Geometry Phase in condensed matter

December 28, 2018

References

- “Geometric Phases in Classical and Quantum Mechanics”, Chruściński and Jamiołkowski, Springer (2004)
- “Topological Insulators and Topological Superconductors”, Bernevig, Princeton (2013)
- “A Short Course on Topological Insulators”, Asbóth, Oroszlány, and Pályi, Springer (2016)
- “Topology and Geometry for Physicists”, Nash and Sen, Dover (1983)

绝热演化

[Michael Berry, "Quantal phase factors accompanying adiabatic changes", Proc. Roy. Soc. London A 392, 45-57, (1984)]

$$\mathcal{H}(t) = \mathcal{H}[\mathrm{R}(t)]$$

$$\mathcal{H}[\mathrm{R}(t)]|\psi_n[\mathrm{R}(t)]\rangle = \mathcal{E}_n[\mathrm{R}(t)]|\psi_n[\mathrm{R}(t)]\rangle \qquad \langle\psi_n(\mathrm{R})|\psi_m(\mathrm{R})\rangle = \delta_{nm}$$

$$\rightarrow \mathcal{H}(t)|\psi_n(t) = \mathcal{E}_n(t)|\psi_n(t)\rangle$$

$$\dot{\mathcal{H}}|\psi_m(t)\rangle + \mathcal{H}(t)|\dot{\psi}_m(t)\rangle = \dot{\mathcal{E}}_m(t)|\psi_m(t)\rangle + \mathcal{E}_m(t)|\dot{\psi}_m(t)\rangle$$

$$\langle\psi_n(t)|\dot{\mathcal{H}}|\psi_m(t)\rangle + \mathcal{E}_n(t)\langle\psi_n(t)|\dot{\psi}_m(t)\rangle = \dot{\mathcal{E}}_m(t)\delta_{nm} + \mathcal{E}_m(t)\langle\psi_n(t)|\dot{\psi}_m(t)\rangle$$

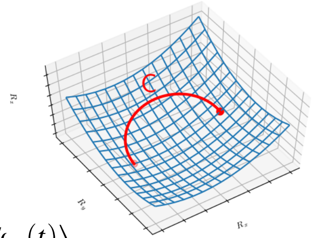
$$\langle\psi_n(t)|\dot{\psi}_m(t)\rangle = \frac{\langle\psi_n(t)|\dot{\mathcal{H}}(t)|\psi_m(t)\rangle}{\mathcal{E}_m(t) - \mathcal{E}_n(t)} \qquad \longleftarrow \mathcal{E}_n \neq \mathcal{E}_m$$

$$\sim 0 \qquad \longleftarrow \dot{H} \ll |\mathcal{E}_m - \mathcal{E}_n|$$

绝热演化

$$
\begin{aligned}
|\psi(t)\rangle &= \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau \leftarrow \text{dynamic phase}} |\psi_m(t)\rangle \\
i\hbar\partial_t|\psi(t)\rangle &= \sum_m [i\hbar\partial_t c_m(t) + \mathcal{E}_m(t)] e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} |\psi_m(t)\rangle \\
&\quad + i\hbar \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} |\dot{\psi}_m(t)\rangle \\
&= \mathcal{H}(t)|\psi(t)\rangle = \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} \mathcal{H}(t)|\psi_m(t)\rangle \\
&= \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} \mathcal{E}_m(t)|\psi_m(t)\rangle \\
0 &= \dot{c}_n(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_n(\tau)d\tau} + \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} \langle\psi_n(t)|\dot{\psi}_m(t)\rangle \\
\dot{c}_n(t) &= -\sum_m c_m(t) e^{\frac{i}{\hbar}\int_0^t [\mathcal{E}_n(\tau)-\mathcal{E}_m(\tau)]d\tau} \langle\psi_n(t)|\dot{\psi}_m(t)\rangle \\
&\simeq -c_n(t)\langle\psi_n(t)|\dot{\psi}_n(t)\rangle \to c_n(t) = e^{i\gamma_n(t)} c_n(0)
\end{aligned}
$$

Adiabatic Berry Phase

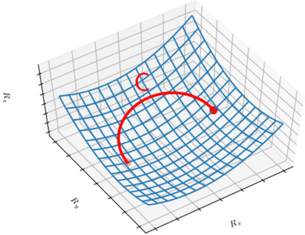


$$|\psi(t)\rangle = \sum_m e^{i\gamma_m(t)} e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} c_m(0)|\psi_m(t)\rangle$$

$$\gamma_n(t) = i\int_0^t \langle\psi_n(\tau)|\dot{\psi}_n(\tau)\rangle d\tau = i\int_0^t \langle\psi_n[R(\tau)]|\partial_R\psi_n[R(\tau)]\rangle \dot{R}(\tau)d\tau$$

$$= i\int_{R(0)}^{R(t)} \langle\psi_n(R)|\partial_R\psi_n(R)\rangle\cdot dR = i\int_C \mathcal{A}_n(R)\cdot dR$$

Adiabatic Berry Phase



$\gamma_m(t)$ 是路径依赖，规范依赖的

$$
\begin{aligned}
|\psi_n(R)\rangle \rightarrow |\psi_n'(R)\rangle &= e^{-i\theta_n(R)}|\psi_n(R)\rangle \\
\mathcal{A}_n'(R) &= i\langle\psi_n(R)|e^{i\theta_n(R)}e^{-i\theta_n(R)}[-i\partial_R\theta_n(R)|\psi_n(R)\rangle + |\partial_R\psi_n(R)\rangle \\
&= \partial_R\theta_n(R) + \mathcal{A}_n(R) \\
\gamma_n'(t) &= \theta_n[R(t)] - \theta_n[R(0)] + \gamma_n(t)
\end{aligned}
$$

Fock 1928 年发现绝热演化导致的额外相位，但是他认为这个相位并不重要且可以忽略：对于任何路径只要 $R(t) \neq R(0)$，我们总可以选择适当的规范 $\theta_n(R)$，使得 $\gamma'(t) = 0$。

Berry Connection/Berry 连接

1984 年 Michael Berry：闭合路径 $R(T) = R(0)$ 中，这个相位无法消除，因此可以导致可观察效应。

$e^{i\theta_n[R(T)]} = e^{i\theta_n[R(0)]} \longrightarrow \theta_n[R(T)] = \theta_n[R(0)] + 2N\pi,$

$N = 0, \pm 1, \pm 2 \cdots$, 和 R 空间上的连通性有关。如果是单连通的话，$N = 0$。

$$\Delta\Theta = \theta_n[R(T)] - \theta_n[R(0)]$$

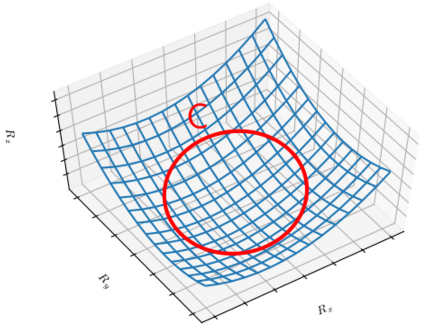
$$= \oint_\gamma \nabla\theta_n(R) \cdot d\mathrm{l}$$

$$\overset{\text{单连通}}{=} \iint \nabla \times \nabla\theta_n(R) \cdot d\mathrm{S} = 0$$

$$\gamma_n(T) \rightarrow \theta_n[R(T)] - \theta_n[R(0)]$$

$$+ \oint_C \mathcal{A}_n \cdot dR$$

$$= 2N\pi + \oint_C \mathcal{A}_n \cdot dR$$



Berry Curvature/Berry 曲率

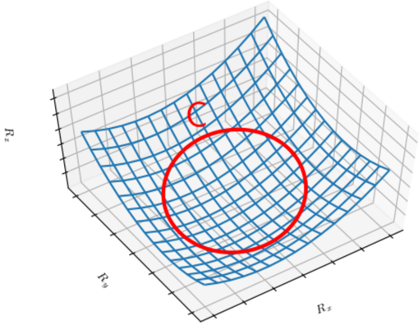
3 维 $R=(R_x,R_y,R_z)$ 空间，Stokes 定理

$$\gamma_n(T) = \oint_C \mathcal{A}_n \cdot dR$$

$$= \int\!\!\int_S \mathbf{\Omega}_n(R) \cdot dS$$

$$\mathbf{\Omega}_n(R) = \nabla_R \times \mathcal{A}_n(R)$$

$$= i\langle \nabla_R \psi_n(R)| \times |\nabla_R \psi_n(R)\rangle$$



- $\mathbf{\Omega}_n(R)$ 定义在 R 空间上
- 非平凡情况下，波函数 $|\psi_n(\mathrm{R})\rangle$ 必然是多分量。
- $\mathbf{\Omega}_n(R)$ 规范不变
  $|\psi_n(\mathrm{R})\rangle$☞$|\psi'_n(\mathrm{R})\rangle = e^{i\theta_n(\mathrm{R})}|\psi_n(\mathrm{R})\rangle$,
  $\mathbf{\Omega}'_n = \mathbf{\Omega}_n + i(\nabla_{\mathrm{R}}\theta_n) \times (\nabla_{\mathrm{R}}\theta_n) = \mathbf{\Omega}_n$

Berry Curvature 的计算

$$\mathcal{H}(R)|\psi_n(R)\rangle = \mathcal{E}_n(\mathrm{R})|\psi_n(\mathrm{R})\rangle \qquad \boldsymbol{\nabla}_R[\mathcal{H}|\psi_n\rangle] = \boldsymbol{\nabla}_R[\mathcal{E}_n|\psi_n\rangle]$$

$$(\boldsymbol{\nabla}_R\mathcal{H})|\psi_n\rangle + \mathcal{H}|\boldsymbol{\nabla}_R\psi_n\rangle = (\boldsymbol{\nabla}_R\mathcal{E}_n)|\psi_n\rangle + \mathcal{E}_n|\boldsymbol{\nabla}_R\psi_n\rangle$$

$$\langle\psi_m|\cdots \rightarrow \langle\psi_m|\boldsymbol{\nabla}_R\mathcal{H}|\psi_n\rangle + \mathcal{E}_m\langle\psi_m|\boldsymbol{\nabla}_R\psi_n\rangle = \boldsymbol{\nabla}_R\mathcal{E}_n\delta_{nm} + \mathcal{E}_n\langle\psi_m|\boldsymbol{\nabla}_R\psi_n\rangle$$

$$\langle\psi_m|\boldsymbol{\nabla}_R\psi_n\rangle = \frac{\langle\psi_m|\boldsymbol{\nabla}_R\mathcal{H}|\psi_n\rangle}{\mathcal{E}_n - \mathcal{E}_m} \qquad m \neq n$$

$$\mathcal{A}_n = i\langle\psi_n|\boldsymbol{\nabla}_R\psi_n\rangle$$

$$\boldsymbol{\Omega}_n = \boldsymbol{\nabla}_R \times \mathcal{A}_n = i\langle\boldsymbol{\nabla}_R\psi_n| \times |\boldsymbol{\nabla}_R\psi_n\rangle = \sum_m i\langle\boldsymbol{\nabla}_R\psi_n|\psi_m\rangle \times \langle\psi_m|\boldsymbol{\nabla}_R\psi_n\rangle$$

$$= i\sum_{m\neq n}\langle\boldsymbol{\nabla}_R\psi_n|\psi_m\rangle \times \langle\psi_m|\boldsymbol{\nabla}_R\psi_n\rangle$$

$$= -i\sum_{m\neq n}\frac{\langle\psi_n|\boldsymbol{\nabla}_R\mathcal{H}|\psi_m\rangle \times \langle\psi_m|\boldsymbol{\nabla}_R\mathcal{H}|\psi_n\rangle}{(\mathcal{E}_n - \mathcal{E}_m)^2}$$

Berry Connection and Berry Curvature 的几何意义

["Holonomy, the Quantum Adiabatic Theorem, and the Berry Phase", Barry Simon, PRL 51, 2167 (1983)]

- 参数 R 构成一个空间 ☞ 底流形（Base manifold）
- 在每个 R 点定义量子态、波函数 $\psi_n(R)\rangle$
- 每个 R 点波函数有相位的自由度，可用另一个参数 $\theta_n(R)$ 描述：$\psi_n(R) \rightarrow e^{i\theta_n(R)}|\psi_n(R)\rangle$
  ☞ 这个相位几何上等价于一条线 ☞ fiber/ray/line
  ☞ 更准确一点说，这个 fiber 等价于一个"直的"圆（S^1）
- 几何体：R 空间和 fiber 的组合 ☞ bundle
  ☞ 整个几何体是 R 空间上的 principle U(1) bundle
  ☞ 所谓的几何拓扑属性都是针对这个 bundle 而言
  - $\mathcal{A}_n(R)$: Connection of line bundle/U(1) bundle
    ☞ 描述不同点上的 fiber 如何连接在一起
  - $\boldsymbol{\Omega}_n(R)$: Curvature of line bundle/U(1) bundle
    ☞ bundle 上的曲率

  ☞ R 空间的几何属性会影响 bundle 的几何属性
  ☞ 通常这两者的几何属性是不同的。

Berry Connection and Berry Curvature 的几何意义

- 欧几里德空间的邻居：距离 $d = |R - R'|$ 最小
  $(x, y, z) \Leftrightarrow (x + \delta x, y + \delta y, z)$
- line bundle 上的邻居：波函数距离最小

$$
\begin{aligned}
|\psi_n(R+\delta R)\rangle &= |\psi_n(R)\rangle + \delta R|\partial_R \psi_n(R)\rangle \\
&= |\psi_n\rangle + \delta R \sum_m |\psi_m\rangle\langle\psi_m|\partial_R\psi_n\rangle \qquad \text{绝热演化 ☞} \\
&\simeq |\psi_n\rangle + \delta R|\psi_n\rangle\langle\psi_n|\partial_R\psi_n\rangle = -i\mathcal{A}_n(R) \\
&= [1 - i\delta R\, \mathcal{A}_n]|\psi_n\rangle = e^{-i\delta R\, \mathcal{A}_n}|\psi_n\rangle
\end{aligned}
$$

$$
e^{i\theta_n(R)}|\psi_n(R)\rangle \Leftrightarrow e^{i\theta_n(R+\delta R)}|\psi_n(R+\delta R)\rangle \simeq e^{i\theta_n(R+\delta R)} e^{-i\delta R \mathcal{A}_n}|\psi_n\rangle
$$

$$
\theta_n(R+\delta R) \Leftrightarrow \theta_n(R) + \delta R\, \mathcal{A}_n(R)
$$

☞ line bundle 上，$\Theta_n(R+\delta R)$ 和 $\Theta_n(R) + \delta R\, \mathcal{A}_n(R)$ 是邻居

☞ $\mathcal{A}_n(R)$ 包含了如何“连接”相邻的 fiber/line/ray 的信息

磁场中的自旋的 Berry phase

参数空间：B，球面（磁场大小不变）或者球（磁场大小可变）

$$\mathrm{B} = (B_x, B_y, B_z) = B(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) = B\hat{e}_r = B\hat{n}$$

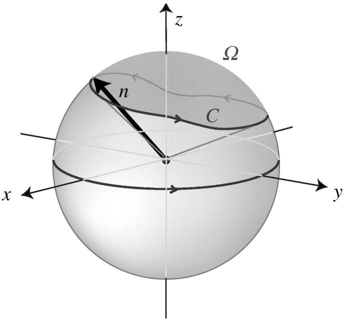
$$\mathcal{H} = \boldsymbol{\sigma}\cdot\mathrm{B} = \begin{pmatrix} B_z & B_x - iB_y \\ B_x + iB_y & -B_z \end{pmatrix}$$

$$|\psi_+\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix}$$

$$\mathcal{A}_\pm = i\langle\psi_\pm|\boldsymbol{\nabla}_\mathrm{B}|\psi_\pm\rangle$$

$$= i\langle\psi_\pm|\hat{e}_r\partial_B + \frac{\hat{e}_\theta}{B}\partial_\theta + \frac{\hat{e}_\phi}{B\sin\theta}\partial_\phi|\psi_\pm\rangle$$

$$= \mp\frac{\sin\theta/2\hat{e}_\phi}{2B\cos\theta/2}$$



$$\boldsymbol{\Omega}_\pm = \boldsymbol{\nabla}\times\mathcal{A}_\pm = \pm\frac{\hat{e}_r}{2B^2} = \pm\frac{\hat{n}}{2B^2}$$

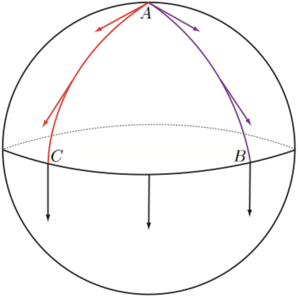
$$\gamma_\pm(T) = \oint\mathcal{A}_\pm\cdot d\mathrm{R} = \int\int_S \Omega_\pm(R)\cdot d\mathrm{S} = \pm\Omega_C$$

$\gamma_\pm$ 的几何含义：球面上矢量顺着轨道“平行移动”之后和原矢量的夹角。

磁场中的自旋的几何：球面上矢量的“平行移动”

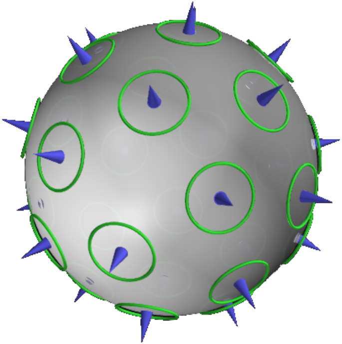
Parallel transport：在曲面上沿某曲线移动矢量，使得移动前后矢量“平行”。大体上：移动时保持矢量和该曲线夹角不变。

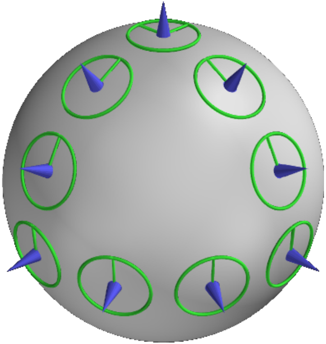
- 球面上的矢量平行移动一圈回到原点，和原矢量有个夹角，$\gamma_C = \Omega_C$ anholomony angle
- $\gamma_C \neq 0$ 是球面弯曲造成，由球面的几何性质决定。
- 经典力学中的几何相位：傅科摆
- $\gamma_C =$ 磁场中自旋 1/2 粒子的 Berry Phase 角度。



磁场中自旋的 line bundle

- 磁场中自旋 1/2 粒子的 line bundle 是球面上的一系列单位圆。
- 这种 bundle 的几何属性和参数空间 $\hat{B} = B\hat{n}$，即球面的切矢量丛完全等价。
- 这是一个非常特殊的情况，通常情况下，这两者并不等价。例拓扑绝缘体的 Bloch bundle 通常不等价于参数空间。





“磁单极” /“Magnetic” monopole

- 真实空间里的磁场：$\mathrm{B} = \boldsymbol{\nabla} \times \mathrm{A}$
- 参数空间里的“有效”磁场：$\boldsymbol{\Omega}_n(\mathrm{R}) = \boldsymbol{\nabla}_{\mathrm{R}} \times \mathcal{A}_n(\mathrm{R})$
- 磁场中的自旋：$\boldsymbol{\Omega}_+(\mathrm{B}) = \hat{B}/(2B^2)$

$$4\pi = \oint\!\!\!\oint_{\mathrm{R}} \boldsymbol{\Omega}_+ \cdot d\mathrm{S}_{\mathrm{B}} = \iiint \boldsymbol{\nabla}_{\mathrm{B}} \cdot \boldsymbol{\Omega}_+ dV_{\mathrm{B}} = 4\pi \iiint \delta(\mathrm{B}) dV_{\mathrm{B}}$$

☞ 点“磁荷”产生的有效“磁场”
☞ $\mathrm{B} \to 0 \longrightarrow \Omega_+(\mathrm{B}) \to \infty$
☞ $\mathcal{A}_+ = \frac{\sin\theta/2}{2B^2\cos\theta/2}\mathrm{e}_\phi \xrightarrow{\theta\to\pi} \infty$
☞ 一般情况下 $\boldsymbol{\nabla}_{\mathrm{R}} \cdot \boldsymbol{\Omega} = \boldsymbol{\nabla}_{\mathrm{R}} \cdot [\boldsymbol{\nabla}_{\mathrm{R}} \times \mathcal{A}] = 0$
☞ 非平凡拓扑必然意味着存在“磁单极”

- 存在“磁单极”的必要条件

$\boldsymbol{\Omega}_n(\mathrm{R}) = -i\sum_{m\neq n} \frac{\langle\psi_n|\boldsymbol{\nabla}_{\mathrm{R}}\mathcal{H}|\psi_m\rangle\times\langle\psi_m|\boldsymbol{\nabla}_{\mathrm{R}}\mathcal{H}|\psi_n\rangle}{[\mathcal{E}_n(\mathrm{R})-\mathcal{E}_m(\mathrm{R})]^2}$

$\Omega_n(\mathrm{R}) \to \infty \Leftarrow \mathcal{E}_n(\mathrm{R}) = \mathcal{E}_m(\mathrm{R})$

☞ 在扩大的参数空间存在能级简并

受对称保护的拓扑性质

- 一般情况下
  $\gamma_c = \oint \mathcal{A} \cdot d\mathrm{l}$ 取值任意
- Chiral symmetry
  磁场只能躺在 $x - y$ 平面 $\mathrm{B} = B(\cos\phi, \sin\phi, 0)$
  ☞ $\sigma_z \mathcal{H} \sigma_z = -\mathcal{H}$
  ☞ $\gamma_C = 2n\pi,\ n = 0, \pm 1, \pm 2, \cdots$

More than 3D

$$
\begin{aligned}
\mathrm{R} &= (R_1, R_2, R_3, \cdots, R_p) \\
\gamma(C) &= \oint_C \mathcal{A}(\mathrm{R}) \cdot d\mathrm{R} = \sum_{\mu=1}^{p} \oint_C \mathcal{A}_i(\mathrm{R}) d\mathrm{R}_i \\
&= \int\int_S \boldsymbol{\Omega}_{\mu\nu}(\mathrm{R}) \cdot d\mathrm{S}_{\mu\nu} \\
\boldsymbol{\Omega}_{\mu\nu} &= \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu \\
d\mathrm{S}_{\mu\nu} &= dR_\mu \wedge dR_\nu = -dR_\nu \wedge dR_\mu
\end{aligned}
$$

电磁场的几何属性

- 参数空间就是时空 (t, r)
- “平直空间”里（无电磁场时）的 Schrödinger 方程

$$i\hbar\partial_t\psi_0(t,\mathrm{r}) = \frac{(-i\hbar\boldsymbol{\nabla}_{\mathrm{r}})^2}{2m}\psi_0(t,\mathrm{r})$$

- “弯曲空间”里（有电磁场时）的 Schrödinger 方程
  ☞ 把 $q\phi = q\phi(t,\mathrm{r}), q\mathrm{A} = q\mathrm{A}(t,\mathrm{r})$ 当成 Berry connection
  ☞ Berry phase

$$\gamma(t,\mathrm{r}) = \frac{q}{\hbar}\int_{(0,0)}^{(t,\mathrm{r})}(\phi,-\mathrm{A})\cdot(dt,d\mathrm{r})$$

$$\psi(t,\mathrm{r}) = e^{i\gamma(t,\mathrm{r})}\psi_0(t,\mathrm{r}) \Leftarrow \psi_0(t,\mathrm{r})$$

$$i\hbar\partial_t\psi = \frac{(-i\hbar\boldsymbol{\nabla}_{\mathrm{r}} + q\mathrm{A})^2}{2m}\psi - q\phi\psi$$

规范变换

$$
\begin{aligned}
\phi &\to \phi'(\mathrm{R},t) = \phi(\mathrm{R},t) + \partial_t \chi(\mathrm{R},t) \\
\mathrm{A} &\to \mathrm{A}'(\mathrm{R},t) = \mathrm{A}(\mathrm{R},t) - \boldsymbol{\nabla}_{\mathrm{R}} \chi(\mathrm{R},t) \\
\mathrm{E} &= \boldsymbol{\nabla}_{\mathrm{R}}\phi + \partial_t \mathrm{A} \to \boldsymbol{\nabla}_{\mathrm{R}}(\phi + \partial_t \chi) + \partial_t(\mathrm{A} - \boldsymbol{\nabla}_{\mathrm{R}}\chi) \\
&= \boldsymbol{\nabla}_{\mathrm{R}}\phi' + \partial_t \mathrm{A}' \\
\mathrm{B} &= \boldsymbol{\nabla}_{\mathrm{R}} \times \mathrm{A} \to \boldsymbol{\nabla}_{\mathrm{R}} \times (\mathrm{A} - \boldsymbol{\nabla}_{\mathrm{R}}\chi) \\
&= \boldsymbol{\nabla}_{\mathrm{R}} \times \mathrm{A}'
\end{aligned}
$$

$$
\begin{aligned}
&\psi \to \psi' = e^{-i\chi}\psi \\
&\quad (i\hbar\partial_t + q\phi)\psi = \frac{(-i\hbar\boldsymbol{\nabla}_{\mathrm{R}} - q\mathrm{A})^2}{2m}\psi \\
&\to (i\hbar\partial_t + q\phi')\psi' = \frac{(-i\hbar\boldsymbol{\nabla}_{\mathrm{R}} - q\mathrm{A}')^2}{2m}\psi'
\end{aligned}
$$

闭合路径里的 Berry Phase

无穷小环

$C = (t,\mathrm{r}) \text{——} (t,\mathrm{r}) + (dt_1, d\mathrm{r}_1) \text{——} (t,\mathrm{r}) + (dt_1 + dt_2, d\mathrm{r}_1 + d\mathrm{r}_2)$
$\text{——} (t,\mathrm{r}) + (dt_2, d\mathrm{r}_2) \text{——} (t,\mathrm{r})$

$$
\begin{aligned}
\frac{\hbar}{q}\delta\gamma_C \simeq\ & [\phi(t,\mathrm{r})dt_1 - \mathrm{A}(t,\mathrm{r}) \cdot d\mathrm{r}_1] \\
& + [\phi(t+dt_1, \mathrm{r}+d\mathrm{r}_1)dt_2 - \mathrm{A}(t+dt_1, \mathrm{r}+d\mathrm{r}_1) \cdot d\mathrm{r}_2] \\
& - [\phi(t+dt_2, \mathrm{r}+d\mathrm{r}_2)dt_1 - \mathrm{A}(t+dt_2, \mathrm{r}+d\mathrm{r}_2) \cdot d\mathrm{r}_1] \\
& - [\phi(t,\mathrm{r})dt_2 - \mathrm{A}(t,\mathrm{r}) \cdot d\mathrm{r}_2] \\
& \simeq [\phi dt_1 - \mathrm{A} \cdot d\mathrm{r}_1] - [\phi dt_2 - \mathrm{A} \cdot d\mathrm{r}_2] \\
& + [(\phi + \partial_t \phi dt_1 + \nabla\phi \cdot d\mathrm{r}_1)dt_2 - (\mathrm{A} + \partial_t \mathrm{A} dt_1 + d\mathrm{r}_1 \cdot \nabla \mathrm{A}) \cdot d\mathrm{r}_2] \\
& - [(\phi + \partial_t \phi dt_2 + \nabla\phi \cdot d\mathrm{r}_2)dt_1 - (\mathrm{A} + \partial_t \mathrm{A} dt_2 + d\mathrm{r}_2 \cdot \nabla \mathrm{A}) \cdot d\mathrm{r}_1] \\
& = -(\nabla\phi + \partial_t \mathrm{A})dt_1 \cdot d\mathrm{r}_2 + (\nabla\phi + \partial_t \mathrm{A})dt_2 \cdot d\mathrm{r}_1 \\
& \quad - d\mathrm{r}_1 \cdot \nabla \mathrm{A} \cdot d\mathrm{r}_2 + d\mathrm{r}_2 \cdot \nabla \mathrm{A} \cdot d\mathrm{r}_1 \\
& = \mathrm{E} \cdot (-dt_1 d\mathrm{r}_2 + dt_2 d\mathrm{r}_1) + \mathrm{B} \cdot (d\mathrm{r}_1 \times d\mathrm{r}_2)
\end{aligned}
$$

电磁场的几何

1918/1919, H. Weyl, after Einstein's geometrization of gravitational force

- 电磁势 ☞ 带电粒子在时空上的连接
- 电磁场 ☞ 带电粒子在时空中的曲率
  - 电场 ☞ 时间 + 真实空间上的曲率
  - 磁场 ☞ 真实空间上的曲率
- Berry phase ☞ 时空上的场 “通量”
  对静磁场，Berry phase 正比于磁通量

$$\gamma(C) = \frac{q}{\hbar}\oint_C \mathrm{A}\cdot d\mathrm{r} = \frac{2\pi}{h/q}\Phi = 2\pi\Phi/\Phi_0$$

$$\Phi_0 = h/q = h/e \qquad \text{flux quantum for electrons}$$

$$\Phi = \oint_C \mathrm{A}\cdot d\mathrm{r} = \int\int_S \mathrm{B}\cdot d\mathrm{S} \qquad \text{Magnetic flux}$$

对静磁场来说，参数空间就是实空间
☞ 容易制造出拓扑非平凡的体系

电磁势的角色

Electromagnetic potentials are not unique ☞ Electromagnetic potentials have no physics significance ☞ Only fields E and H can be observed, when they both vanish, there cannot be any electromagnetic effects on a charged particle.

- O. Heaviside

  "A and its scalar potential parasite ϕ sometimes causing great mathematical complexity and indistinctiveness; and it is, for practical reasons, best to murder the whole lot, or, at any rate, merely employ them as subsidiary functions $\cdots$ Thus ϕ and A are murdered, so to speak, with a great gain in definiteness and conciseness."

- Whittaker

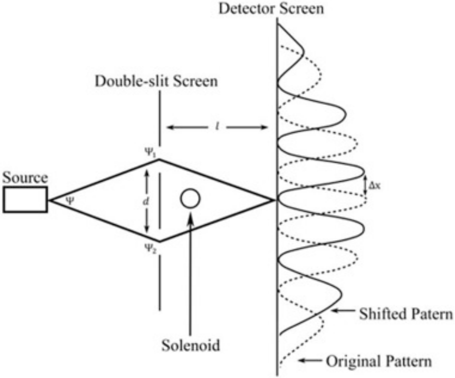
  "As the potentials do not possess any physical significance, it is desirable to remove them from the equations. This was done afterwards by Maxwell himself, who in 1868 proposed to base the electromagnetic theory of light solely on the equations $\nabla \times \mathrm{H} = 4\pi\mathrm{S}$, $\nabla \times \mathrm{E} = -\partial_t \mathrm{B}$ together with the equations which define S in terms of E, and B in terms of H."

Berry Phase 的观测：A-B effect

W. Ehrenberg and R. E. Siday, “The Refractive Index in Electron Optics and the Principles of Dynamics”, Proceedings of the Physical Society. Series B. 62, 8 (1949); Y. Aharonov and D Bohm, “Significance of electromagnetic potentials in quantum theory”, Phys. Rev. 115, 485 (1959).

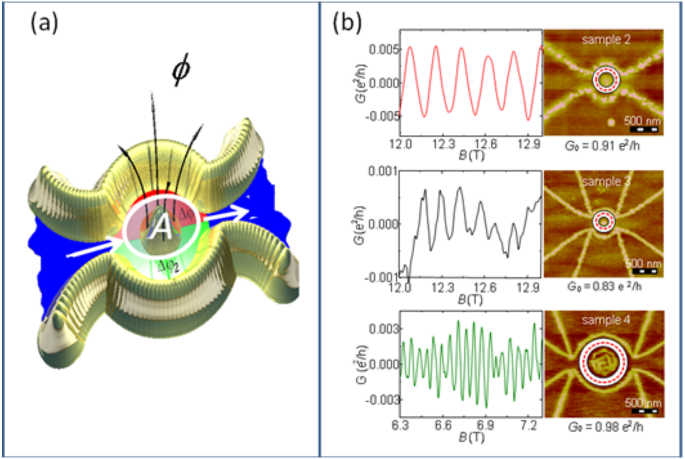
- 电子的双缝干涉条纹
- 线圈外无电磁场 ☞ 经典角度线圈是否通电流对干涉条纹无影响
- 量子角度通电流之后磁通不为零 ☞ 不同路径相位差（Berry phase）☞ 干涉条纹移动

$$\Delta\varphi = \gamma(C) = 2\pi\Phi/\Phi_0$$
$$\Delta x = \frac{\lambda l}{d}\frac{\Delta\varphi}{2\pi} = \frac{\lambda l}{d}\frac{\Phi}{\Phi_0}$$



Berry Phase 的观测：纳米环里的电导震荡

[Giesbers et al, “Correlation-induced single-flux-quantum penetration in quantum rings”, Nat. Phys. 6, 173 (2010)]



$$G/G_0 = |t_1 e^{i\gamma_1} + t_2 e^{i\gamma_2}|^2 = |t_1|^2 + 2|t_2|^2 + 2|t_1 t_2| \cos[\theta_{12} + (\gamma_2 - \gamma_1)]$$
$$= T_1 + T_2 + 2\sqrt{T_1 T_2} \cos[\theta_{12} + 2\pi\Phi/\Phi_0]$$

纳米环里的持续电流

- 有时间反演不变的体系中，热力学平衡态下不可能存在电流
- 加上磁场之后破坏时间反演不变，可能存在平衡电流

半径为 R 的纳米环，中心有磁通 Φ：

$$\mathrm{A} = \Phi/(2\pi R)\hat{e}_\phi \qquad \Phi = \oint \mathrm{A}\cdot d\mathrm{l}$$

$$\mathcal{H} = \frac{(-i\hbar + e\mathrm{A})^2}{2m^*} = \frac{\hbar^2}{2m^*}\left[\frac{-i\partial_\phi}{R} + \frac{e\Phi}{Rh}\right]^2 = \frac{\hbar^2}{2m^*R^2}\left(-i\partial_\phi + \frac{\Phi}{\Phi_0}\right)^2$$

$$\Psi_l(\phi) = e^{il\phi} \qquad E_l\Psi_l = \mathcal{H}\Psi_l = \frac{\hbar^2}{2m^*R^2}(l + \Phi/\Phi_0)^2$$

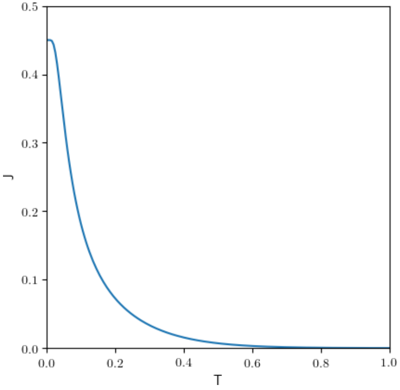
$$\mathrm{I}_l = I_l\hat{e}_\phi = -\frac{e}{m^*}\langle\Psi_l|\mathrm{p} + e\mathrm{A}|\Psi_l\rangle = -\frac{\partial E_l(\mathrm{A})}{\partial \mathrm{A}} = 2\pi R\frac{\partial E_l}{\partial \Phi}\hat{e}_\phi$$

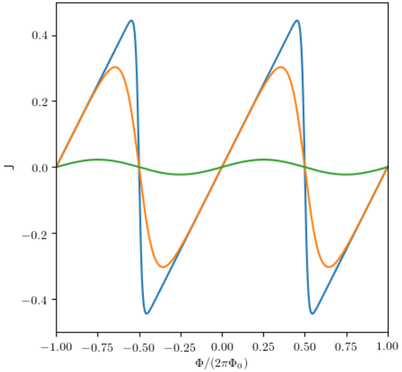
$$\propto (l + \Phi/\Phi_0)\hat{e}_\phi$$

纳米环里的持续电流

$$E_l \propto (l+\Phi/\Phi_0)^2 \qquad I_l \propto (l+\Phi/\Phi_0) \qquad I = \frac{1}{Z}\sum_l I_l e^{-\beta E_l}$$

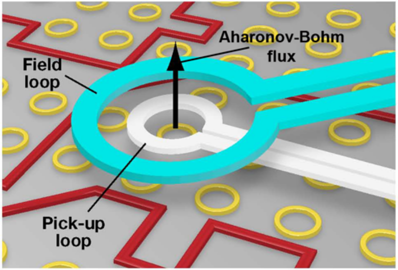
- 无磁场：$\Phi = 0$
  $E_l = E_{-l}$, $I_l = -I_{-l}$， $I = 0$
- 有磁场：$\Phi \neq 0$
  $E_l \neq E_{-l}$， $I_l \neq -J_l$， $I \neq 0$

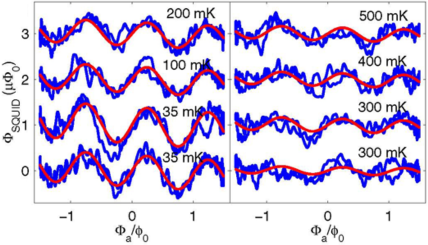




纳米环里的持续电流

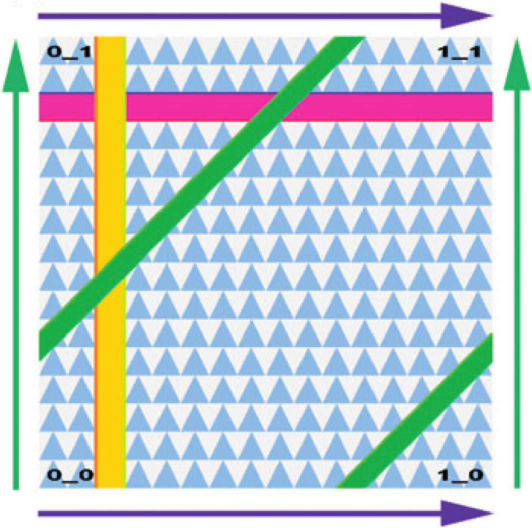
M. Büttiker, Y. Imry and R. Landauer, “Josephson behavior in small normal one-dimensional rings”, Phys. Lett. A 96, 365 (1983); H. Bluhm et al, “Persistent Currents in Normal Metal Rings”, PRL 102, 136802 (2009)





$\Phi = 0$ 时量子环里电子的 line bundle

C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)



$\Phi = 0$ 时量子环里电子的 line bundle

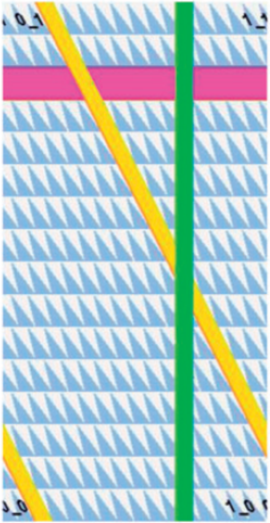
C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)

$\Phi = 0$ 时量子环里电子的 line bundle

C. H. Séquin, "Topological tori as abstract art", Journal of Mathematics and the Arts 6, 191–209, (2012)

$\Phi = \Phi_0$ 时量子环里电子的 line bundle

C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)



$\Phi = \Phi_0$ 时量子环里电子的 line bundle

C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)

$\Phi = \Phi_0$ 时量子环里电子的 line bundle

C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)

$\Phi = \Phi_0$ 时量子环里电子的 line bundle

C. H. Séquin, “Topological tori as abstract art”, Journal of Mathematics and the Arts 6, 191–209, (2012)

Charge pumping

$$\mathcal{H}[\Phi] = \frac{\hbar^2}{2m^* R^2}[-i\partial_\phi + \Phi/\Phi_0]^2$$

$$\Psi_l(\Phi,\phi) = e^{il\phi} \qquad\qquad E_l(\Phi) = \frac{\hbar^2}{2m^* R^2}(l + \Phi/\Phi_0)^2$$

规范变换

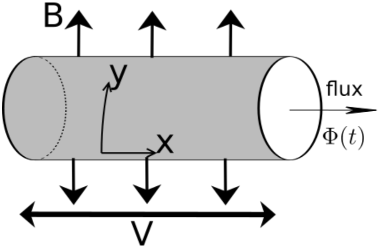
$$\Psi_l'(\Phi,\phi) = \Psi_l(\phi)e^{in\phi} = e^{i(l+n)\phi}$$

$$\begin{aligned}
\mathcal{H}'[\Phi] = e^{in\phi}\mathcal{H}[\Phi]e^{-in\phi} &= \frac{\hbar^2}{2m^* R^2}[-i\partial_\phi - n + \Phi/\Phi_0]^2 \\
&= \frac{\hbar^2}{2m^* R^2}[-i\partial_\phi + (\Phi - n\Phi_0)/\Phi_0]^2 \\
&= \mathcal{H}[\Phi - n\Phi_0]
\end{aligned}$$

$$\Psi_l'(\Phi,\phi) = \Psi_{l+n}(\Phi - n\Phi_0,\phi) \qquad\qquad E_l'(\Phi) = E_{l+n}(\Phi - n\Phi_0)$$

$\Phi + n\Phi_0 \to \Phi$ 系统的本征态/本征能量/平衡物理量没有任何变化，但是把所有的量子数为 l 的态变成量子数为 $l+n$ 的态。

Laughlin's gedankenexperiment: 量子 Hall 效应的规范不变解释



$\hat{e}_r \to \hat{z} \qquad \hat{e}_\phi \to \hat{y}$

$y = R\phi \qquad L_y = 2\pi R$

$k_y = 2\pi l/L_y \qquad \mathrm{A} = (Bx + \Phi/L_y)\hat{e}_\phi$

☞$\mathrm{B} = B\hat{z} + Bx/R\hat{x} \to 0$ if $R \to \infty$

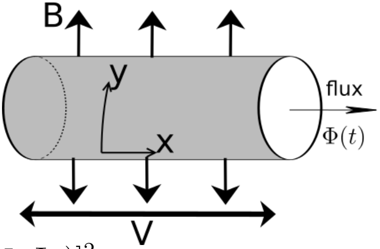
$$\mathcal{H}[\Phi] = \frac{p_x^2}{2m^*} + \frac{[p_y + eBx + h\Phi/(L_y\Phi_0)]^2}{2m^*} + V_{imp}(x,y)$$

$$\to e^{i2\pi\Delta\Phi y/(L_y\Phi_0)}\mathcal{H}e^{-i2\pi\Delta\Phi y/(L_y\Phi_0)}$$

$$\to \frac{p_x^2}{2m^*} + \frac{[p_y + eBx + h(\Phi-\Delta\Phi)/(L_y\Phi_0)]^2}{2m^*} + V_{imp}(x,y) = \mathcal{H}[\Phi - \Delta\Phi]$$

- 没有杂质时，对于每一个被占据的 Landau 能级
  - Landau 规范下，波函数 在 y 方向扩展 $k_y = 2l\pi/L_y$，x 方向局域于 $x_0(k_y) = -k_y l_B^2$。
  - $\Phi(t)$ 改变 Φ_0 后，量子数 l 改变 1 ☞ k_y 改变 $2\pi/L_y$
    ☞ x 方向的中心移动 $-2\pi l_B^2/L_y$
    ☞ 考虑 x 方向的边界，有一个电子从右边跑到左边

Laughlin's gedankenexperiment: 量子 Hall 效应的规范不变解释



$$\hat{e}_r \to \hat{z} \qquad \hat{e}_\phi \to \hat{y}$$

$$y = R\phi \qquad L_y = 2\pi R$$

$$\mathcal{H}' = \frac{p_x^2}{2m^*} + \frac{[p_y + eBx + h(\Phi - \Delta\Phi)/(L_y\Phi_0)]^2}{2m^*} + V_{imp}(x, y)$$

- 没有杂质时，对于每一个被占据的 Landau 能级，$\Phi(t)$ 改变 Φ_0 后，有一个电子从样品的一边被 pump 到另一边
  - 系统能量改变的复杂算法

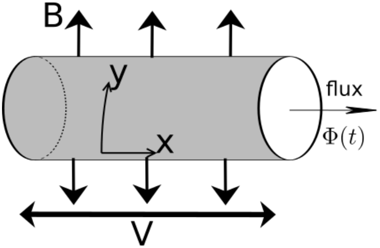
    $$\Delta E = \sum_n \sum_{k_y} \Delta E_n(k_y) = \sum_n \sum_{k_y} \frac{-\hbar\Delta k_y E}{B}$$

    $$= \sum_{n=1}^{\nu} \frac{-\hbar\Delta k_y E}{B} \frac{L_x}{\Delta k_y l_B^2 {=\hbar/(eB)}} = \nu e E L_x = \nu e V$$
  - 系统能量改变的简单算法

    有 ν 个电子从样品一头跑到另一头，每个电子能量改变 eV，总能量改变 νeV
  - y 方向电流

    $$I_y = \frac{\Delta E}{\Delta\Phi} = \frac{\nu eV}{h/e} = \nu\frac{e^2}{h}V \qquad R_{xy} = R_K/\nu$$

Laughlin's gedankenexperiment: 量子 Hall 效应的规范不变解释



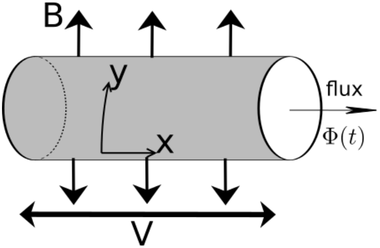
$\hat{e}_r \to \hat{z}$ $\qquad$ $\hat{e}_\phi \to \hat{y}$

$y = R\phi$ $\qquad$ $L_y = 2\pi R$

$$\mathcal{H}' = \frac{p_x^2}{2m^*} + \frac{[p_y + eBx + h(\Phi - \Delta\Phi)/(L_y\Phi_0)]^2}{2m^*} + V_{imp}(x, y)$$

- 没有杂质时，对于每一个被占据的 Landau 能级，$\Phi(t)$ 改变 Φ_0 后，有一个电子从样品的一边被 pump 到另一边
- 有杂质时，无法计算本征态，本征能量。但是通过作规范变换，$\Phi(t)$ 改变 Φ_0 后，同样可以得出结论 ν 个电子从样品的一边被 pump 到另一边。
  - ☞ 系统能量改变 νeV
  - ☞ 电流 $I_y = \nu(e^2/h)V$
  - ☞ 只要 $\sigma_{xx} = 0$，必然有 $R_{xy} = R_K/\nu$

Laughlin's gedankenexperiment: 量子 Hall 效应的规范不变解释



Fine prints

- ☞ 有 ν 个电子 $x = 0 \to x = L_x$
- ☞ 系统能量改变 νeV
- ☞ 电流 $I_y = \nu(e^2/h)V$
- ☞ 只要 $\sigma_{xx} = 0$ ，必然有 $R_{xy} = R_K/\nu$

- ☞ 有 ν 个电子 $x = 0 \to x = L_x$
- ☞ $I_x \neq 0$，$\sigma_{xx} \neq 0$?
- ☞ $E_y = \partial_t A_y \to I_x \neq 0$

Zak phase: 晶体里的 Berry phase

J. Zak, "Berry's phase for energy bands in solids", PRL 62, 2747 (1989)

$$\mathcal{H} = \frac{(-i\hbar\boldsymbol{\nabla})^2}{2m} + V(\mathrm{r})$$
$$|\psi_n(\mathrm{k})\rangle = e^{i\mathrm{k}\cdot\hat{\mathrm{r}}}|u_n(\mathrm{k})\rangle$$
$$☞\mathcal{H}(\mathrm{k}) = e^{-i\mathrm{k}\cdot\hat{\mathrm{r}}}\mathcal{H}e^{i\mathrm{k}\cdot\hat{\mathrm{r}}} = \frac{(\hbar\mathrm{k} - i\boldsymbol{\nabla})^2}{2m} + V(\mathrm{r})$$
$$☞\mathcal{H}(\mathrm{k})|u_n(\mathrm{k})\rangle = E_n(\mathrm{k})|u_n(\mathrm{k})\rangle$$

- 参数空间: k, 1st BZ
  - 一维：“直的”圆，S^1
  - 二维：“直的”环面，T^2
  - 三维：“直的”三维环面，T^3
- Berry connection： $\mathcal{A}_{n\mu}(\mathrm{k}) = i\langle u_n(\mathrm{k})|\partial_{k_\mu} u_n(\mathrm{k})\rangle$
- Berry curvature： $\boldsymbol{\Omega}_{\mu\nu}(\mathrm{k}) = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu$

几何相位的应用：晶体的电极化理论

- 分子/原子团（有限体系）的电极化

$$\mathrm{P} = \sum_i q_i(\mathrm{r}_i + \mathrm{R}_0) = (\sum_i q_i \mathrm{r}_i) + \mathrm{R}_0 \sum_i q_i = 0 = \sum_i q_i \mathrm{r}_i$$

几何相位的应用：晶体的电极化理论

- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞

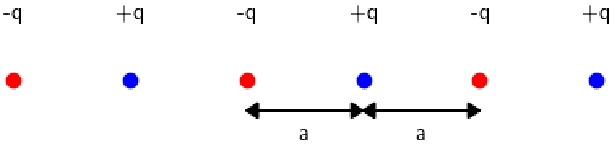
$$\mathrm{P} = \sum_{li} q_i \mathrm{r}_{li} = \sum_{li} q_i(\mathrm{R}_l + \mathrm{r}_i) = \sum_{l}\sum_{i}(q_i\mathrm{r}_i) + \sum_{l} \mathrm{R}_l \Big(\sum_{i} q_i\Big) = 0$$

$$= N\Omega\Big(\sum_i q_i \mathrm{r}_i\Big)/\Omega = N\Omega\mathrm{p} = V\mathrm{p}$$

$$\mathrm{p} = \mathrm{P}/(N\Omega)$$ 单位体积的电极化

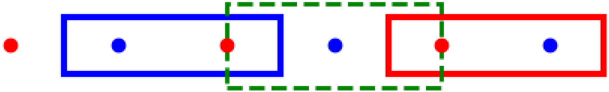
几何相位的应用：晶体的电极化理论

- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞



几何相位的应用：晶体的电极化理论

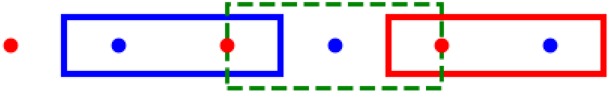
- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞



$p_0 = [(-q)*(-a)/2 + (-q)*(+a)/2 + (q)*(0)]/a = 0$

几何相位的应用：晶体的电极化理论

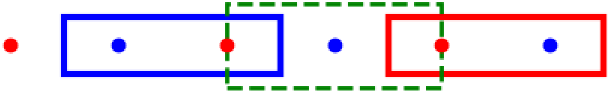
- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞



$$\mathrm{p}_0 = [(-q)*(-a)/2+(-q)*(+a)/2+(q)*(0)]/a = 0$$
$$\mathrm{p}_1 = [(+q)*(-a/2)+(-q)*(a/2)]/a = -q$$

几何相位的应用：晶体的电极化理论

- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞



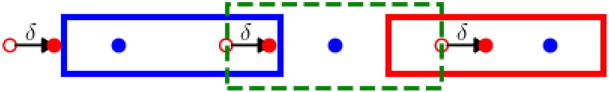
$$\mathrm{p}_0 = [(-q)*(-a)/2 + (-q)*(+a)/2 + (q)*(0)]/a = 0$$

$$\mathrm{p}_1 = [(+q)*(-a/2) + (-q)*(a/2)]/a = -q$$

$$\mathrm{p}_2 = [(-q)*(-a/2) + (q)*(a/2)]/a = q$$

几何相位的应用：晶体的电极化理论

- 分子/原子团（有限体系）的电极化
- 晶体（周期结构）中的电极化，N 个晶胞

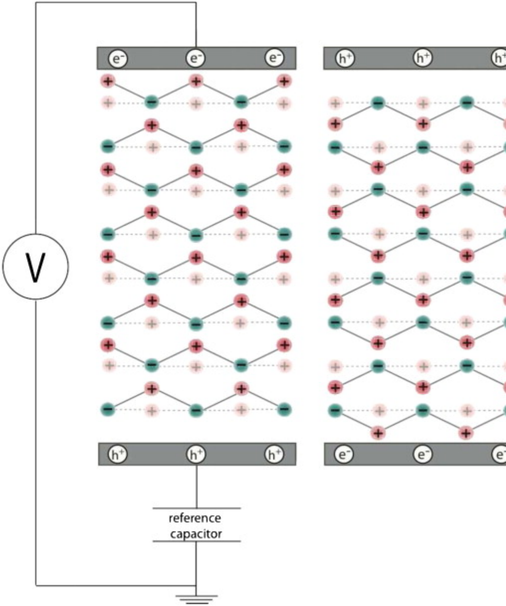


$$\mathrm{p}_0 = [(-q)*(-a)/2 + (-q)*(+a)/2 + (q)*(0)]/a = 0$$
$$\mathrm{p}_1 = [(+q)*(-a/2) + (-q)*(a/2)]/a = -q$$
$$\mathrm{p}_2 = [(-q)*(-a/2) + (q)*(a/2)]/a = q$$

$$\delta\mathrm{p}_1 = [(+q)*(-a/2+\delta) + (-q)*(a/2) + qa]/a = q\delta/a$$
$$\delta\mathrm{p}_2 = [(-q)*(-a/2) + (+q)*(a/2+\delta) - qa]/a = q\delta/a$$

电偶极矩的测量: Sawyer-Tower method

- 晶体的绝对电偶极矩是多值的，没有物理意义
  $p_N = Nqa,$
  $N = 0, \pm 1, \pm 2, \cdots$
- 电偶极矩的改变量有物理意义
  $\delta p = q\delta + p_N$
- 物理上也只能测量电偶极矩该变量，不能测量绝对值



Modern theory of polarization

λ: 晶格位移量 R_j☞$\mathrm{R}_j(\lambda)$，$|\psi_n(\mathrm{k})\rangle \rightarrow |\psi_n(\mathrm{k},\lambda)\rangle$

$$\mathrm{p}_{tot}(\lambda) = \frac{1}{N}\int \rho_{tot}(\mathrm{r})\mathrm{r}\, d\mathrm{r} = \frac{1}{N}\left\{\sum_{lj} z_j[\mathrm{R}_l + \mathrm{R}_j(\lambda)] - e\int \rho_{el}(\mathrm{r})\mathrm{r}\, d\mathrm{r}\right\}$$

$$\begin{aligned}
\mathrm{p}_{el}(\lambda) &= \frac{1}{N}\int \rho_{el}(\mathrm{r})\mathrm{r}\, d\mathrm{r} = -\frac{e}{N}\sum_n \int d\mathrm{k}\, \langle\psi_n(\mathrm{k},\lambda)|\mathrm{r}|\psi_n(\mathrm{k},\lambda)\rangle \\
&= -\frac{e}{N}\sum_n\sum_l \mathrm{R}_l - ei\sum_{n\mathrm{k}}\langle u_n(\mathrm{k},\lambda)|\partial_{\mathrm{k}} u_n(\mathrm{k},\lambda)\rangle \\
&= -\frac{e}{N}\sum_n\sum_l \mathrm{R}_l - e\sum_n \int d\mathrm{k}\, \boldsymbol{\Omega}_n(\mathrm{k},\lambda)\text{☞}\gamma_n(\lambda)
\end{aligned}$$

$$\partial_\lambda \mathrm{p}_{el}(\lambda) = -e\sum_n \partial_\lambda \gamma_n(\lambda)$$

$$\Delta\mathrm{p}_{el}(\delta) = -e\sum_n \int_0^\delta \partial_\lambda\gamma_n(\lambda)\, d\lambda = -e\sum_n[\gamma_n(\delta) - \gamma_n(0)]$$

$$\Delta p = \Delta p_n + \Delta p_{el} = e\sum_j z_j[\mathrm{R}_j(\delta) - \mathrm{R}_j(0)] - e\sum_n[\gamma_n(\delta) - \gamma_n(0)]$$