continuum of ground states can be labeled by two angles \( \theta_1 \) and \( \theta_2 \), and that we only need to know the values of \( \sum_{t=1}^{k} n_{t} \) (\( k = 0, 1, ..., N \)) modulo \( q \). We will see shortly that these two facts will lead to the existence of the \( q \) different lowest energy bands.

For each path of \( N \) steps, let us define \( l_s \) (\( s = 0, 1, ..., q-1 \)) as the number of times the particle landing on a site congruent to \( s \) modulo \( q \). The total number of steps is then \( N = \sum_{s=0}^{(q-1)} l_s \).
Show that, with the above definition, (32) can be expressed as
\[ G(\theta_1, \theta_2, \nu) = \frac{1}{1 - 2(Ke^{-SE/h})z^{-1} \cos \theta_1} \sum_{N=0}^{\infty} \prod_{i=1}^{N} \left\{ \sum_{n_i=\pm 1} e^{i\theta_2 \sum_{j=1}^{n_j} t_s^i} \right\} e^{i\theta_2 \sum_{s=0}^{q-1} N} \prod_{s=0}^{q-1} t_{s_s^i}, \tag{33} \]
where \( z = e^{i\nu} \) and
\[ t_s = \frac{Ke^{-SE/h}}{z - 2(Ke^{-SE/h}) \cos (2\pi s - \theta_1)}. \tag{34} \]

(d) To sum the expression (33) further, let us define the \( q \)-dimensional vector
\[ F_s(N) = \prod_{i=1}^{N} \left\{ \sum_{n_i=\pm 1} \right\} \left[ e^{i\theta_2 \sum_{j=1}^{n_j} t_s^i} \delta_{s-\sum_{k=1}^{n_k}} \right], \quad (s = 0, 1, \ldots, q - 1) \tag{35} \]
where the Kronecker delta has to be evaluated modulo \( q \).

Show that, after working out the recursive relation for \( \vec{F}(N) \),
\[ \vec{F}(N) = A \cdot \vec{F}(0), \tag{36} \]
where \( A \) is a \( q \) by \( q \) matrix given by
\[
A = \begin{pmatrix}
0 & t_0e^{-i\theta_2} & 0 & 0 & \cdots & t_0e^{+i\theta_2} \\
t_1e^{+i\theta_2} & 0 & t_1e^{-i\theta_2} & 0 & \cdots & 0 \\
0 & t_2e^{+i\theta_2} & 0 & t_2e^{-i\theta_2} & & \\
& & \ddots & & \ddots & \\
0 & \cdots & t_{q-2}e^{+i\theta_2} & 0 & t_{q-2}e^{-i\theta_2} & t_{q-2}e^{+i\theta_2} \\
t_{q-1}e^{-i\theta_2} & 0 & \cdots & t_{q-1}e^{+i\theta_2} & 0 & t_{q-1}e^{-i\theta_2}
\end{pmatrix} \tag{37}
\]
and the \( q \)-dimensional vector \( \vec{F}(0) \) describes the starting configuration below
\[
\vec{F}(0) = \begin{pmatrix}
1 \\
0 \\
\vdots \\
0
\end{pmatrix}. \tag{38}
\]

Using the equation (36), verify that the function \( G(\theta_1, \theta_2, \nu) \) can be expressed as
\[ G(\theta_1, \theta_2, \nu) = \frac{1}{1 - 2(Ke^{-SE/h})z^{-1} \cos \theta_1} \left( \begin{pmatrix}
1 \\
1 \\
\vdots \\
1
\end{pmatrix} \cdot \frac{1}{1_q - A} \cdot \begin{pmatrix}
1 \\
0 \\
\vdots \\
0
\end{pmatrix} \right), \tag{39} \]
where \( 1_q \) denotes the \( q \)-dimensional identity matrix.
Substituting (39) into (31), show that the energy levels of $q$ different lowest bands are given by

$$E = \frac{\hbar}{2} \sqrt{\omega_c^2 + 4\omega_o^2} - \hbar \mathcal{E}(\theta_1, \theta_2, s; \alpha),$$

where $\mathcal{E}(\theta_1, \theta_2, s; \alpha)$ are the eigenvalues of the $q \times q$ matrix $\mathbf{H}$ below

$$\mathbf{H} = (K e^{-s E/\hbar})$$

\[
\begin{pmatrix}
 r_0 & e^{-i \theta_2} & 0 & 0 & \cdots & e^{+i \theta_2} \\
 e^{+i \theta_2} & r_1 & e^{-i \theta_2} & 0 & \cdots & 0 \\
 0 & e^{+i \theta_2} & r_2 & e^{-i \theta_2} & \vdots \\
 \vdots & \ddots & \ddots & \ddots & \ddots \\
 0 & \cdots & e^{+i \theta_2} & r_{q-2} & e^{-i \theta_2} \\
 e^{-i \theta_2} & 0 & \cdots & e^{+i \theta_2} & r_{q-1}
\end{pmatrix}
\]

with $r_s = 2 \cos(2\pi \alpha s - \theta_1)$ ($s = 0, 1, 2, \ldots, q - 1$). Componentwise, the eigenvalue equation can be expressed as

$$e^{-i \theta_2} g(s + 1) + e^{+i \theta_2} g(s - 1) + 2 \cos(2\pi \alpha s - \theta_1) g(s) = \frac{\mathcal{E}}{K e^{-s E/\hbar}} g(s)$$

with $g(s + q) = g(s)$. (42) is the well-known Harper’s equation.

The spectrum of the Harper equation was analyzed mainly by Hofstadter using transfer-matrix techniques. In particular, Hofstadter’s work emphasized the fractal and self-similar structure of the resulting spectrum. Figure 1 shows the graph of the spectrum of Harper’s equation as a function of $\alpha$. Can you see a butterfly there?