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

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

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

$$V(\vec{x} + \vec{l}) = V(\vec{x}) , \tag{2}$$

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

$$V(\vec{x}) = -V_0\left[\cos(2\pi x/a) + \cos(2\pi y/a) - 2\right] \text{ with } V_0 \geq 0 . \tag{3}$$

[**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

$$U_x^{(0)} = e^{ip_x a/\hbar}$$
$$U_y^{(0)} = e^{ip_y a/\hbar} \tag{4}$$

do not commute with the Hamiltonian (1).

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

(b) <u>Show</u> that U_x and U_y no longer commute with each other;

$$U_x U_y = e^{2\pi i\alpha} U_y U_x , \tag{5}$$

where $2\pi\alpha = \frac{eBa^2}{\hbar c}$. 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

$$\alpha = \frac{p}{q} \tag{6}$$

with p, q integers, one can show that

$$\left[U_x^q, U_y \right] = 0 \ . \tag{7}$$

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

$$|\vec{n}\rangle \equiv \left| (n_x, n_y) \right\rangle \ . \tag{8}$$

Using (8), <u>construct</u> q different approximate ground states,

$$\left| \vec{\theta} = (\theta_x, \theta_y), j \right\rangle \qquad (j = 0, 1, .., q-1) \ , \tag{9}$$

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

$$\left\langle \vec{\theta}, j \middle| e^{-HT/\hbar} \middle| \vec{\theta}', j' \right\rangle \ . \tag{10}$$

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

$$\left\langle (n_x, n_y) \middle| e^{-HT/\hbar} \middle| (0,0) \right\rangle \propto \lim_{T \to \infty} \int D\vec{x}(\tau) \ e^{-S_{\mathrm{E}}[\vec{x}(\tau)]/\hbar} \ , \tag{11}$$

subject to the boundary conditions

$$\vec{x}(-T/2) = (0,0) \ , \qquad \vec{x}(+T/2) = (n_x, n_y) \ . \tag{12}$$

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) <u>Show</u> that the instanton equations of motion are given by

$$\frac{d^2}{d\xi^2}\bar{x} = g^2 \left[-i\frac{d}{d\xi}\bar{y} + 2\pi \sin\left(2\pi\bar{x}\right) \right] \ ,$$

$$\frac{d^2}{d\xi^2}\bar{y} = g^2 \left[+i\frac{d}{d\xi}\bar{x} + 2\pi \sin\left(2\pi\bar{y}\right) \right] \ , \tag{13}$$

where $\bar{x} = x/a$, $\bar{y} = y/a$, and $\xi = t_{\rm E}/\tau$ with $\tau = 2\pi\alpha\hbar/V_0$. 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., $g = 2\pi\omega_c/\omega_o$.

(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

$$\bar{x}(\xi) = n_x + x_{\rm R}(\xi) \ , \qquad \bar{y}(\xi) = n_y + iy_{\rm I}(\xi) \ , \tag{14}$$

with $x_{\rm R}(-\infty) = 0$, $x_{\rm R}(+\infty) = \pm 1$ and $y_{\rm I}(\pm\infty) = 0$. <u>Explain</u> why the above ansatz is legitimate to choose.

Substituting (14) into (13), the instanton equations become purely real:

$$\frac{d^2}{d\xi^2}x_{\rm R} = g^2 \left[\frac{d}{d\xi}y_{\rm I} + 2\pi \sin\left(2\pi x_{\rm R}\right) \right] \ ,$$

$$\frac{d^2}{d\xi^2}y_{\rm I} = g^2 \left[\frac{d}{d\xi}x_{\rm R} + 2\pi \sinh\left(2\pi y_{\rm I}\right) \right] \ . \tag{15}$$

<u>Show</u> that the Euclidean action for such a complex instanton solution in the x direction (15) is given by

$$S_{{\rm E}x}/\hbar = \mathfrak{Re}\left[S_{{\rm E}x}/\hbar \right] + i\mathfrak{Im}\left[S_{{\rm E}x}/\hbar \right] \tag{16}$$

with

$$\mathfrak{Re}\left[S_{{\rm E}x}/\hbar \right] = 2\pi\alpha \int_{-\infty}^{+\infty} d\xi \ \left[\frac{1}{2g^2}\left\{ \left(\frac{dx_{\rm R}}{d\xi}\right)^2 - \left(\frac{dy_{\rm I}}{d\xi}\right)^2 \right\} - y_{\rm I}\frac{dx_{\rm R}}{d\xi} \right.$$
$$\left. -\left\{ \cos\left(2\pi x_{\rm R}\right) + \cosh\left(2\pi y_{\rm I}\right) - 2 \right\} \right] \ , \tag{17}$$

and

$$\mathfrak{Im}\left[S_{{\rm E}x}/\hbar \right] = 2\pi\alpha n_y \Delta x_{\rm R} \qquad (\Delta x_{\rm R} \equiv x_{\rm R}(+\infty) - x_{\rm R}(-\infty) = \pm 1) \ .. \tag{18}$$

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(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 $g^2 \to \infty$,

$$\pm 2\pi x_{\mathrm{R}}(\xi) \simeq 2\tan^{-1}(\sqrt{2}\sinh(4\pi^2\xi)) + \pi ,$$
$$2\pi y_I(\xi) \simeq -\cosh^{-1}(1 + 2\operatorname{sech}(8\pi^2\xi)) . \tag{19}$$

and

$$\mathfrak{Re}\left[S_{\mathrm{E}x}/\hbar\right] = \alpha \int_0^1 dx_{\mathrm{R}} \ \cosh^{-1}\left[2 - \cos(2\pi x_{\mathrm{R}})\right] \simeq (7.32772)\frac{\alpha}{2\pi} . \tag{20}$$

(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 $S_{\mathrm{E}y}$ has no imaginary part, and agrees with the real part of $S_{\mathrm{E}x}$ obtained above.

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

$$\int dt \ K_x e^{-S_{\mathrm{E}}/\hbar} e^{-2\pi i \alpha n_y \delta x_R} , \tag{21}$$

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

$$\int dt \ K_y e^{-S_{\mathrm{E}}/\hbar} , \tag{22}$$

where $S_{\mathrm{E}} = \mathfrak{Re}[S_{\mathrm{E}x}] = S_{\mathrm{E}y}$, 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

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

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

$$D = m \begin{pmatrix} -\frac{d^2}{dt_{\mathrm{E}}^2} & -i\omega_c \frac{d}{dt_{\mathrm{E}}} \\ +i\omega_c \frac{d}{dt_{\mathrm{E}}} & -\frac{d^2}{dt_{\mathrm{E}}^2} \end{pmatrix} , \tag{24}$$

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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, <u>show</u> that, for large T,

$$\det\left[D + V''(\vec{l})\right]^{-1/2} \propto e^{-\frac{1}{2}\sqrt{\omega_c^2 + 4\omega_0^2}\,T} \ , \tag{26}$$

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

$$\left\langle (n_x, n_y) \middle| e^{-HT/\hbar} \middle| (0,0) \right\rangle \propto e^{-\frac{1}{2}\sqrt{\omega_c^2 + 4\omega_0^2}\,T} \sum_{\substack{\text{all possible} \\ \text{paths}}} \int_{-T/2}^{T/2} dt_1 \int_{-T/2}^{t_1} dt_2 \cdots \int_{-T/2}^{t_{M+N-1}} dt_{M+N}$$

$$\left(K e^{-S_\mathrm{E}/\hbar}\right)^{M+N} \exp\left[-2\pi i \alpha \sum_{k=1}^{M+N} (y_k \Delta x_k)/a^2\right] \ , \tag{27}$$

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 $\pm$ directions. y_k denotes the initial y coordinate of the k-th instanton and Δx_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 ith 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 ith 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 ath step during the ith 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

$$\vec{x}_f - \vec{x}_i = a\Big(\sum_{i=0}^{N}\sum_{a=1}^{M_i} m_{ia}, \sum_{i=1}^{N} n_i\Big) \ . \tag{29}$$

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

$$e^{-\frac{1}{2}\sqrt{\omega_c^2+4\omega_0^2}\,T} \sum_{N=0}^{\infty} \cdot \prod_{i=0}^{N}\Big\{\sum_{M_i=0}^{\infty}\Big\} \cdot \prod_{j=1}^{N}\Big\{\sum_{n_j=\pm1}\Big\} \cdot \prod_{k=0}^{N}\prod_{a=1}^{M_k}\Big\{\sum_{m_{ka}=\pm1}\Big\}\Big[\delta_{n_y - \sum_{r=1}^{N} n_r} \times$$

$$\delta_{n_x - \sum_{s=0}^{N}\sum_{c=1}^{M_s} m_{sc}} \cdot \frac{1}{(M+N)!}\left(KTe^{-S_E/\hbar}\right)^{M+N} \cdot \exp\Big(-2\pi i\alpha \sum_{l=0}^{N}\sum_{b=1}^{M_l} m_{lb}\sum_{t=1}^{l} n_t\Big)\Big] \ , \tag{30}$$

where $\sum_{i=1}^{0} n_i$ is defined to be 0.

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

$$\big\langle(n_x, n_y)\big|e^{-HT/\hbar}\big|(0,0)\big\rangle \propto e^{-\frac{1}{2}\sqrt{\omega_c^2+4\omega_0^2}\,T}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\theta_1}{2\pi}\int_0^{2\pi}\frac{d\nu}{2\pi}$$

$$e^{-i\theta_1 n_x}e^{-i\theta_2 n_y}\cdot e^{Te^{i\nu}}\cdot G(\theta_1, \theta_2, \nu) \tag{31}$$

with

$$G(\theta_1, \theta_2, \nu) = \sum_{N=0}^{\infty}\cdot\prod_{i=1}^{N}\Big\{\sum_{n_i=\pm1}\Big\}\Big[e^{-i\nu N}\cdot\left(KE^{-S_E/\hbar}\right)^{N}\cdot e^{i\theta_2\sum_{j=1}^{N} n_j}\times$$

$$\prod_{k=0}^{N}\Big\{1 - 2KE^{-S_E/\hbar}e^{-i\nu}\cos\Big(2\pi\alpha\sum_{t=1}^{k} n_t - \theta_1\Big)\Big\}^{-1}\Big]\ . \tag{32}$$

(c) When $\alpha = p/q$, (32) implies that the continuum of ground states can be labeled by two angles θ_1 and θ_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 $N = \sum_{s=0}^{(q-1)} l_s$.

<u>Show</u> that, with the above definition, (32) can be expressed as

$$G(\theta_1, \theta_2, \nu) = \frac{1}{1 - 2(Ke^{-S_E/\hbar})z^{-1}\cos\theta_1} \sum_{N=0}^{\infty} \cdot \prod_{i=1}^{N}\left\{\sum_{n_i=\pm 1}\right\} e^{i\theta_2 \sum_{j=1}^{N} n_j} \prod_{s=0}^{q-1} t_s^{l_s}, \quad (33)$$

where $z = e^{i\nu}$ and

$$t_s = \frac{Ke^{-S_E/\hbar}}{z - 2(Ke^{-S_E/\hbar})\cos\left(2\pi\alpha s - \theta_1\right)} \ . \quad (34)$$

(d) To sum the epxression (33) further, let us define the q-dimensional vector

$$F_s(N) = \prod_{i=1}^{N}\left\{\sum_{n_i=\pm 1}\right\}\left[e^{i\theta_2 \sum_{j=1}^{N} n_j} \prod_{s=0}^{q-1} t_s^{l_s} \cdot \delta_{s - \sum_{k=1}^{N} n_k}\right], (s = 0, 1, .., q-1) \quad (35)$$

where the Kronecker delta has to be evaluated modulo q.

<u>Show</u> that, after working out the recursive relation for $\vec{F}(N)$,

$$\vec{F}(N) = \mathbf{A} \cdot \vec{F}(0) \ , \quad (36)$$

where $\mathbf{A}$ is a q by q matrix given by

$$\mathbf{A} = \begin{pmatrix} 0 & t_0 e^{-i\theta_2} & 0 & 0 & \cdots & t_0 e^{+i\theta_2} \\ t_1 e^{+i\theta_2} & 0 & t_1 e^{-i\theta_2} & 0 & \cdots & 0 \\ 0 & t_2 e^{+i\theta_2} & 0 & t_2 e^{-i\theta_2} & & \vdots \\ \vdots & & & \ddots & & \\ 0 & \cdots & & t_{q-2} e^{+i\theta_2} & 0 & t_{q-2} e^{-i\theta_2} \\ t_{q-1} e^{-i\theta_2} & 0 & \cdots & & t_{q-1} e^{+i\theta_2} & 0 \end{pmatrix} \quad (37)$$

and the q-dimensional vector $\vec{F}(0)$ describes the starting configuration below

$$\vec{F}(0) = \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \ . \quad (38)$$

Using the equation (36), <u>verify</u> that the function $G(\theta_1, \theta_2, \nu)$ can be expressed as

$$G(\theta_1, \theta_2, \nu) = \frac{1}{1 - 2(Ke^{-S_E/\hbar})z^{-1}\cos\theta_1}\begin{pmatrix}1 & 1 & \cdots & 1\end{pmatrix} \cdot \frac{1}{\mathbf{1_q} - \mathbf{A}} \cdot \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad (39)$$

where $\mathbf{1_q}$ denotes the q-dimensional identity matrix.

[**4**] Substituting (39) into (31), <u>show</u> that the energy levels of q different lowest bands are given by

$$E = \frac{\hbar}{2}\sqrt{\omega_c^2 + 4\omega_o^2} - \hbar\mathcal{E}(\theta_1, \theta_2, s; \alpha) \ , \tag{40}$$

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

$$\mathbf{H} = (Ke^{-S_{\mathrm{E}}/\hbar})\begin{pmatrix} r_0 & e^{-i\theta_2} & 0 & 0 & \cdots & e^{+i\theta_2} \\ e^{+i\theta_2} & r_1 & e^{-i\theta_2} & 0 & \cdots & 0 \\ 0 & e^{+i\theta_2} & r_2 & e^{-i\theta_2} & & \vdots \\ \vdots & & & \ddots & & \\ 0 & \cdots & & e^{+i\theta_2} & r_{q-2} & e^{-i\theta_2} \\ e^{-i\theta_2} & 0 & \cdots & & e^{+i\theta_2} & r_{q-1} \end{pmatrix} \tag{41}$$

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

$$e^{-i\theta_2}g(s+1) + e^{+i\theta_2}g(s-1) + 2\cos(2\pi\alpha s - \theta_1)g(s) = \frac{\mathcal{E}}{Ke^{-S_{\mathrm{E}}/\hbar}}g(s) \tag{42}$$

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 trasnfer-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 α. *Can you see a butterfly there?*

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