Lectures on Berry phase related phyiscs

Fumiyuki Ishii

Kanazawa University

June 17, 2018

Contents of lectures

Topics

- Berry phase and physical properties
- Berry curvature and anomalous Hall conductivity
- Topological invariant: Chern number and Z_2
- Computing Chern number as local quantity
- Computing Z_2 number as local quantity

Time-dependent Schrödinger equation

$$H(t+T) = H(t)$$

$$i\hbar\frac{\partial\psi}{\partial t} = H(t)\psi$$

$$H(t)\phi_n(t) = E_n(t)\phi_n(t)$$

$$\psi = \sum_n C_n(t)\phi_n(t) \simeq C_n(t)\phi_n(t)$$

$$i\hbar\left(\phi_n\frac{dC_n}{dt} + C_n\frac{d\phi_n}{dt}\right) = H(t)C_n\phi_n = E_nC_n\phi_n$$

$$\frac{d\phi_n}{dt} \simeq 0$$

$$i\hbar\frac{dC_n}{dt} \simeq E_nC_n$$

Time-dependent Schrödinger equation

$$i\hbar\frac{dC_n}{dt} = E_n C_n$$

$$\log C_n = -\frac{i}{\hbar}\int_0^t E_n(s)ds$$

$$C_n = \exp\left(-\frac{i}{\hbar}\int_0^t E_n(s)ds\right)$$

$$\psi = \exp\left(-\frac{i}{\hbar}\int_0^t E_n(s)ds\right)\phi_n$$

$$\psi \to \psi e^{i\theta(t)}$$

$$C_n \to C_n e^{i\theta(t)}$$

Time-dependent Schrödinger equation

$$i\hbar\left(\phi_n\frac{dC_n}{dt}+C_n\frac{d\phi_n}{dt}\right)=E_nC_n\phi_n$$

$$i\hbar\left(e^{i\theta(t)}\phi_n\frac{dC_n}{dt}+C_ne^{i\theta(t)}\phi_n\left(i\frac{d\theta(t)}{dt}\right)+C_ne^{i\theta(t)}\frac{d\phi_n}{dt}\right)$$
$$=E_nC_ne^{i\theta(t)}\phi_n$$

$$i\hbar\left(\phi_n\frac{dC_n}{dt}+C_n\phi_n\left(i\frac{d\theta(t)}{dt}\right)+C_n\frac{d\phi_n}{dt}\right)=E_nC_n\phi_n$$

$$\phi_n\left(\frac{d\theta(t)}{dt}\right)=i\frac{d\phi_n}{dt}$$

$$\int dr\phi_n^*\phi_n\left(\frac{d\theta(t)}{dt}\right)=\int dr\left(i\phi_n^*\frac{d\phi_n}{ds}\right)$$

Berry phase

Time-dependent Schrödinger equation

$$\int dr \phi_n^* \phi_n \left(\frac{d\theta(t)}{dt} \right) = \int dr \left(i\phi_n^* \frac{d\phi_n}{ds} \right)$$

$$\theta(t) = \int_0^t ds \int dr \left(i\phi_n^* \frac{d\phi_n}{ds} \right)$$

Berry phase

$$\theta(T) - \theta(0) = \frac{1}{\hbar} \int_0^T ds \int dr \phi_n^* \frac{\partial \phi_n}{\partial s} \neq 0$$

$$\frac{\partial}{\partial t} = \frac{dx}{dt} \frac{\partial}{\partial x}$$

$$\theta(x(T)) - \theta(x(0)) = \frac{1}{\hbar} \int_{x(0)}^{x(T)} dx' \int dr \phi_n^* \frac{\partial \phi_n}{\partial x'} \neq 0$$

Phase of Wavefunction

Guage transformation: phase and vector potential

$$\psi \to e^{\frac{ie\theta(\boldsymbol{r},t)}{\hbar}}\psi$$

$$H = \frac{1}{2m}(\boldsymbol{p} + e\boldsymbol{A})^2 - e\phi$$

$$i\hbar\frac{\partial\psi(\boldsymbol{r},t)}{\partial t} = H\psi(\boldsymbol{r},t)$$

$$\boldsymbol{A} \to \boldsymbol{A} - \nabla\theta(\boldsymbol{r},t)$$

$$\phi \to \phi + \frac{\partial\theta}{\partial t}$$

$$\boldsymbol{j} = \frac{\hbar}{2mi}\left(\nabla\psi^*(\boldsymbol{r},t)\psi(\boldsymbol{r},t) - \psi(\boldsymbol{r},t)^*\nabla\psi(\boldsymbol{r},t)\right) + \frac{e}{m}\left(\boldsymbol{A}|\psi(\boldsymbol{r},t)|^2 - |\psi(\boldsymbol{r},t)|^2\nabla\theta(\boldsymbol{r},t)\right)$$

c.f. Peierls substitution method: computing magnetic field effect whithin LCAO method

Phase of Wavefunction

Difference in phase of wavefunctions

$$e^{-i\Delta\theta} = \frac{\langle\phi(t)|\phi(t')\rangle}{|\langle\phi(t)|\psi(t')\rangle|}$$

$$\Delta\theta : \text{Real}$$

$$\log e^{-i\Delta\theta} = -i\Delta\theta = \text{Im}\log\langle\phi(t)|\phi(t')\rangle$$

$$\Delta t = t' - t \ll 1$$

$$\log\left(\langle\phi(t)|\phi(t+\Delta t)\rangle\right) \simeq \langle\phi(t)|\nabla_t\phi(t)\rangle\Delta t$$

$$\theta(T) - \theta(0) = \sum_{s=1}^{s=M} \Delta\theta_{s,s+1}$$

$$\rightarrow \oint_C \boldsymbol{A}(t)dt$$

$$\boldsymbol{A}(t) = i\langle\phi(t)|\nabla_t|\phi(t)\rangle$$

Electric currents and polarization

Electric currents in classical picture

$$\boldsymbol{J} = \frac{Ne}{V}\frac{d\boldsymbol{r}}{dt}$$

Electric polarization as integrated current I

$$\begin{aligned}\int_0^{\Delta t} \boldsymbol{J} dt &= \frac{Ne(\boldsymbol{r}(\Delta t) - \boldsymbol{r}(0))}{V} \\ &= \boldsymbol{P}(\Delta t) - \boldsymbol{P}(\mathbf{0})\end{aligned}$$

Electric currents and polarization II

Electric currents as derivative of electric polarization

$$\boldsymbol{J} = \frac{d\boldsymbol{P}}{dt}$$

Electric polarization expressed by wave function

$$\begin{aligned}
\frac{d\boldsymbol{P}}{dt} &= \frac{Ne}{V}\frac{d}{dt}\int d\boldsymbol{r}\psi(t)^*\boldsymbol{r}\psi(t) \\
&= \frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\left(\frac{d\psi(t)^*}{dt}\right)\psi(t) + \int d\boldsymbol{r}\boldsymbol{r}\psi(t)^*\left(\frac{d\psi(t)}{dt}\right)
\end{aligned}$$

Electric currents and polarization III

Time-dependent Schrödinger equation

$$\left(\frac{d\psi}{dt}\right) = \frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi$$

$$\left(\frac{d\psi^*}{dt}\right) = -\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi^*$$

Electric polarization expressed by wave function

$$\begin{aligned}\frac{dP}{dt} &= \frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\left(-\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi^*(t)\right)\psi(t) \\ &+\frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\psi(t)^*\left(\frac{1}{i\hbar}\left(-\frac{\hbar^2}{2m}\nabla^2 + v\right)\psi(t)\right)\end{aligned}$$

Electric currents and polarization IV

Electric polarization expressed by wave function

$$\begin{aligned}\frac{d\boldsymbol{P}}{dt} &= -\frac{Ne}{V}\frac{\hbar}{2mi}\int d\boldsymbol{r}\boldsymbol{r}\left(\nabla^2\psi^*(t)\psi(t) - \psi(t)^*\nabla^2\psi(t)\right) \\ &= -\frac{Ne}{V}\frac{\hbar}{2mi}\int d\boldsymbol{r}\boldsymbol{r}\nabla\cdot\left(\nabla\psi^*(t)\psi(t) - \psi(t)^*\nabla\psi(t)\right) \\ &= -\frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\nabla\cdot\boldsymbol{j}\end{aligned}$$

Probability current

$$\boldsymbol{j} = \frac{\hbar}{2mi}\left(\nabla\psi^*(t)\psi(t) - \psi(t)^*\nabla\psi(t)\right)$$

Electric currents and polarization V

Electric polarization (OBC) and continuity equation

$$\begin{aligned}
\frac{d\boldsymbol{P}}{dt} &= -\frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\nabla\cdot\boldsymbol{j} \\
\frac{d}{dt}\frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\rho &= -\frac{Ne}{V}\int d\boldsymbol{r}\boldsymbol{r}\nabla\cdot\boldsymbol{j} \\
\frac{d\rho}{dt} &= -\nabla\cdot\boldsymbol{j}
\end{aligned}$$

Probability current and phase of wavefunction

$$\psi(\boldsymbol{r},t) = |\psi(\boldsymbol{r},t)|\, e^{i\theta(\boldsymbol{r},t)}$$

$$\boldsymbol{j} = -\frac{\hbar}{m}|\psi(\boldsymbol{r},t)|^2\nabla\theta(\boldsymbol{r},t)$$