Thouless pumping

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(Dated: October 10, 2019)

We shall find that the Berry phase appears when a quantum state undergoes an adiabatic evolution with a time-dependent 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 [1–4]

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 revisit the Berry phase by analyzing the adiabatic evolution of a *quantum state* $|\uparrow(t)\rangle$, which is the lowest energy eigenstate of a time-dependent Hamiltonian $H(t)$.

A. Adiabatic changes of a quantum state

Let the time-dependent Hamiltonian be

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

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

$$\underbrace{|\uparrow(0)\rangle}_{\text{for magnetic moment}} = \underbrace{|\Downarrow(0)\rangle}_{\text{for spin}} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2}$$

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

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

with the energy $\epsilon_\uparrow(t) = \epsilon_\Downarrow(t) = -\frac{1}{2}\hbar\gamma_s B(t)$. Here, at t the magnetic field is assumed to be

$$\boldsymbol{B}(t) = B(t)\begin{bmatrix} \sin\theta(t)\sin\phi(t) \\ \sin\theta(t)\cos\phi(t) \\ \cos\theta(t) \end{bmatrix}. \tag{4}$$

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,

$$|\uparrow(T)\rangle = e^{-i\Phi(T)}|\uparrow(0)\rangle. \tag{5}$$

We shall see that the phase can be written as [5]

$$\Phi(T) = \underbrace{\Phi(0)}_{\text{initial phase}} + \underbrace{\frac{1}{\hbar}\int_0^T dt\epsilon_\uparrow(t)}_{\text{dynamical phase}} - \underbrace{\gamma_\uparrow}_{\text{Berry phase}}. \tag{6}$$

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The starting point is the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H(t)|\psi(t)\rangle, \tag{7}$$

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

$$|\psi(t)\rangle = e^{-i\Phi(t)}|\uparrow(t)\rangle \tag{8}$$

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 equivalent to performing a *projection operation* on the state $|\psi(t)\rangle$ to restrict it to the eigenstates $|\uparrow(t)\rangle$ [1]. Plugging this form of wave function into Eq. (7) and operate $\langle\uparrow(t)|$ from the left we have

$$\hbar\frac{\partial\Phi(t)}{\partial t} + i\hbar\left\langle\uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle = \epsilon_\uparrow(t). \tag{9}$$

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

$$\hbar\left(\Phi(T)-\Phi(0)\right) + \hbar\int_0^T dt\; i\left\langle\uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle = \int_0^T dt\epsilon_\uparrow(t), \tag{10}$$

which indeed indicates Eq.(6) with the Berry phase [5]:

$$\begin{aligned}
\gamma_\uparrow &= \int_0^T dt\; i\left\langle\uparrow(t)\middle|\frac{\partial}{\partial t}\middle|\uparrow(t)\right\rangle \\
&= \int_0^T dt\left(i\left\langle\uparrow(\boldsymbol{\sigma}(t))\middle|\frac{\partial}{\partial\boldsymbol{\sigma}(t)}\middle|\uparrow(\boldsymbol{\sigma}(t))\right\rangle\right)\dot{\boldsymbol{\sigma}}(t) \\
&= \oint_{\mathrm{C}} d\boldsymbol{\sigma}\cdot\underbrace{\left(i\left\langle\uparrow(\boldsymbol{\sigma})\middle|\frac{\partial}{\partial\boldsymbol{\sigma}}\middle|\uparrow(\boldsymbol{\sigma})\right\rangle\right)}_{\boldsymbol{A}_\uparrow:\ \text{Berry connection}} \\
&= \int_{\mathcal{A}} d\boldsymbol{S}\cdot\underbrace{(\boldsymbol{\nabla}\times\boldsymbol{A}_\uparrow)}_{\boldsymbol{\Omega}_\uparrow:\ \text{Berry curvature}}\quad.
\end{aligned} \tag{11}$$

This establishes the close link between the Berry phase and adiabatic evolution of the quantum state $|\uparrow(t)\rangle$. Note that $\gamma_\uparrow$ does not depend on the velocity $\dot{\boldsymbol{\sigma}}$ 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 $\boldsymbol{\sigma}$, 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.

1. *From Euler angle representation*

We know from the last lecture that

$$\begin{aligned}
\Omega_\uparrow(\phi,\theta) &= \boldsymbol{\nabla}\times\boldsymbol{A}_\uparrow(\phi,\theta) \\
&= \boldsymbol{\nabla}\times\begin{bmatrix}0\\0\\\frac{1-\cos\theta}{\sin\theta}\end{bmatrix} == \begin{bmatrix}\frac{1}{\frac{1}{2}\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\left(\frac{1-\cos\theta}{\sin\theta}\right)\right)\\0\\0\end{bmatrix} = \begin{bmatrix}2\\0\\0\end{bmatrix} = 2\boldsymbol{e}_r.
\end{aligned} \tag{12}$$

2. From spinor representation

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

$$
\begin{aligned}
\boldsymbol{A}_\uparrow \equiv \boldsymbol{A}_\Downarrow &= i\left\langle \uparrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \middle| \uparrow(\boldsymbol{\sigma}) \right\rangle \\
&= i\left\langle \Downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \middle| \Downarrow(\boldsymbol{\sigma}) \right\rangle \\
&= i\left(\left[-e^{i\frac{\phi}{2}} \sin\frac{\theta}{2}, e^{-i\frac{\phi}{2}} \cos\frac{\theta}{2} \right] \cdot \left(\boldsymbol{\nabla} \begin{bmatrix} -e^{-i\frac{\phi}{2}} \sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}} \cos\frac{\theta}{2} \end{bmatrix} \right) \right) \\
&= i\left(\left[-e^{i\frac{\phi}{2}} \sin\frac{\theta}{2}, e^{-i\frac{\phi}{2}} \cos\frac{\theta}{2} \right] \cdot \left(\boldsymbol{e}_\theta \frac{1}{\frac{1}{2}} \frac{\partial}{\partial\theta} \begin{bmatrix} -e^{-i\frac{\phi}{2}} \sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}} \cos\frac{\theta}{2} \end{bmatrix} + \boldsymbol{e}_\phi \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial\phi} \begin{bmatrix} -e^{-i\frac{\phi}{2}} \sin\frac{\theta}{2} \\ e^{i\frac{\phi}{2}} \cos\frac{\theta}{2} \end{bmatrix} \right) \right) \\
&= i\left(\left[-e^{i\frac{\phi}{2}} \sin\frac{\theta}{2}, e^{-i\frac{\phi}{2}} \cos\frac{\theta}{2} \right] \cdot \left(\begin{bmatrix} -e^{-i\frac{\phi}{2}} \cos\frac{\theta}{2} \\ -e^{i\frac{\phi}{2}} \sin\frac{\theta}{2} \end{bmatrix} \boldsymbol{e}_\theta + \frac{1}{\sin\theta} \begin{bmatrix} ie^{-i\frac{\phi}{2}} \sin\frac{\theta}{2} \\ ie^{i\frac{\phi}{2}} \cos\frac{\theta}{2} \end{bmatrix} \boldsymbol{e}_\phi \right) \right) \\
&= i\left(\left(\sin\frac{\theta}{2}\cos\frac{\theta}{2} - \cos\frac{\theta}{2}\sin\frac{\theta}{2} \right) \boldsymbol{e}_\theta + \frac{1}{\sin\theta} \left(-i\sin^2\frac{\theta}{2} + i\cos^2\frac{\theta}{2} \right) \boldsymbol{e}_\phi \right) \\
&= -\frac{\cos\theta}{\sin\theta} \boldsymbol{e}_\phi.
\end{aligned} \tag{13}
$$

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

$$
\begin{aligned}
\boldsymbol{\Omega}_\uparrow(\boldsymbol{\sigma}) &= \boldsymbol{\nabla} \times \boldsymbol{A}_\uparrow \\
&= \boldsymbol{\nabla} \times \left(i\left\langle \uparrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \middle| \uparrow(\boldsymbol{\sigma}) \right\rangle \right) \\
&= \boldsymbol{\nabla} \times \begin{bmatrix} 0 \\ 0 \\ -\frac{\cos\theta}{\sin\theta} \end{bmatrix} = \begin{bmatrix} \frac{1}{\frac{1}{2}\sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \left(-\frac{\cos\theta}{\sin\theta} \right) \right) \\ 0 \\ 0 \end{bmatrix} \\
&= \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix} = 2\boldsymbol{e}_r.
\end{aligned} \tag{14}
$$

3. From first-order correction to the adiabatic eigenstates

From the vector identity

$$
\boldsymbol{\nabla} \times (f \boldsymbol{\nabla} g) = \boldsymbol{\nabla} f \times \boldsymbol{\nabla} g, \tag{15}
$$

the second expression in Eq. (14) can also be written as

$$
\begin{aligned}
\boldsymbol{\Omega}_\uparrow(\boldsymbol{\sigma}) &= \boldsymbol{\nabla} \times \left(i \langle \uparrow(\boldsymbol{\sigma}) | \boldsymbol{\nabla} | \uparrow(\boldsymbol{\sigma}) \rangle \right) \\
&= i \langle \boldsymbol{\nabla} \uparrow(\boldsymbol{\sigma}) | \times | \boldsymbol{\nabla} \uparrow(\boldsymbol{\sigma}) \rangle \\
&= i\left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| \times \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle \\
&= i \sum_{m=\uparrow,\downarrow} \left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| m(\boldsymbol{\sigma}) \right\rangle \times \left\langle m(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle \qquad (16) \\
&= i \left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| \downarrow(\boldsymbol{\sigma}) \right\rangle \times \left\langle \downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle, \qquad (17)
\end{aligned}
$$

where last equality comes from the fact that

$$
\left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| \uparrow(\boldsymbol{\sigma}) \right\rangle = -\left\langle \uparrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle. \tag{18}
$$

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:

$$\left\langle \downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle = \frac{1}{\epsilon_\uparrow(\boldsymbol{\sigma}) - \epsilon_\downarrow(\boldsymbol{\sigma})} \left\langle \downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial H(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} \middle| \uparrow(\boldsymbol{\sigma}) \right\rangle \tag{19}$$

$$\left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| \downarrow(\boldsymbol{\sigma}) \right\rangle = \frac{1}{\epsilon_\uparrow(\boldsymbol{\sigma}) - \epsilon_\downarrow(\boldsymbol{\sigma})} \left\langle \uparrow(\boldsymbol{\sigma}) \middle| \frac{\partial H(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} \middle| \downarrow(\boldsymbol{\sigma}) \right\rangle, \tag{20}$$

where $|\uparrow(\boldsymbol{\sigma})\rangle$ ($|\downarrow(\boldsymbol{\sigma})\rangle$) and $\epsilon_\uparrow(\boldsymbol{\sigma})$ ($\epsilon_\downarrow(\boldsymbol{\sigma})$) are the eigenstate and the eigenvalue of the Hamiltonian $H(t) = H(\boldsymbol{\sigma}(t))$ in Eq. (1). The relation can be obtained by differentiating the eigenequation

$$H(\boldsymbol{\sigma})|\uparrow(\boldsymbol{\sigma})\rangle = \epsilon_\uparrow(\boldsymbol{\sigma})|\uparrow(\boldsymbol{\sigma})\rangle \tag{21}$$

by $\boldsymbol{\sigma}$ and then by projecting on the state $\langle\downarrow(\boldsymbol{\sigma})|$. With Eqs. (19) and (20), the Berry curvature Eq. (17) becomes

$$\begin{aligned} \boldsymbol{\Omega}_\uparrow(\boldsymbol{\sigma}) &= i \left\langle \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \middle| \downarrow(\boldsymbol{\sigma}) \right\rangle \times \left\langle \downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial}{\partial \boldsymbol{\sigma}} \uparrow(\boldsymbol{\sigma}) \right\rangle \\ &= \frac{i}{(\epsilon_\uparrow(\boldsymbol{\sigma}) - \epsilon_\downarrow(\boldsymbol{\sigma}))^2} \left\langle \uparrow(\boldsymbol{\sigma}) \middle| \frac{\partial H(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} \middle| \downarrow(\boldsymbol{\sigma}) \right\rangle \times \left\langle \downarrow(\boldsymbol{\sigma}) \middle| \frac{\partial H(\boldsymbol{\sigma})}{\partial \boldsymbol{\sigma}} \middle| \uparrow(\boldsymbol{\sigma}) \right\rangle, \end{aligned} \tag{22}$$

suggesting that when $\epsilon_\uparrow(\boldsymbol{\sigma}) \sim \epsilon_\downarrow(\boldsymbol{\sigma})$ the Berry curvature $\Omega_\uparrow(\boldsymbol{\sigma})$ becomes large. Note that the advantage of the last formula Eq. (22) is that there is no differentiation on the wave function.

II. THOULESS PUMPING [1, 4]

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

$$H(t) = \frac{p}{2m} + V(x,t), \tag{23}$$

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:

$$|\psi_{n,k}(x,t)\rangle = e^{ikx}|u_{n,k}(x,t)\rangle, \tag{24}$$

with the *twisted* periodic boundary condition:

$$|\psi_{n,k}(x+a,t)\rangle = e^{ika}|\psi_{n,k}(x,t)\rangle \tag{25}$$

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. (25), we can use the cell-periodic part $|u_{n,k}(x,t)\rangle$ of the Bloch form Eq. (24) as the instantaneous eigenstates. This is basically a gauge-transformation. The boundary condition for $|u_{n,k}(x,t)\rangle$ is the ordinary one,

$$|u_{n,k}(x+a,t)\rangle = |u_{n,k}(x,t)\rangle, \tag{26}$$

at the expense of the Hamiltonian Eq. (23) being changed into k-dependent form

$$H(k,t) = e^{-ikx}H(t)e^{ikx} = \frac{1}{2m}(p+\hbar k)^2 + V(x,t). \tag{27}$$

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

$$\begin{aligned} e^{-ikx}pe^{ikx} &= e^{-ikx}\left(-i\hbar\frac{\partial}{\partial x}\right)e^{ikx} \\ &= \hbar k - i\hbar\frac{\partial}{\partial x} = \hbar k + p. \end{aligned} \tag{28}$$

A. Zero-order current: j_0

The velocity of the electron can be given by

$$v = -\frac{i}{\hbar}\left[x, H\right]. \tag{29}$$

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

$$\begin{aligned}
v^{(0)}_{n,k} &\equiv \langle u_{n,k}|e^{-ikx} v e^{ikx}|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|e^{-ikx}\left[x, H\right]e^{ikx}|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\left[x, e^{-ikx}He^{ikx}\right]|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\left[x, \frac{1}{2m}\left((p+\hbar k)^2 + V(x)\right)\right]|u_{n,k}\rangle \\
&= -\frac{i}{\hbar}\langle u_{n,k}|\underbrace{\left[x, \frac{1}{2m}\left(\left(-i\hbar\frac{\partial}{\partial x} + \hbar k\right)^2 + V(x)\right)\right]}_{i\hbar\frac{p+\hbar k}{m}}|u_{n,k}\rangle \\
&= \langle u_{n,k}|\frac{1}{m}\left(p+\hbar k\right)|u_{n,k}\rangle \\
&= \frac{1}{\hbar}\langle u_{n,k}|\frac{\partial H}{\partial k}|u_{n,k}\rangle \\
&= \frac{1}{\hbar}\frac{\partial \epsilon_{n,k}}{\partial k}.
\end{aligned} \tag{30}$$

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

$$\begin{aligned}
j_0 &= -e\sum_n \int_{\mathrm{BZ}} \frac{dk}{2\pi} v^{(0)}_{n,k} \\
&= -e\sum_n \frac{1}{\hbar}\int_{\mathrm{BZ}} \frac{dk}{2\pi}\frac{\partial \epsilon_{n,k}}{\partial k} \\
&= -e\sum_n \frac{1}{h}\int_{\mathrm{BZ}} d\epsilon_{n,k} \\
&= -e\sum_n \frac{1}{h}\left[\epsilon_{k=\frac{2\pi}{a},n} - \epsilon_{k=0,n}\right] = 0.
\end{aligned} \tag{31}$$

B. First-order current: j_1

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

$$|u^{(1)}_{k,n}\rangle = |u_{n,k}\rangle - i\hbar\sum_{n'\neq n}\frac{|u_{n',k}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle}{\epsilon_{n,k} - \epsilon_{k,n'}}. \tag{32}$$

Thus the first-order correction to the velocity reads

$$\begin{aligned}
v^{(1)}_{n,k} &\equiv \frac{1}{\hbar}\langle u_{n,k}|\frac{\partial H}{\partial k}|\left(-i\hbar\sum_{n'\neq n}\frac{|u_{n',k}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle}{\epsilon_{n,k} - \epsilon_{k,n'}}\right) + \frac{1}{\hbar}\left(i\hbar\sum_{n'\neq n}\frac{\left\langle \frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\langle u_{n',k}|}{\epsilon_{n,k} - \epsilon_{k,n'}}\right)|\frac{\partial H}{\partial k}|u_{n,k}\rangle \\
&= -i\sum_{n'\neq n}\frac{1}{\epsilon_{n,k} - \epsilon_{k,n'}}\left(\left\langle u_{n,k}|\frac{\partial H}{\partial k}|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle - \left\langle\frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}|\frac{\partial H}{\partial k}|u_{n,k}\right\rangle\right).
\end{aligned} \tag{33}$$

Now, let us exploit the similar relations as Eqs.(19) and (20):

$$\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial k}\right\rangle = \frac{1}{\epsilon_{n,k}-\epsilon_{k,n'}}\left\langle u_{n',k}\middle|\frac{\partial H}{\partial k}\middle|u_{n,k}\right\rangle \tag{34}$$

$$\left\langle \frac{\partial u_{n,k}}{\partial k}\middle|u_{n',k}\right\rangle = \frac{1}{\epsilon_{n,k}-\epsilon_{k,n'}}\left\langle u_{n,k}\middle|\frac{\partial H}{\partial k}\middle|u_{n',k}\right\rangle, \tag{35}$$

to get

$$\begin{aligned} v^{(1)}_{n,k} &= -i\sum_{n'\neq n}\left(\left\langle \frac{\partial u_{n,k}}{\partial k}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial k}\right\rangle\right) \\ &= -i\left(\left\langle \frac{\partial u_{n,k}}{\partial k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t}\middle|\frac{\partial u_{n,k}}{\partial k}\right\rangle\right). \end{aligned} \tag{36}$$

Remembering that

$$\begin{aligned} &\sum_{n'\neq n}\left(\left\langle \frac{\partial u_{n,k}}{\partial k}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle - \left\langle \frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial k}\right\rangle\right) \\ &= \sum_{n'\neq n}\left.\left[\begin{array}{c}\left\langle \frac{\partial u_{n,k}}{\partial k}\middle|u_{n',k}\right\rangle \\ \left\langle \frac{\partial u_{n,k}}{\partial t}\middle|u_{n',k}\right\rangle \\ 0\end{array}\right]\times\left[\begin{array}{c}\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial k}\right\rangle \\ \left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle \\ 0\end{array}\right]\right|_z \\ &= \sum_{n'\neq n}\left\langle \frac{\partial u_{n,k}}{\partial \boldsymbol{\sigma}}\middle|u_{n',k}\right\rangle\times\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial \boldsymbol{\sigma}}\right\rangle, \end{aligned} \tag{37}$$

and comparing the form of the Berry curvature in Eq. (16) we can recognize that $v^{(1)}_{n,k}$ is nothing but the Berry curvature:

$$v^{(1)}_{n,k} = -\Omega_{n,k}. \tag{38}$$

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*:

$$j_1 = -e\sum_n\int_{\rm BZ}\frac{dk}{2\pi}v^{(1)}_{n,k} = e\sum_n\int_{\rm BZ}\frac{dk}{2\pi}\Omega_{n,k} \tag{39}$$

C. Quantization of charge transport [1, 6]

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:

$$c_n = \int_0^T dt\int_{\rm BZ}\frac{dk}{2\pi}\Omega_{n,k}. \tag{40}$$

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

$$c_n = \frac{1}{2\pi}\int_0^1 dx\int_0^1 dy\;\Omega(x,y), \tag{41}$$

where

$$\Omega(x,y) = \frac{\Omega_{n,k}}{TG}. \tag{42}$$

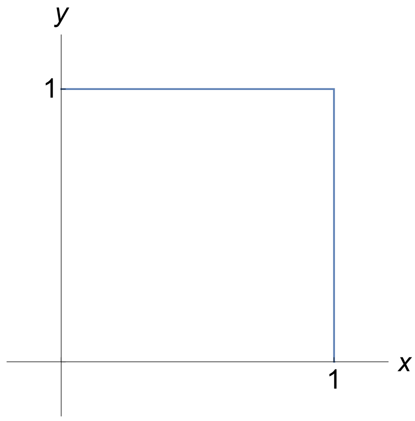

FIG. 1: Path $(0,0) \to (1,0) \to (1,1) \to (0,1) \to (0,0)$ is used to evaluate the integral Eq. (43).

We can now use the Stokes theorem to obtain the line integral form of Eq. (41), that is,

$$\begin{aligned} c_n &= \frac{1}{2\pi} \oint_C dl A(x,y) \\ &= \frac{1}{2\pi} \left(\int_0^1 dx A(x,0) + \int_0^1 dy A(1,y) + \int_1^0 dx A(x,1) + \int_1^0 dy A(0,y) \right) \\ &= \frac{1}{2\pi} \left(\int_0^1 dx \left(A(x,0) - A(x,1) \right) + \int_0^1 dy \left(A(1,y) - A(0,y) \right) \right), \end{aligned} \tag{43}$$

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

$$A(x,y) = i \left\langle u(x,y) \right| \boldsymbol{\nabla} \left| u(x,y) \right\rangle . \tag{44}$$

Here a question regarding the gauge choice arises. We have tacitly assumed the so-called *parallel transport gauge* (see Appendix A), 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, 4]:

$$|u(x,1)\rangle = e^{i\theta_x(x)} |u(x,0)\rangle \tag{45}$$

$$|u(1,y)\rangle = e^{i\theta_y(y)} |u(0,y)\rangle . \tag{46}$$

Thus,

$$\begin{aligned} A(x,0) - A(x,1) &= i \left\langle u(x,0) \middle| \frac{\partial}{\partial x} \middle| u(x,0) \right\rangle + i \left\langle u(x,1) \middle| \frac{\partial}{\partial x} \middle| u(x,1) \right\rangle \\ &= i \left\langle u(x,0) \middle| \frac{\partial}{\partial x} \middle| u(x,0) \right\rangle + i \left\langle u(x,0) \middle| e^{-i\theta_x(x)} \frac{\partial}{\partial x} e^{i\theta_x(x)} \middle| u(x,0) \right\rangle \\ &= \frac{\partial \theta_x(x)}{\partial x}, \end{aligned} \tag{47}$$

and similarly

$$A(0,y) - A(1,y) = \frac{\partial \theta_y(y)}{\partial y} . \tag{48}$$

Consequently, the line integral Eq. (43) becomes

$$\begin{aligned} c_n &= \frac{1}{2\pi} \left(\int_0^1 \frac{\partial \theta_x(x)}{\partial x} dx - \int_0^1 dy \frac{\partial \theta_y(y)}{\partial y} \right) \\ &= \frac{1}{2\pi} \left(\int_0^1 d\theta_x(x) - \int_0^1 d\theta_y(y) \right) \\ &= \frac{1}{2\pi} \left(\theta_x(1) - \theta_x(0) - \theta_y(1) + \theta_y(0) \right) . \end{aligned} \tag{49}$$

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

$$|u(0,0)\rangle = \exp\left[i\left(\theta_x(0)+\theta_y(1)-\theta_x(1)-\theta_y(0)\right)\right]|u(0,0)\rangle, \tag{50}$$

since the wave function acqires 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 $(0,0)$. We thus conclude that

$$\theta_y(0)+\theta_x(1)-\theta_y(1)-\theta_x(0) = 2\pi Z, \tag{51}$$

where Z is integer, and the line integral Eq. (49) becomes

$$c_n = Z. \tag{52}$$

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* [6].

Appendix A: First-order correction of the quantum adiabatic theorem [1, 4]

Here we derive $\left|u^{(1)}_{n,k}\right\rangle$ in Eq. (32) with the perturbation thoey. The relevent time-dependent Schrödinger equation reads

$$i\hbar\frac{\partial}{\partial t}\left|\psi_k(t)\right\rangle = H_k(t)\left|\psi_k(t)\right\rangle. \tag{A1}$$

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

$$\left|\psi_k(t)\right\rangle = \sum_n \exp\left[-\frac{i}{\hbar}\int_{t_0}^t dt'\epsilon_{n,k}\right] a_{n,k}(t)\left|u_{n,k}(t)\right\rangle, \tag{A2}$$

where $a_{n,k}$ are the coefficients. By plugging Eq. (A2) into Eq. (A1) and multiply $\langle u_{n',k}|$ from the left we find that the coefficients $a_{n,k}$ satisfy

$$\dot{a}_{n',k}(t) = -\sum_n a_{n,k}(t)\exp\left[-\frac{i}{\hbar}\int_{t_0}^t dt'\left(\epsilon_{n,k}-\epsilon_{n',k}\right)\right]\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle. \tag{A3}$$

Now we use the *parallel transport gauge* [1, 4], that is, the phase of $|u_{n,k}\rangle$ is chosen to be satisfy

$$\left\langle u_{n,k}(t)\middle|\frac{\partial}{\partial t}\middle|u_{n,k}(t)\right\rangle = 0 \tag{A4}$$

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

$$\dot{a}_{n,k}(t) = 0 \tag{A5}$$

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.*

The first-order correction of this situation is crucial for the Thouless pumping and can be obtained in the following way. Suppose we have $a_{n,k}(0) = 1$ and $a_{n',k}(0) = 0$ for $n' \neq n$. In this case Eq. (A5) is still intact but we have from Eq. (A3) with $a_{n,k}(t) \sim 1$

$$\dot{a}_{n',k}(t) = -\exp\left[-\frac{i}{\hbar}\int_{t_0}^t dt'\left(\epsilon_{n,k}-\epsilon_{n',k}\right)\right]\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle. \tag{A6}$$

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

$$a_{n',k}(t) = -\exp\left[-\frac{i}{\hbar}\int_{t_0}^t dt'\left(\epsilon_{n,k}-\epsilon_{n',k}\right)\right]\left(\frac{i\hbar\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle}{\epsilon_{n,k}-\epsilon_{n',k}}\right). \tag{A7}$$

Plugging this results for $a_{n',k}(t)$ and $a_{n,k}(t) = 1$ into Eq. (A2), we have

$$|\psi_k(t)\rangle = \exp\left[-\frac{i}{\hbar}\int_{t_0}^{t} dt' \epsilon_{n,k}\right]\left(\underbrace{|u_{n,k}(t)\rangle - i\hbar\sum_{n'\neq n}\frac{|u_{n',k}\rangle\left\langle u_{n',k}\middle|\frac{\partial u_{n,k}}{\partial t}\right\rangle}{\epsilon_{n,k}-\epsilon_{n',k}}}_{\left|u^{(1)}_{n,k}\right\rangle}\right). \tag{A8}$$

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