Thouless pumping

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We shall find that the Berry phase appears when a quantum state is modified by adiabatic changes of Hamiltonian. This sets the stage to explore the yet another interesting quantization phenomenon, the *Thouless pumping*. Here the parameter space is torus and spaned by the time t and the wave number k, both of which are periodic.

I. BERRY PHASE AND ADIABATIC CHANGES OF A QUANTUM STATE [1–3]

So far we investigated the Berry phase with path integral method, which basically means that we treated the *inherently quantum-mechanical* electron spin as the classical megnetic moment, $\boldsymbol{n} = \frac{\boldsymbol{m}}{m_0} = \begin{bmatrix} \sin\theta\cos\phi \\ \sin\theta\sin\phi \\ \cos\theta \end{bmatrix}$. Now, we shall re-discover the same Berry phase by analyzing the *adiabatic changes* of a quantum state $|\uparrow(t)\rangle$ which is one of the eigenstates of the spin.

A. Adiabatic changes of a quantum state

Let the time-varing Hamiltonian be

$$H(t) = \boldsymbol{m}\cdot\boldsymbol{B}(t) = \gamma\boldsymbol{\sigma}\cdot\boldsymbol{B}(t). \tag{1}$$

Suppose that the magnetic field at $t=0$ is $\boldsymbol{B}(0) = B(0)\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$ and the spin starts at $t=0$ in one of the eignestates

$$|\uparrow(0)\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \tag{2}$$

with the energy $\epsilon_\uparrow(0) = \frac{1}{2}\gamma B(0)$ $(\gamma < 1)$. When the time-variation of the Hamiltonian $H(t)$ is *abiabatic* the spin state remains in the instantaneous eigenstate of $H(t)$, that is,

$$|\uparrow(t)\rangle = \begin{bmatrix} e^{-i\frac{\phi(t)}{2}}\cos\frac{\theta(t)}{2} \\ -ie^{i\frac{\phi(t)}{2}}\sin\frac{\theta(t)}{2} \end{bmatrix}, \tag{3}$$

with the energy $\epsilon_\uparrow(t) = \frac{1}{2}\gamma B(t)$. Here, at t the magnetic field is assumed to be $\boldsymbol{B}(t) = B(t)\begin{bmatrix} \sin\theta(t)\sin\phi(t) \\ \sin\theta(t)\cos\phi(t) \\ \cos\theta(t) \end{bmatrix}$.

Now suppose that, at the end of the evolution $t=T$, the Hamiltonian returns to the original one, that is, $H(T) = H(0)$ and thus the state must come back to the original state with some phase factor, that is,

$$|\uparrow(T)\rangle = e^{-i\Phi(T)}|\uparrow(0)\rangle. \tag{4}$$

We shall see that the phase can be written as [4]

$$\Phi(T) = \underbrace{\Phi(0)}_{\text{initial phase}} + \underbrace{\frac{1}{\hbar}\int_0^T dt\epsilon_\uparrow(t)}_{\text{dynamical phase}} + \underbrace{\gamma_\uparrow}_{\text{Berry phase}}. \tag{5}$$

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The starting point is the time-dependent Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{6}$$

where the wave function $|\psi(t)\rangle$ can be assumed to be the instantaneous eigenstate $|\uparrow(t)\rangle$ with some phase factor, that is,

$$|\psi(t)\rangle = e^{-i\Phi(t)}|\uparrow(t)\rangle \tag{7}$$

since $|\psi(t)\rangle$ changes adiabatically from $|\uparrow(0)\rangle$ to $|\uparrow(T)\rangle$ in a course of time evolution. This adiabatic approximation is essentially a *projection operation*, by which the state $|\psi(t)\rangle$ is restricted onto the one of the eigenstates $|\uparrow(t)\rangle$ [1]. Plugging this form of wave function into Eq. (6) and operate $\langle\uparrow(t)|$ from the left we have

$$\hbar\frac{\partial\Phi(t)}{\partial t} + i\hbar\left\langle \uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle = \epsilon_\uparrow(t). \tag{8}$$

By integrating both sides with respenct to t from 0 to T we have

$$\hbar\left(\Phi(T)-\Phi(0)\right) + \hbar\int_0^T dt\; i\left\langle \uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle = \int_0^T dt\epsilon_\uparrow(t), \tag{9}$$

which indeed indicates Eq.(5) with the Berry phase [4]:

$$\begin{aligned}\gamma_\uparrow &= -\int_0^T dt\; i\left\langle \uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle \\ &= \int_0^T dt\left(-i\left\langle \uparrow(\boldsymbol{R}(t))\middle|\frac{\partial}{\partial \boldsymbol{R}(t)}\middle|\uparrow(\boldsymbol{R}(t))\right\rangle\right)\dot{\boldsymbol{R}}(t) \\ &= \oint_{\mathrm{C}} d\boldsymbol{R}\cdot\underbrace{\left(-i\left\langle \uparrow(\boldsymbol{R})\middle|\frac{\partial}{\partial \boldsymbol{R}}\middle|\uparrow(\boldsymbol{R})\right\rangle\right)}_{\boldsymbol{A}_\uparrow:\ \text{Berry connection}} \\ &= \int_{\mathcal{A}} d\boldsymbol{S}\cdot\underbrace{\left(\nabla\times\boldsymbol{A}_\uparrow\right)}_{\boldsymbol{\Omega}_\uparrow:\ \text{Berry curvature}}.\end{aligned} \tag{10}$$

This establishes the close link between the Berry phase and adiabatic changes of the quantum state $|\uparrow(t)\rangle$. Note that $\gamma_\uparrow$ does not depend on the velocity $\dot{\boldsymbol{R}}$ in this setting and stems from the *geometry* of the space where the eigenstates $|\uparrow(t)\rangle$ lives. Thus, the Berry phase is also called the *geometric phase*.

B. Calcution of Berry curvatures

Unlike the Berry connection, the Berry curvature and the Berry phase are gauge-independent and observable. Especially the Berry curvature can be evaluated locally at $\boldsymbol{R}$, that is, in the Euler angle representation, at (ϕ,θ). Let us explore several ways in which the Berry curvature $\Omega_\uparrow$ can be calculated. We know from the last lecture that

$$\begin{aligned}\Omega_\uparrow(\phi,\theta) &= \nabla\times\boldsymbol{A}_\uparrow(\phi,\theta) \\ &= \nabla\times\begin{bmatrix}0\\0\\\frac{1-\cos\theta}{\sin\theta}\end{bmatrix} == \begin{bmatrix}\frac{1}{\frac{1}{2}\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\left(\frac{1-\cos\theta}{\sin\theta}\right)\right)\\0\\0\end{bmatrix} = \begin{bmatrix}2\\0\\0\end{bmatrix} = 2\boldsymbol{e}_r.\end{aligned} \tag{11}$$

1. *From spinor representation*

The Berry connection $\boldsymbol{A}_\uparrow$ can be written in terms of spinor representation as

$$\begin{aligned}
\boldsymbol{A}_\uparrow &= -i\left\langle \uparrow(\boldsymbol{R})\middle|\frac{\partial}{\partial \boldsymbol{R}}\middle|\uparrow(\boldsymbol{R})\right\rangle \\
&= -i\left(\left[e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2}, ie^{-i\frac{\phi}{2}}\sin\frac{\theta}{2}\right]\cdot\left(\nabla\begin{bmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ -ie^{i\frac{\phi}{2}}\sin\frac{\theta}{2}\end{bmatrix}\right)\right) \\
&= -i\left(\left[e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2}, ie^{-i\frac{\phi}{2}}\sin\frac{\theta}{2}\right]\cdot\left(\frac{1}{\frac{1}{2}}\frac{\partial}{\partial\theta}\begin{bmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ -ie^{i\frac{\phi}{2}}\sin\frac{\theta}{2}\end{bmatrix}\boldsymbol{e}_\theta + \frac{1}{\frac{1}{2}\sin\theta}\frac{\partial}{\partial\phi}\begin{bmatrix} e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ -ie^{i\frac{\phi}{2}}\sin\frac{\theta}{2}\end{bmatrix}\boldsymbol{e}_\phi\right)\right) \\
&= -i\left(\left[e^{-i\frac{\phi}{2}}\cos\frac{\theta}{2}, ie^{-i\frac{\phi}{2}}\sin\frac{\theta}{2}\right]\cdot\left(\begin{bmatrix} -e^{-i\frac{\phi}{2}}\sin\frac{\theta}{2} \\ -ie^{i\frac{\phi}{2}}\cos\frac{\theta}{2}\end{bmatrix}\boldsymbol{e}_\theta + \frac{1}{\sin\theta}\begin{bmatrix} -ie^{-i\frac{\phi}{2}}\cos\frac{\theta}{2} \\ e^{i\frac{\phi}{2}}\sin\frac{\theta}{2}\end{bmatrix}\boldsymbol{e}_\phi\right)\right) \\
&= -i\left(\left(-\cos\frac{\theta}{2}\sin\frac{\theta}{2}+\sin\frac{\theta}{2}\cos\frac{\theta}{2}\right)\boldsymbol{e}_\theta + i\frac{1}{\sin\theta}\left(-\cos^2\frac{\theta}{2}+\sin^2\frac{\theta}{2}\right)\boldsymbol{e}_\phi\right) \\
&= -\frac{\cos\theta}{\sin\theta}\boldsymbol{e}_\phi.
\end{aligned} \tag{12}$$

With this Berry connection, we arrive at the same Berry curvature:

$$\begin{aligned}
\boldsymbol{\Omega}_\uparrow(\boldsymbol{R}) &= \nabla\times\left(-i\left\langle \uparrow(\boldsymbol{R})\middle|\frac{\partial}{\partial \boldsymbol{R}}\middle|\uparrow(\boldsymbol{R})\right\rangle\right) \\
&= \nabla\times\begin{bmatrix} 0 \\ 0 \\ -\frac{\cos\theta}{\sin\theta}\end{bmatrix} = \begin{bmatrix} \frac{1}{\frac{1}{2}\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\left(-\frac{\cos\theta}{\sin\theta}\right)\right) \\ 0 \\ 0\end{bmatrix} \\
&= \begin{bmatrix} 2 \\ 0 \\ 0\end{bmatrix} = 2\boldsymbol{e}_r.
\end{aligned} \tag{13}$$

2. *From first-order correction to the adiabatic eigenstates*

From the vector identity

$$\nabla\times(f\nabla g) = \nabla f\times\nabla g, \tag{14}$$

the second expression in Eq. (13) can also be written as

$$\begin{aligned}
\boldsymbol{\Omega}_\uparrow(\boldsymbol{R}) &= \nabla\times\left(-i\left\langle\uparrow(\boldsymbol{R})|\nabla|\uparrow(\boldsymbol{R})\right\rangle\right) \\
&= -i\langle\nabla\uparrow(\boldsymbol{R})|\times|\nabla\uparrow(\boldsymbol{R})\rangle \\
&= -i\left\langle\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\middle|\times\middle|\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\right\rangle \qquad (15)\\
&= -i\sum_{m=\uparrow,\downarrow}\left\langle\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\middle|m(\boldsymbol{R})\right\rangle\times\left\langle m(\boldsymbol{R})\middle|\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\right\rangle \\
&= -i\left\langle\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\middle|\downarrow(\boldsymbol{R})\right\rangle\times\left\langle\downarrow(\boldsymbol{R})\middle|\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\right\rangle, \qquad (16)
\end{aligned}$$

where last equality comes from

$$\left\langle\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\middle|\uparrow(\boldsymbol{R})\right\rangle = -\left\langle\uparrow(\boldsymbol{R})\middle|\frac{\partial}{\partial\boldsymbol{R}}\uparrow(\boldsymbol{R})\right\rangle. \tag{17}$$

This form allows us to explore the relation between the Berry courvature and degeneracy points. To see this relation, let us exploit the following relations:

$$\left\langle m(\boldsymbol{R}) \middle| \frac{\partial}{\partial \boldsymbol{R}} \uparrow(\boldsymbol{R}) \right\rangle = \frac{1}{\epsilon_\uparrow(\boldsymbol{R}) - \epsilon_m(\boldsymbol{R})} \left\langle m(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| \uparrow(\boldsymbol{R}) \right\rangle \tag{18}$$

$$\left\langle \frac{\partial}{\partial \boldsymbol{R}} \uparrow(\boldsymbol{R}) \middle| m(\boldsymbol{R}) \right\rangle = \frac{1}{\epsilon_\uparrow(\boldsymbol{R}) - \epsilon_m(\boldsymbol{R})} \left\langle \uparrow(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| m(\boldsymbol{R}) \right\rangle, \tag{19}$$

where $|m(\boldsymbol{R})\rangle$ and $\epsilon_m(\boldsymbol{R})$ are the eigenstates and the eigenvalues of the Hamiltonian $H(t) = H(\boldsymbol{R}(t))$ in Eq. (1). The relation can be obtained by differentiating the eigenequation

$$H(\boldsymbol{R})|m(\boldsymbol{R})\rangle = \epsilon_m(\boldsymbol{R})|m(\boldsymbol{R})\rangle \tag{20}$$

by $\boldsymbol{R}$. With Eqs. (18) and (19), the Berry curvature Eq. (16) becomes

$$\begin{aligned} \boldsymbol{\Omega}_\uparrow(\boldsymbol{R}) &= -i \sum_{m=\uparrow,\downarrow} \frac{1}{(\epsilon_\uparrow(\boldsymbol{R}) - \epsilon_m(\boldsymbol{R}))^2} \left\langle \uparrow(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| m(\boldsymbol{R}) \right\rangle \times \left\langle m(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| \uparrow(\boldsymbol{R}) \right\rangle \\ &= -\frac{i}{(\epsilon_\uparrow(\boldsymbol{R}) - \epsilon_\downarrow(\boldsymbol{R}))^2} \left\langle \uparrow(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| \downarrow(\boldsymbol{R}) \right\rangle \times \left\langle \downarrow(\boldsymbol{R}) \middle| \frac{\partial H(\boldsymbol{R})}{\partial \boldsymbol{R}} \middle| \uparrow(\boldsymbol{R}) \right\rangle, \end{aligned} \tag{21}$$

suggesting that when $\epsilon_\uparrow(\boldsymbol{R}) \sim \epsilon_\downarrow(\boldsymbol{R})$ the Berry curvature $\Omega_\uparrow(\boldsymbol{R})$ becomes large and $\Omega_\uparrow(\boldsymbol{R})$ becomes divergent at the degeracy point where $\epsilon_\uparrow(\boldsymbol{R}) = \epsilon_\downarrow(\boldsymbol{R})$. The advantage of the last formula Eq. (21) is that there is no differentiation on the wave function.

II. THOULESS PUMPING [1]

Now we shall extend our interest to solid state physics and explore the Berry phase accompanying Bloch electron.The model Hamiltonian is one for a 1D electron in a slowly varing periodic potential

$$H(t) = \frac{p}{2m} + V(x,t), \tag{22}$$

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

$$|\psi_{n,k}(x,t)\rangle = e^{ikx}|u_{n,k}(x,t)\rangle, \tag{23}$$

with the *twisted* boundary conditions:

$$|\psi_{n,k}(x+a,t)\rangle = e^{ika}|\psi_{n,k}(x,t)\rangle \tag{24}$$

where n stands for the band index and k does for the wave number. To rectify the *twisted* boundary condition we can use the periodic part $|u_{n,k}(x,t)\rangle$ of the Bloch form Eq. (23) as the instantaneous eigenstates. This is basically a gauge-transformation. The boundary condition for $|u_{n,k}(x,t)\rangle$ is the ordinary one,

$$|u_{n,k}(x+a,t)\rangle = |u_{n,k}(x,t)\rangle, \tag{25}$$

while the Hamiltonian Eq. (22) changes into k-dependent form

$$H(k,t) = e^{-ikx}H(t)e^{ikx} = \frac{1}{2m}(p + \hbar k)^2 + V(x,t), \tag{26}$$

since

$$\begin{aligned} e^{-ikx}pe^{ikx} &= e^{-ikx}\left(-i\hbar\frac{\partial}{\partial x}\right)e^{ikx} \\ &= \hbar k - i\hbar\frac{\partial}{\partial x} = \hbar k + p. \end{aligned} \tag{27}$$

The velocity of the electron can be given by

$$v = -\frac{i}{\hbar}\left[x, H\right]. \tag{28}$$

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

$$\begin{aligned}
v_{k,n}^{(0)} &\equiv \langle u_{k,n}|e^{-ikx} v e^{ikx}|u_{k,n}\rangle \\
&= -\frac{i}{\hbar}\langle u_{k,n}|e^{-ikx}\left[x, H\right]e^{ikx}|u_{k,n}\rangle \\
&= -\frac{i}{\hbar}\langle u_{k,n}|\left[x, e^{-ikx} H e^{ikx}\right]|u_{k,n}\rangle \\
&= -\frac{i}{\hbar}\langle u_{k,n}|\left[x, \frac{1}{2m}\left((p+\hbar k)^2 + V(x)\right)\right]|u_{k,n}\rangle \\
&= -\frac{i}{\hbar}\langle u_{k,n}|\left[x, \frac{1}{2m}\left(\left(-i\hbar\frac{\partial}{\partial x} + \hbar k\right)^2 + V(x)\right)\right]|u_{k,n}\rangle \\
&= \frac{1}{m}\langle u_{k,n}|\left(p+\hbar k\right)|u_{k,n}\rangle \\
&= \frac{1}{\hbar}\langle u_{k,n}|\frac{\partial H}{\partial k}|u_{k,n}\rangle \\
&= \frac{1}{\hbar}\frac{\partial \epsilon_{k,n}}{\partial k}.
\end{aligned} \tag{29}$$

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

$$\begin{aligned}
j_0 &= -e\sum_n \int_{\mathrm{BZ}} \frac{dk}{2\pi} v_{k,n}^{(0)} \\
&= -e\sum_n \frac{1}{\hbar}\int_{\mathrm{BZ}} \frac{dk}{2\pi}\frac{\partial \epsilon_{k,n}}{\partial k} \\
&= -e\sum_n \frac{1}{h}\int_{\mathrm{BZ}} d\epsilon_{k,n} = 0.
\end{aligned} \tag{30}$$

So let us look at the first-order correction to the adiabatic eigenstates $|u_{k,n}\rangle$. The purtabation theory tells us that the first-order approximation of the adiabatic eigenstates can be given by

$$|u_{k,n}\rangle - i\hbar\sum_{n'=n}\frac{|u_{k,n'}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{k,n}}{\partial t}\right\rangle}{\epsilon_{k,n}-\epsilon_{k,n'}}. \tag{31}$$

Thus the first-order correction to the velocity reads

$$\begin{aligned}
v_{k,n}^{(1)} &\equiv \frac{1}{\hbar}\langle u_{k,n}|\frac{\partial H}{\partial k}|\left(-i\hbar\sum_{n'=n}\frac{|u_{k,n'}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{k,n}}{\partial t}\right\rangle}{\epsilon_{k,n}-\epsilon_{k,n'}}\right) + \frac{1}{\hbar}\left(i\hbar\sum_{n'=n}\frac{\left\langle\frac{\partial u_{k,n}}{\partial t}\middle|u_{n',k}\right\rangle\langle u_{k,n'}|}{\epsilon_{k,n}-\epsilon_{k,n'}}\right)|\frac{\partial H}{\partial k}|u_{k,n}\rangle \\
&= -i\sum_{n=n'}\frac{1}{\epsilon_{k,n}-\epsilon_{k,n'}}\left(\left\langle u_{k,n}|\frac{\partial H}{\partial k}|u_{k,n'}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{k,n}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{k,n}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{k,n'}|\frac{\partial H}{\partial k}|u_{k,n}\right\rangle\right).
\end{aligned} \tag{32}$$

Now, let us exploit the similar relations as Eqs.(18) and (19):

$$\begin{aligned}
\left\langle u_{k,n'}\middle|\frac{\partial u_{k,n}}{\partial k}\right\rangle &= \frac{1}{\epsilon_{k,n}-\epsilon_{k,n'}}\left\langle u_{k,n'}\middle|\frac{\partial H}{\partial k}\middle|u_{k,n}\right\rangle && (33)\\
\left\langle\frac{\partial u_{k,n}}{\partial k}\middle|u_{k,n'}\right\rangle &= \frac{1}{\epsilon_{k,n}-\epsilon_{k,n'}}\left\langle u_{k,n}\middle|\frac{\partial H}{\partial k}\middle|u_{k,n'}\right\rangle, && (34)
\end{aligned}$$

to get

$$\begin{aligned}
v_{k,n}^{(1)} &= -i\sum_{n=n'}\left(\left\langle\frac{\partial u_{k,n}}{\partial k}\middle|u_{k,n'}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{k,n}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{k,n}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{k,n'}\middle|\frac{\partial u_{k,n}}{\partial k}\right\rangle\right) \\
&= -i\left(\left\langle\frac{\partial u_{k,n}}{\partial k}\middle|\frac{\partial u_{k,n}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{k,n}}{\partial t}\middle|\frac{\partial u_{k,n}}{\partial k}\right\rangle\right).
\end{aligned} \tag{35}$$

Comparing the last form with the form of the Berry curvature in Eq. (15) we can recognize that $v_{k,n}^{(1)}$ is nothing but the Berry curvature:

$$v_{k,n}^{(1)} = \Omega_{k,n}. \tag{36}$$

This Berry curvature measures the curvature of the space spaned by the time t and the wave number k. Here t assumes the periodic boundary conditions $t + T = t$ and k assumes the periodic boundary conditions $k + G = k$ where $G = \frac{2\pi}{a}$, the parameter space is torus. Integrating over the Brilloin zone we have the Berry-curvature induced *abiabatic current*:

$$j_1 = -e \sum_n \int_{\text{BZ}} \frac{dk}{2\pi} v_{k,n}^{(1)} = -e \sum_n \int_{\text{BZ}} \frac{dk}{2\pi} \Omega_{k,n} \tag{37}$$

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

$$c_n = \int_0^T dt \int_{\text{BZ}} \frac{dk}{2\pi} \Omega_{k,n}. \tag{38}$$

The quantitiy $2\pi c_n$ 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

$$c_n = \frac{1}{2\pi} \int_0^1 dx \int_0^1 dy \; \Omega(x, y), \tag{39}$$

where

$$\Omega(x, y) = \frac{\Omega_{k,n}}{TG}. \tag{40}$$

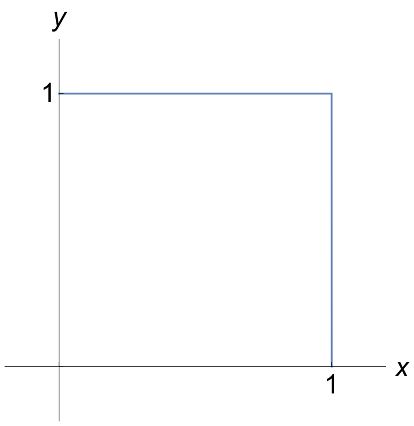

FIG. 1: Path $(0, 0) \to (1, 0) \to (1, 1) \to (0, 1) \to (0, 0)$ is used to evaluate the integral Eq. (41).

We can now use the Stokes theorem to obtain the line integral form of Eq. (39), that is,

$$\begin{aligned} c_n &= \frac{1}{2\pi} \oint_{\text{C}} dl A(x, y) \\ &= \frac{1}{2\pi} \left(\int_0^1 dx A(x, 0) + \int_0^1 dy A(1, y) + \int_1^0 dx A(x, 1) + \int_1^0 dy A(0, y) \right) \\ &= \frac{1}{2\pi} \left(\int_0^1 dx \left(A(x, 0) - A(x, 1) \right) + \int_0^1 dy \left(A(1, y) - A(0, y) \right) \right), \end{aligned} \tag{41}$$

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

$$A(x, y) = -i \left\langle u(x, y) | \nabla | u(x, y) \right\rangle. \tag{42}$$

Here a question regarding the gauge choice arises since we are now interested in the gauge-dependent Berry connection $A(x,y)$. We employ the so-called *periodic gauge* [1]:

$$
\begin{aligned}
|u(x,1)\rangle &= e^{i\theta_x(x)}|u(x,0)\rangle &(43)\\
|u(1,y)\rangle &= e^{i\theta_y(y)}|u(0,y)\rangle. &(44)
\end{aligned}
$$

Thus, we have

$$
\begin{aligned}
A(x,0)-A(x,1) &= -i\left\langle u(x,0)\left|\frac{\partial}{\partial x}\right|u(x,0)\right\rangle + i\left\langle u(x,1)\left|\frac{\partial}{\partial x}\right|u(x,1)\right\rangle \\
&= -i\left\langle u(x,0)\left|\frac{\partial}{\partial x}\right|u(x,0)\right\rangle + i\left\langle u(x,0)\left|e^{-i\theta_x(x)}\frac{\partial}{\partial x}e^{i\theta_x(x)}\right|u(x,0)\right\rangle \\
&= -\frac{\partial\theta_x(x)}{\partial x}, \qquad (45)
\end{aligned}
$$

and similarly

$$
A(0,y)-A(1,y) = -\frac{\partial\theta_y(y)}{\partial y}. \qquad (46)
$$

Consequently, the line integral Eq. (41) becomes

$$
\begin{aligned}
c_n &= -\frac{1}{2\pi}\left(\int_0^1 \frac{\partial\theta_x(x)}{\partial x}dx - \int_0^1 dy\frac{\partial\theta_y(y)}{\partial y}\right) \\
&= -\frac{1}{2\pi}\left(\int_0^1 d\theta_x(x) - \int_0^1 d\theta_y(y)\right) \\
&= -\frac{1}{2\pi}\left(\theta_x(1)-\theta_x(0)-\theta_y(1)+\theta_y(0)\right). \qquad (47)
\end{aligned}
$$

On the other hand, the single-valuedness of the wave function requires

$$
|u(0,0)\rangle = \exp\left[i\left(\theta_x(0)+\theta_y(1)-\theta_x(1)-\theta_y(0)\right)\right]|u(0,0)\rangle, \qquad (48)
$$

since the wave function acqires the phase $\theta_x(0)$ from $(0,0)$ to $(1,0)$, $\theta_y(1)$ from $(1,0)$ to $(1,1)$, $-\theta_x(1)$ from $(1,1)$ to $(0,1)$, and $-\theta_y(0)$. We thus conclude that

$$
\theta_x(0)+\theta_y(1)-\theta_x(1)-\theta_y(0) = 2\pi Z, \qquad (49)
$$

where Z is integer, and the line integral Eq. (47) becomes

$$
c_n = Z. \qquad (50)
$$

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* [5].

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