Thouless pumping

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We have learned that the Berry phase appears when a quantum state undergoes an adiabatic evolution with a time-dependent Hamiltonian. We shall explore the yet another interesting quantization phenomenon, the *Thouless pumping* of Bloch electrons, accompanying a *periodic* adiabatic time-evolution of a 1D *periodic* lattice potential. Here the parameter space is torus spanned by the time t and the wave number k.

I. 1D BLOCH ELECTRON [1, 2]

Now we shall extend our interest to solid state physics and explore the Berry phase associated with a periodic time-evolution of a 1D Bloch electron. The model Hamiltonian is

$$H(t) = \frac{p^2}{2m} + V(x,t), \tag{1}$$

where the potential $V(x,t)$ assumes the periodic boundary condition $V(x+a,t) = V(x,t)$ all the time, where a is the lattice constant. According to Bloch's theorem the instantaneous eigenstates can be given by the Bloch form:

$$|\psi_{n,k}(x,t)\rangle = e^{ikx}|u_{n,k}(x,t)\rangle, \tag{2}$$

with the *twisted* periodic boundary condition:

$$|\psi_{n,k}(x+a,t)\rangle = e^{ika}|\psi_{n,k}(x,t)\rangle \tag{3}$$

where n stands for the band index and k does for the wave number. To eliminate the extra phase factor e^{ika} in the twisted periodic boundary condition, Eq. (3), we can use the cell-periodic part $|u_{n,k}(x,t)\rangle$ of the Bloch form Eq. (2) as the instantaneous eigenstates. This is basically a gauge-transformation. The boundary condition for $|u_{n,k}(x,t)\rangle$ is the ordinary one,

$$|u_{n,k}(x+a,t)\rangle = |u_{n,k}(x,t)\rangle, \tag{4}$$

at the expense of the Hamiltonian Eq. (1) being changed into k-dependent form

$$H(k,t) = e^{-ikx}H(t)e^{ikx} = \frac{1}{2m}\left(p+\hbar k\right)^2 + V(x,t). \tag{5}$$

The k-dependent Hamiltonian can be derived from the fact that

$$\begin{aligned} e^{-ikx}pe^{ikx} &= e^{-ikx}\left(-i\hbar\frac{\partial}{\partial x}\right)e^{ikx} \\ &= \hbar k - i\hbar\frac{\partial}{\partial x} = \hbar k + p. \end{aligned} \tag{6}$$

A. Quantum adiabatic theorem [1, 2]

Let us consider a time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\left|\psi_k(t)\right\rangle = H(k,t)\left|\psi_k(t)\right\rangle. \tag{7}$$

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The state $|\psi_k(t)\rangle$ can be expanded using the instantaneous eigenstates $|u_{n,k}(t)\rangle$ as

$$|\psi_k(t)\rangle = \sum_n \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \epsilon_{n,k}\right] a_{n,k}(t)\,|u_{n,k}(t)\rangle\,, \tag{8}$$

where $a_{n,k}$ are the coefficients. By plugging Eq. (8) into Eq. (7) and multiply $\langle u_{n',k}|$ from the left we find that the coefficients $a_{n,k}$ satisfy

$$\dot{a}_{n',k}(t) = -\sum_n a_{n,k}(t) \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left(\epsilon_{n,k} - \epsilon_{n',k}\right)\right] \left\langle u_{n',k}(t)\middle|\frac{\partial}{\partial t}\middle|u_{n,k}(t)\right\rangle. \tag{9}$$

Now we use the *parallel transport gauge* [1, 2], that is, the phase of $|u_{n,k}(t)\rangle$ is chosen to be satisfy

$$\left\langle u_{n,k}(t)\middle|\frac{\partial}{\partial t}\middle|u_{n,k}(t)\right\rangle = 0 \tag{10}$$

except for the edge region. This means that the Berry connection is zero in the bulk but non-zero at the edge. This brings us to the conclusion that

$$\dot{a}_{n,k}(t) = 0 \tag{11}$$

when $a_{n,k}(0) = 1$, that is, the state is initially in the eigenstate $|u_{n,k}\rangle$. Thus $|u_{n,k}\rangle$ stays in the same state. This is the *quantum adiabatic theorem.*

B. Zero-order current: j_0

The velocity of the electron can then be given by

$$\dot{x} = v = -\frac{i}{\hbar}\left[x, H(t)\right]. \tag{12}$$

The velocity of the electron in a state of given k and band index n can then be obtained by

$$\begin{aligned}
v_{n,k}^{(0)} &\equiv \langle u_{n,k}|e^{-ikx} v e^{ikx}|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|e^{-ikx}\left[x, H(t)\right] e^{ikx}|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\left[x, \underbrace{e^{-ikx}H(t)e^{ikx}}_{H(k,t)}\right]|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\left[x, \frac{1}{2m}\left((p+\hbar k)^2 + V(x,t)\right)\right]|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\underbrace{\left[x, \frac{1}{2m}\left(\left(-i\hbar\frac{\partial}{\partial x} + \hbar k\right)^2 + V(x,t)\right)\right]}_{i\hbar\frac{p+\hbar k}{m}}|u_{n,k}\rangle \\
&= \langle u_{n,k}|\frac{1}{m}\left(p+\hbar k\right)|u_{n,k}\rangle \\
&= \frac{1}{\hbar}\langle u_{n,k}|\frac{\partial H}{\partial k}|u_{n,k}\rangle \\
&= \frac{1}{\hbar}\frac{\partial \epsilon_{n,k}}{\partial k}.
\end{aligned} \tag{13}$$

Integrating over the Brillouin zone we have the zero total current:

$$\begin{aligned} j_0 &= -e\sum_n \int_{\mathrm{BZ}} \frac{dk}{2\pi} v^{(0)}_{n,k} \\ &= -e\sum_n \frac{1}{\hbar}\int_{\mathrm{BZ}} \frac{dk}{2\pi}\frac{\partial \epsilon_{n,k}}{\partial k} \\ &= -e\sum_n \frac{1}{h}\int_{\mathrm{BZ}} d\epsilon_{n,k} \\ &= -e\sum_n \frac{1}{h}\left[\epsilon_{k=\frac{\pi}{a},n} - \epsilon_{k=-\frac{\pi}{a},n}\right] = 0. \end{aligned} \tag{14}$$

C. First-order correction [1, 2]

The first-order correction of this situation is crucial for now. Suppose that, at time $t = 0$, $a_{n,k}(0) = 1$ and $a_{n',k}(0) = 0$ for $n' \neq n$. We have from Eq. (9) with $a_{n,k}(t) \sim 1$

$$\dot{a}_{n',k}(t) = -\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left(\epsilon_{n,k} - \epsilon_{n',k}\right)\right]\left\langle u_{n',k}\middle|\frac{\partial}{\partial t}\middle|u_{n,k}\right\rangle. \tag{15}$$

The solution of this integro-differential equation can be obtained by assuming that $\langle u_{n',k}|\frac{\partial}{\partial t}|u_{n,k}\rangle$ is more or less constant as compared with the exponential part. The resultant solution is given by

$$a_{n',k}(t) = -\frac{i\hbar}{\epsilon_{n,k} - \epsilon_{n',k}}\exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \left(\epsilon_{n,k} - \epsilon_{n',k}\right)\right]\left\langle u_{n',k}\middle|\frac{\partial}{\partial t}\middle|u_{n,k}\right\rangle. \tag{16}$$

Plugging this results for $a_{n',k}(t)$ and $a_{n,k}(t) = 1$ into Eq. (8), we have

$$|\psi_k(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \epsilon_{n,k}\right]\left(\underbrace{|u_{n,k}(t)\rangle - i\hbar\sum_{n'\neq n}\frac{|u_{n',k}\rangle\langle u_{n',k}|\frac{\partial}{\partial t}|u_{n,k}\rangle}{\epsilon_{n,k} - \epsilon_{n',k}}}_{\left|u^{(1)}_{n,k}(t)\right\rangle}\right). \tag{17}$$

We can see that the refined eigenstate $\left|u^{(1)}_{n,k}(t)\right\rangle$ contains not only the contribution from the state $|u_{n,k}(t)\rangle$ but also the contributions from the states of other bands $|u_{n',k}(t)\rangle$. The first-order correction to the velocity, Eq. (13), now reads

$$\begin{aligned} v^{(1)}_{n,k} &\equiv \frac{1}{\hbar}\langle u_{n,k}|\frac{\partial H}{\partial k}|\left(-i\hbar\sum_{n'\neq n}\frac{|u_{n',k}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle}{\epsilon_{n,k} - \epsilon_{k,n'}}\right) + \frac{1}{\hbar}\left(i\hbar\sum_{n'\neq n}\frac{\left\langle\frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\langle u_{n',k}|}{\epsilon_{n,k} - \epsilon_{k,n'}}\right)|\frac{\partial H}{\partial k}|u_{n,k}\rangle \\ &= -i\sum_{n'\neq n}\frac{1}{\epsilon_{n,k} - \epsilon_{k,n'}}\left(\left\langle u_{n,k}\middle|\frac{\partial H}{\partial k}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial H}{\partial k}\middle|u_{n,k}\right\rangle\right). \end{aligned} \tag{18}$$

II. ADIABATIC VELOCITY, BERRY CURVATURE, AND DEGENERACY

A. Adiabatic velocity

We shall now find the interesting relationship between the adiabatic velocity, Eq. (18), and the Berry curvature. To see the relationship, let us differentiate the eigen-equation

$$H(k,t)|u_{n,k}(t)\rangle = \epsilon_{n,k}(t)|u_{n,k}(t)\rangle \tag{19}$$

with respect to $\boldsymbol{R} = \begin{bmatrix} k \\ t \end{bmatrix}$, i.e.,

$$\frac{\partial H(k,t)}{\partial \boldsymbol{R}} |u_{n,k}(t)\rangle + H(k,t) \left| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle = \frac{\partial \epsilon_{n,k}(t)}{\partial \boldsymbol{R}} |u_{n,k}(t)\rangle + \epsilon_{n,k}(t) \left| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle . \tag{20}$$

Then, by projecting on to the state $|u_{n',k}(t)\rangle$, we have

$$\left\langle u_{n',k}(t) \middle| \frac{\partial H(k,t)}{\partial \boldsymbol{R}} \middle| u_{n,k}(t) \right\rangle + \underbrace{\left\langle u_{n',k}(t) \middle| H(k,t) \middle| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle}_{\epsilon_{n',k}(t)\left\langle u_{n',k}(t) \middle| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle} = \underbrace{\frac{\partial \epsilon_{n,k}(t)}{\partial \boldsymbol{R}} \langle u_{n',k}(t) | u_{n,k}(t) \rangle}_{0} + \epsilon_{n,k}(t) \left\langle u_{n',k}(t) \middle| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle .$$

We have thus the following relation:

$$\left\langle u_{n',k}(t) \middle| \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \right\rangle = \frac{1}{\epsilon_{n,k}(t) - \epsilon_{n',k}(t)} \left\langle u_{n,k}(t) \middle| \frac{\partial H(k,t)}{\partial \boldsymbol{R}} \middle| u_{n',k}(t) \right\rangle . \tag{21}$$

Similarly, the following relation also hold:

$$\left\langle \frac{\partial u_{n,k}(t)}{\partial \boldsymbol{R}} \middle| u_{n',k}(t) \right\rangle = \frac{1}{\epsilon_{n,k}(t) - \epsilon_{n',k}(t)} \left\langle u_{n',k}(t) \middle| \frac{\partial H(k,t)}{\partial \boldsymbol{R}} \middle| u_{n,k}(t) \right\rangle . \tag{22}$$

By exploiting these relations the adiabatic velocity, Eq. (18), becomes

$$\begin{aligned} v_{n,k}^{(1)} &= -i \sum_{n' \neq n} \left(\left\langle \frac{\partial u_{n,k}}{\partial k} \middle| u_{n',k} \right\rangle \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial t} \right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t} \middle| u_{n',k} \right\rangle \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial k} \right\rangle \right) \\ &= -i \left(\left\langle \frac{\partial u_{n,k}}{\partial k} \middle| \frac{\partial u_{n,k}}{\partial t} \right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t} \middle| \frac{\partial u_{n,k}}{\partial k} \right\rangle \right) . \end{aligned} \tag{23}$$

B. Berry Curvature

Let us further perform the following manipulations with a mock-up matrix form,

$$\begin{aligned} v_{n,k}^{(1)} &= -i \sum_{n' \neq n} \left(\left\langle \frac{\partial u_{n,k}}{\partial k} \middle| u_{n',k} \right\rangle \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial t} \right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t} \middle| u_{n',k} \right\rangle \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial k} \right\rangle \right) \\ &= -i \sum_{n' \neq n} \left(\underbrace{\begin{bmatrix} \left\langle \frac{\partial u_{n,k}}{\partial k} \middle| u_{n',k} \right\rangle \\ \left\langle \frac{\partial u_{n,k}}{\partial t} \middle| u_{n',k} \right\rangle \\ 0 \end{bmatrix}}_{\left\langle \frac{\partial u_{n,k}}{\partial \boldsymbol{R}} \middle| u_{n',k} \right\rangle} \times \underbrace{\begin{bmatrix} \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial k} \right\rangle \\ \left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial t} \right\rangle \\ 0 \end{bmatrix}}_{\left\langle u_{n',k} \middle| \frac{\partial u_{n,k}}{\partial \boldsymbol{R}} \right\rangle} \right)_z \\ &= -i \left(\left\langle \frac{\partial u_{n,k}}{\partial \boldsymbol{R}} \right| \times \left| \frac{\partial u_{n,k}}{\partial \boldsymbol{R}} \right\rangle \right)_z \\ &= -\left(\underbrace{\frac{\partial}{\partial \boldsymbol{R}}}_{\boldsymbol{\nabla}_{k,t}} \times \underbrace{\left(i \left\langle u_{n,k} \middle| \frac{\partial}{\partial \boldsymbol{R}} \middle| u_{n,k} \right\rangle \right)}_{\boldsymbol{A}_{n,k}(t)} \right)_z \\ &= -\Omega_{n,k}(t), \end{aligned} \tag{24}$$

where we found the Berry connection $\boldsymbol{A}_{n,k}(t)$ and the Berry curvature $\Omega_{n,k}(t)$ appear. The adiabatic velocity, Eq. (18), is thus nothing but the Berry curvature itself. Note that this Berry curvature here measures the curvature of the space spanned by the time t and the wave number k.

C. Degeneracy

With Eqs. (21) and (22), the Berry curvature $\Omega_{n,k}(t)$ can also be written by

$$\begin{aligned}\Omega_{n,k}(t) &= i\sum_{n'=n}\left\langle \frac{\partial}{\partial \boldsymbol{R}}u_{n,k}(t)\middle|u_{n',k}(t)\right\rangle \times \left\langle u_{n',k}(t)\middle|\frac{\partial}{\partial \boldsymbol{R}}u_{n,k}(t)\right\rangle \\ &= \sum_{n'=n}\frac{i}{\left(\epsilon_{n,k}(t)-\epsilon_{n',k}(t)\right)^2}\left\langle u_{n,k}(t)\middle|\frac{\partial H(k,t)}{\partial \boldsymbol{R}}\middle|u_{n',k}(t)\right\rangle \times \left\langle u_{n',k}(t)\middle|\frac{\partial H(k,t)}{\partial \boldsymbol{R}}\middle|u_{n,k}(t)\right\rangle,\end{aligned} \tag{25}$$

suggesting that whenever $\epsilon_{n,k}(\boldsymbol{R}) \sim \epsilon_{n',k}(\boldsymbol{R})$ (the degeneracy points!) the Berry curvature $\Omega_{n,k}(t)$ becomes large. Note that the advantage of the last formula Eq. (25) is that there is no differentiation on the wave function.

III. QUANTIZATION OF CHARGE TRANSPORT [1, 3]

Now we shall consider a cyclic time-evolution, that is, t assumes the periodic boundary conditions $t+T=t$. Since k also assumes the periodic boundary conditions $k+G=k$ where $G=\frac{2\pi}{a}$, the parameter space is now *torus*. Integrating over the Brillouin zone we have the Berry-curvature induced *adiabatic current*:

$$j_1 = -e\sum_n\int_{\mathrm{BZ}}\frac{dk}{2\pi}v^{(1)}_{n,k} = e\sum_n\int_{\mathrm{BZ}}\frac{dk}{2\pi}\Omega_{n,k}. \tag{26}$$

Let us see the number of charges transported by the nth-band adiabatic current per one-cycle of periodic time evolution. To see this, we shall integrate the $\frac{j_1}{e}$ over the one cycle of periodic time-evolution:

$$c_n = \int_0^T dt\int_{\mathrm{BZ}}\frac{dk}{2\pi}\Omega_{n,k}. \tag{27}$$

The quantity $2\pi c_n$ is nothing but the Berry phase of this problem since the value is obtained by integrating the Berry curvature over the surface of the parameter space. By rescaling $t\to x=\frac{t}{T}$ and $k\to y=\frac{k}{G}$, we have

$$c_n = \frac{1}{2\pi}\int_0^1 dx\int_0^1 dy\ \Omega(x,y), \tag{28}$$

where

$$\Omega(x,y) = \frac{\Omega_{n,k}}{TG}. \tag{29}$$

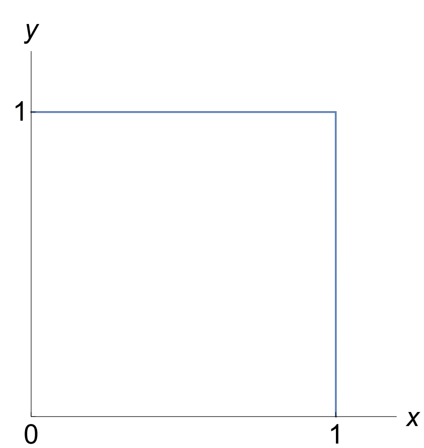

FIG. 1. Path $(0,0)\to(1,0)\to(1,1)\to(0,1)\to(0,0)$ is used to evaluate the integral Eq. (30).

We can now use the Stokes theorem to obtain the line integral form of Eq. (28), that is,

$$\begin{aligned} c_n &= \frac{1}{2\pi}\oint_{\mathrm{C}} dl A(x,y) \\ &= \frac{1}{2\pi}\left(\int_0^1 dx A(x,0) + \int_0^1 dy A(1,y) + \int_1^0 dx A(x,1) + \int_1^0 dy A(0,y)\right) \\ &= \frac{1}{2\pi}\left(\int_0^1 dx\left(A(x,0)-A(x,1)\right) + \int_0^1 dy\left(A(1,y)-A(0,y)\right)\right), \end{aligned} \tag{30}$$

where the line integral is along the path $(0,0)\to(1,0)\to(1,1)\to(0,1)\to(0,0)$ in Fig. 1. Here, the Berry connection $A(x,y)$ is given by

$$A(x,y) = i\left\langle u(x,y)\right|\boldsymbol{\nabla}\left|u(x,y)\right\rangle. \tag{31}$$

Now, a question regarding the gauge choice arises. We have so far tacitly used the *parallel transport gauge*, with which we have $A(x,y)=0$ in the bulk but $A(x,y)\neq 0$ at the edge, that is, we have used the following boundary conditions [1, 2]:

$$|u(x,1)\rangle = e^{i\theta_x(x)}|u(x,0)\rangle \tag{32}$$

$$|u(1,y)\rangle = e^{i\theta_y(y)}|u(0,y)\rangle. \tag{33}$$

Thus,

$$\begin{aligned} A(x,0)-A(x,1) &= i\left\langle u(x,0)\middle|\frac{\partial}{\partial x}\middle|u(x,0)\right\rangle - i\left\langle u(x,1)\middle|\frac{\partial}{\partial x}\middle|u(x,1)\right\rangle \\ &= i\left\langle u(x,0)\middle|\frac{\partial}{\partial x}\middle|u(x,0)\right\rangle - i\left\langle u(x,0)\middle|e^{-i\theta_x(x)}\frac{\partial}{\partial x}e^{i\theta_x(x)}\middle|u(x,0)\right\rangle \\ &= \frac{\partial\theta_x(x)}{\partial x}, \end{aligned} \tag{34}$$

and similarly

$$A(0,y)-A(1,y) = \frac{\partial\theta_y(y)}{\partial y}. \tag{35}$$

Consequently, the line integral Eq. (30) becomes

$$\begin{aligned} c_n &= \frac{1}{2\pi}\left(\int_0^1 \frac{\partial\theta_x(x)}{\partial x}dx - \int_0^1 dy\frac{\partial\theta_y(y)}{\partial y}\right) \\ &= \frac{1}{2\pi}\left(\int_0^1 d\theta_x(x) - \int_0^1 d\theta_y(y)\right) \\ &= \frac{1}{2\pi}\left(\theta_x(1)-\theta_x(0)-\theta_y(1)+\theta_y(0)\right). \end{aligned} \tag{36}$$

Since the wave function acquires the phase $\theta_y(0)$ from $(0,0)$ to $(1,0)$, $\theta_x(1)$ from $(1,0)$ to $(1,1)$, $-\theta_y(1)$ from $(1,1)$ to $(0,1)$, and $-\theta_x(1)$ from $(0,1)$ to $(0,0)$, the single-valuedness of the wave function requires $(\theta_x(0)+\theta_y(1)-\theta_x(1)-\theta_y(0)) = 2\pi Z$.

We thus conclude that

$$\theta_y(0)+\theta_x(1)-\theta_y(1)-\theta_x(0) = 2\pi Z, \tag{37}$$

where Z is integer, which leads to the line integral in Eq. (36) being

$$c_n = Z. \tag{38}$$

This proves the initial statement that the number of charges transported by the nth-band adiabatic current per one-cycle of periodic time evolution is quantized. This kind of quantized charge transport is called *Thouless pumping* [3].

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