第六章　凝聚态物理里的几何相位

6.1　绝热演化

6.2　Berry Phase/Berry Connection

6.3　磁场中自旋 1/2 粒子的 Berry phase

6.4　几何相位的应用：晶体的电极化理论

6.5　Zak phase：晶体里的 Berry phase

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)

波函数的全局相位

$$i\hbar\partial_t|\psi\rangle = \mathcal{H}(\boldsymbol{Q})|\psi\rangle \qquad \boxed{\boldsymbol{Q} = (\boldsymbol{Q}_1, \boldsymbol{Q}_2, \cdots, \boldsymbol{Q}_p)\text{：外界参数}}$$

$$\varepsilon_n(\boldsymbol{Q})|\psi_n(\boldsymbol{Q})\rangle = \mathcal{H}(\boldsymbol{Q})|\psi_n(\boldsymbol{Q})\rangle$$

$$\langle\psi_n(\boldsymbol{Q})|\psi_m\rangle = \delta_{nm} \qquad \sum_m |\psi_m(\boldsymbol{Q})\rangle\langle\psi_m(\boldsymbol{Q})| = 1$$

$$|\psi_n(\boldsymbol{Q})\rangle \Rightarrow |\psi'_n(\boldsymbol{Q})\rangle = e^{i\theta_n(\boldsymbol{Q})}|\psi_n(\boldsymbol{Q})\rangle \qquad \boxed{\text{全局相位}}$$

$$\varepsilon_n(\boldsymbol{Q})|\psi'_n(\boldsymbol{Q})\rangle = \mathcal{H}(\boldsymbol{Q})|\psi'_n(\boldsymbol{Q})\rangle$$

- $\boldsymbol{Q}$ 不发生改变时，全局相位对 Schrödinger 完全没有影响
- 改变全局相位 $\theta(\boldsymbol{Q})$（规范变换）不改变 Schrödinger 方程以及可测量物理量
- 能否测量？ ⇒ 绝热演化：让 $\boldsymbol{Q}$ 缓慢改变
  $\boldsymbol{Q} = \boldsymbol{Q}(t) = (Q_1(t), Q_2(t), \cdots,)$
- 不同参数下，能量本征态会发生改变

$$\langle\psi_n(\boldsymbol{Q})|\psi_m(\boldsymbol{Q})\rangle = \delta_{nm} \qquad \langle\psi_n(\boldsymbol{Q})|\psi_m(\boldsymbol{Q}')\rangle \neq \delta_{nm'}$$

绝热演化

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

- 选择每一个时刻的能量本征态为基

$$Q(t) = Q \qquad \mathcal{H}(Q)|\psi_n(Q)\rangle = \varepsilon_n(Q)|\psi_n(Q)\rangle$$

$$Q(t') = Q' \qquad \mathcal{H}(Q')|\psi_n(Q')\rangle = \varepsilon_n(Q')|\psi_n(Q')\rangle$$

- 波函数时间演化

$$\mathcal{H}(t) = \mathcal{H}[Q(t)] \qquad \mathcal{H}[Q(t)]|\psi_n[Q(t)]\rangle = \mathcal{E}_n[Q(t)]|\psi_n[Q(t)]\rangle$$

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

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

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

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

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

绝热演化

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

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

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

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

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

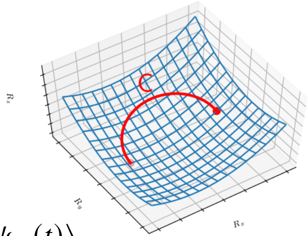
$$0 = \dot{c}_n(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_n(\tau)d\tau} + \sum_m c_m(t) e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} \langle\psi_n(t)|\dot{\psi}_m(t)\rangle$$

$$\dot{c}_n(t) = -\sum_m c_m(t) e^{\frac{i}{\hbar}\int_0^t [\mathcal{E}_n(\tau)-\mathcal{E}_m(\tau)]d\tau} \langle\psi_n(t)|\dot{\psi}_m(t)\rangle$$

只保留 $m = n$

$$\simeq -c_n(t)\langle\psi_n(t)|\dot{\psi}_n(t)\rangle \rightarrow c_n(t) = e^{i\gamma_n(t)} c_n(0)$$

Adiabatic Berry Phase

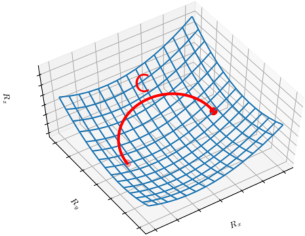


$$|\psi(t)\rangle = \sum_m e^{i\gamma_m(t)} e^{-\frac{i}{\hbar}\int_0^t \mathcal{E}_m(\tau)d\tau} c_m(0)|\psi_m(t)\rangle$$

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

$$= i\int_{\boldsymbol{Q}(0)}^{\boldsymbol{Q}(t)} \langle\psi_n(\boldsymbol{Q})|\partial_{\boldsymbol{Q}}\psi_n(\boldsymbol{Q})\rangle \cdot d\boldsymbol{Q} = i\int_C \mathcal{A}_n(\boldsymbol{Q})\cdot d\boldsymbol{Q}$$

Adiabatic Berry Phase



$\gamma_m(t)$ 是路径依赖，规范依赖的

$$|\psi_n(\boldsymbol{Q})\rangle \rightarrow |\psi'_n(\boldsymbol{Q})\rangle = e^{-i\theta_n(\boldsymbol{Q})}|\psi_n(\boldsymbol{Q})\rangle$$

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

- 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 $\boldsymbol{Q}(t) \neq \boldsymbol{Q}(0)$，我们总可以选择适当的规范 $\theta_n(\boldsymbol{Q})$，使得 $\gamma'(t) = 0$。
- 1984 年 Michael Berry：闭合路径 $\boldsymbol{Q}(T) = \boldsymbol{Q}(0)$ 中，这个相位无法消除，因此可以导致可观察效应。

Berry Curvature/Berry 曲率

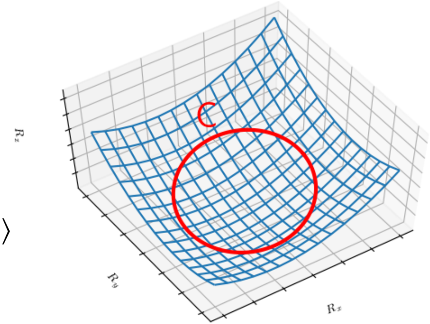
3 维 $\boldsymbol{Q} = (Q_x, Q_y, Q_z)$ 空间，Stokes 定理

$$\gamma_n(T) = \oint_C \mathcal{A}_n \cdot d\boldsymbol{Q}$$

$$= \int\int_S \boldsymbol{\Omega}_n(\boldsymbol{Q}) \cdot dS$$

$$\boldsymbol{\Omega}_n(\boldsymbol{Q}) = \boldsymbol{\nabla}_{\boldsymbol{Q}} \times \mathcal{A}_n(\boldsymbol{Q})$$

$$= i\langle \boldsymbol{\nabla}_{\boldsymbol{Q}} \psi_n(\boldsymbol{Q})| \times |\boldsymbol{\nabla}_{\boldsymbol{Q}} \psi_n(\boldsymbol{Q})\rangle$$



- $\boldsymbol{\Omega}_n(\boldsymbol{Q})$ 定义在 $\boldsymbol{Q}$ 空间上
- 非平凡情况下，波函数 $|\psi_n(\boldsymbol{Q})\rangle$ 必然是多分量。
- $\boldsymbol{\Omega}_n(\boldsymbol{Q})$ 规范不变

$$|\psi_n(\boldsymbol{Q})\rangle \Rightarrow |\psi'_n(\boldsymbol{Q})\rangle = e^{i\theta_n(\boldsymbol{Q})}|\psi_n(\boldsymbol{Q})\rangle$$

$$\boldsymbol{\Omega}'_n = \boldsymbol{\Omega}_n + i[(\boldsymbol{\nabla}_{\boldsymbol{Q}}\theta_n) \times \mathcal{A} + \mathcal{A} \times (\boldsymbol{\nabla}_{\boldsymbol{Q}}\theta_n)] + i(\boldsymbol{\nabla}_{\boldsymbol{Q}}\theta_n) \times (\boldsymbol{\nabla}_{\boldsymbol{Q}}\theta_n)$$

$$= \boldsymbol{\Omega}_n$$

Berry Curvature 的计算

$$\mathcal{H}(\boldsymbol{Q})|\psi_n(\boldsymbol{Q})\rangle = \mathcal{E}_n(\boldsymbol{Q})|\psi_n(\boldsymbol{Q})\rangle \qquad \boldsymbol{\nabla}_{\boldsymbol{Q}}[\mathcal{H}|\psi_n\rangle] = \boldsymbol{\nabla}_{\boldsymbol{Q}}[\mathcal{E}_n|\psi_n\rangle]$$

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

$$\langle\psi_m|\cdots \to \langle\psi_m|\boldsymbol{\nabla}_{\boldsymbol{Q}}\mathcal{H}|\psi_n\rangle + \mathcal{E}_m\langle\psi_m|\boldsymbol{\nabla}_{\boldsymbol{Q}}\psi_n\rangle$$

$$= \boldsymbol{\nabla}_{\boldsymbol{Q}}\mathcal{E}_n\delta_{nm} + \mathcal{E}_n\langle\psi_m|\boldsymbol{\nabla}_{\boldsymbol{Q}}\psi_n\rangle$$

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

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

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

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

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

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 $\boldsymbol{Q}$ 构成一个空间 ⇒ 底流形（Base manifold）
- 在每个 $\boldsymbol{Q}$ 点定义量子态、波函数 $|\psi_n(\boldsymbol{Q})\rangle$
- 每个 $\boldsymbol{Q}$ 点波函数有相位的自由度，可用另一个参数 $\theta_n(\boldsymbol{Q})$ 描述：$|\psi_n(\boldsymbol{Q})\rangle \to e^{i\theta_n(\boldsymbol{Q})}|\psi_n(\boldsymbol{Q})\rangle$
  ⇒ 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：$\boldsymbol{Q}$ 空间和 fiber 的组合 ⇒ bundle
  ⇒ 整个几何体是 $\boldsymbol{Q}$ 空间上的 principal U(1) bundle
  ⇒ 所谓的几何拓扑属性都是针对这个 bundle 而言 U(1) bundle over $\boldsymbol{Q}$ space
  - $\mathcal{A}_n(\boldsymbol{Q})$: Connection of line bundle/U(1) bundle
    ⇒ 描述不同点上的 fiber 如何连接在一起
  - $\boldsymbol{\Omega}_n(\boldsymbol{Q})$: Curvature of line bundle/U(1) bundle
    ⇒ bundle 上的曲率

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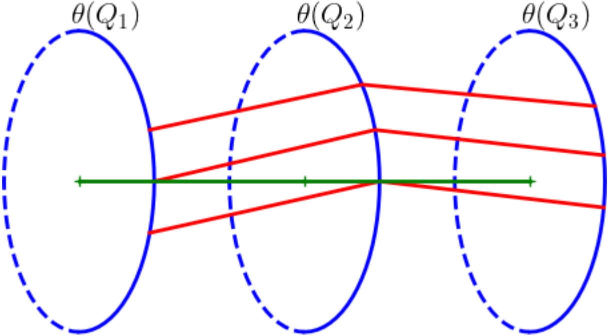


$$|\psi_n(\boldsymbol{Q}+\delta\boldsymbol{Q})\rangle = |\psi_n(\boldsymbol{Q})\rangle + \delta\boldsymbol{Q}\partial_{\boldsymbol{Q}}|\psi_n(\boldsymbol{Q})\rangle$$

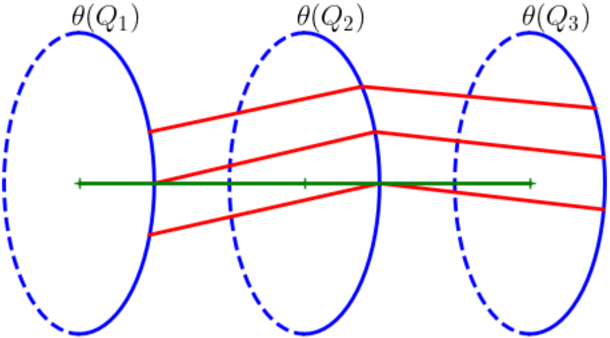
$$= |\psi_n(\boldsymbol{Q})\rangle + \delta\boldsymbol{Q}\sum_m |\psi_m(\boldsymbol{Q})\rangle\langle\psi_m(\boldsymbol{Q})|\partial_{\boldsymbol{Q}}\psi_n(\boldsymbol{Q})\rangle$$

$$\simeq |\psi_n(\boldsymbol{Q})\rangle - i\delta\boldsymbol{Q}|\psi_n(\boldsymbol{Q})\rangle[i\langle\psi_n(\boldsymbol{Q})|\partial_{\boldsymbol{Q}}|\psi_n(\boldsymbol{Q})\rangle] = \mathcal{A}_n(\boldsymbol{Q})$$

$$= [1 - i\delta\boldsymbol{Q}\mathcal{A}_n(\boldsymbol{Q})]|\psi_n(\boldsymbol{Q})\rangle \simeq e^{-i\delta\boldsymbol{Q}\cdot\mathcal{A}_n(\boldsymbol{Q})}|\psi_n(\boldsymbol{Q})\rangle$$

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)]



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

$$\theta_n(\boldsymbol{Q}+\delta\boldsymbol{Q}) \Leftrightarrow \theta_n(\boldsymbol{Q})+\delta\boldsymbol{Q}\ \mathcal{A}_n(\boldsymbol{Q})$$

$\Rightarrow \mathcal{A}_n(\boldsymbol{Q})$ 包含了如何 “连接”“相邻” 的 fiber/line/ray 的信息

Berry Connection and Berry Curvature 的几何意义

绝热演化 $\Rightarrow$ U(1) bundle 上的平行移动（Parallel transport）
$\Rightarrow$ 尽可能保持波函数不改变 $\Leftrightarrow$ 使得波函数的“距离”尽可能小

$$
\begin{aligned}
d &= \left| e^{i\theta_n(\boldsymbol{Q}+\delta\boldsymbol{Q})} |\psi_n(\boldsymbol{Q}+\delta\boldsymbol{Q})\rangle - e^{i\theta_n(\boldsymbol{Q})} |\psi_n(\boldsymbol{Q})\rangle \right| \\
&= \left| |\psi_n(\boldsymbol{Q}+\delta\boldsymbol{Q})\rangle - e^{-i[\theta_n(\boldsymbol{Q}+\delta\boldsymbol{Q})-\theta_n(\boldsymbol{Q})]\boxed{=\delta\theta}} |\psi_n(\boldsymbol{Q})\rangle \right| \\
&= \left| |\psi_n(\boldsymbol{Q})\rangle + \delta\boldsymbol{Q} \sum_m |\psi_m\rangle\langle\psi_m|\partial_{\boldsymbol{Q}}\psi_n\rangle - e^{-i\delta\theta}|\psi_n\rangle \right| \\
&= \left| [e^{-i\delta\boldsymbol{Q}\cdot\mathcal{A}_n} - e^{-i\delta\theta}]|\psi_n\rangle + \delta\boldsymbol{Q} \sum_{m\neq n} (\langle\psi_m|\partial_{\boldsymbol{Q}}\psi_n\rangle)|\psi_m\rangle \right|
\end{aligned}
$$

$\Rightarrow$ 要使得 d 最小，必须 $\delta\theta = \delta\boldsymbol{Q} \cdot \mathcal{A}_n(\boldsymbol{Q})$

磁场中自旋 1/2 粒子的 Berry phase

参数空间：$\boldsymbol{B}$，球面（磁场大小不变）或者球（磁场大小可变）

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

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

$\hat{e}_r = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$

$\hat{e}_\theta = (\cos\theta\cos\phi, \cos\theta\sin\phi, -\sin\theta)$

$\hat{e}_\phi = (-\sin\phi, \cos\phi, 0)$

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

$$\partial_B|\psi_\pm\rangle = 0$$

$$\partial_\theta|\psi_+\rangle = \frac{1}{2}\begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2}e^{i\phi} \end{pmatrix} = \frac{1}{2}|\psi_-\rangle \qquad \partial_\theta|\psi_-\rangle = \frac{1}{2}\begin{pmatrix} -\cos\frac{\theta}{2}e^{-i\phi} \\ -\sin\frac{\theta}{2} \end{pmatrix} = -\frac{1}{2}|\psi_+\rangle$$

$$\partial_\phi|\psi_+\rangle = i\begin{pmatrix} 0 \\ \sin\frac{\theta}{2}e^{i\phi} \end{pmatrix} \qquad \partial_\phi|\psi_-\rangle = i\begin{pmatrix} \sin\frac{\theta}{2}e^{-i\phi} \\ 0 \end{pmatrix}$$

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

$$= \mp\frac{\sin^2\theta/2}{\sin\theta}\hat{e}_\phi = \mp\frac{\sin\theta/2\hat{e}_\phi}{2B\cos\theta/2} = \mp\frac{1}{2B}\tan\frac{\theta}{2}\hat{e}_\phi$$

磁场中自旋 1/2 粒子的 Berry phase

$$\mathbf{\Omega}_\pm = \nabla \times \mathcal{A}_\pm = \left(\hat{e}_r\partial_B + \frac{\hat{e}_\theta}{B}\partial_\theta + \frac{\hat{e}_\phi}{B\sin\theta}\partial_\phi\right) \times \left(\frac{\mp}{2B}\tan\frac{\theta}{2}\hat{e}_\phi\right)$$

$$= \pm\frac{\hat{e}_r \times \hat{e}_\phi}{2B^2}\tan\frac{\theta}{2} \mp \frac{\hat{e}_\theta \times \hat{e}_\phi}{4B^2\cos^2\theta/2} \mp \frac{\tan\frac{\theta}{2}}{2B^2\sin\theta}\hat{e}_z$$

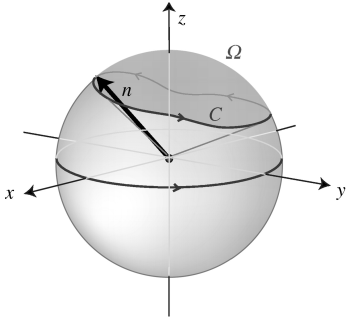
$$\hat{e}_r \times \hat{e}_\phi = -\hat{e}_\theta \qquad \hat{e}_\theta \times \hat{e}_\phi = \hat{e}_r \qquad \hat{e}_\phi \times \partial_\phi \hat{e}_\phi = \hat{e}_z = \cos\theta\hat{e}_r - \sin\theta\hat{e}_\theta$$

$$\Omega_\pm = \mp\frac{1}{4B^2}\left(\frac{1}{\cos^2\theta/2} + \frac{\cos\theta}{\sin\theta}\tan\frac{\theta}{2}\right)\hat{e}_r$$

$$= \mp\frac{\hat{e}_r}{2B^2} = \mp\frac{\hat{n}}{2B^2}$$

$$\gamma_\pm(T) = \oint \mathcal{A}_\pm \cdot d\mathbf{R}$$

$$= \int\int_S \Omega_\pm(R)\cdot d\mathbf{S} = \mp\Omega_C/2$$

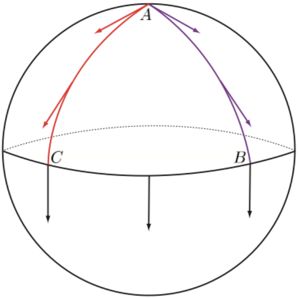


☞ $\gamma_\pm$ 的几何含义：球面上切矢量“平行移动”之后和原矢量的夹角。

磁场中的自旋的几何：球面上矢量的“平行移动”

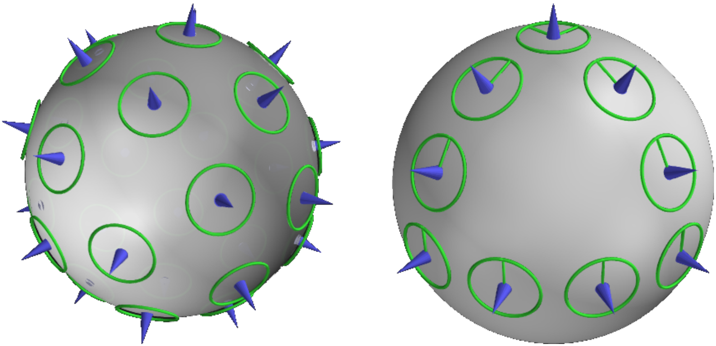
Parallel transport：在曲面上沿某曲线移动矢量，使得移动前后矢量“平行”。大体上：移动时保持矢量和该曲线夹角不变。

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



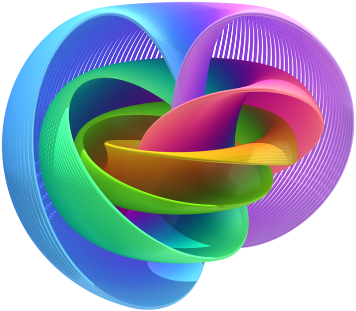
磁场中自旋的 line bundle

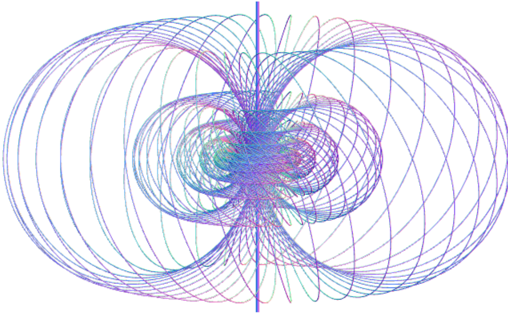
- 磁场中自旋 1/2 粒子的 line bundle 是球面上的一系列单位圆。
- 这种 bundle 的几何属性和参数空间（$\hat{B} = B\hat{n}$，即球面）的切矢量丛完全等价。
- 这是一个非常特殊的情况，通常情况下，这两者并不等价。例拓扑绝缘体的 Bloch bundle 通常不等价于参数空间的切矢量丛。

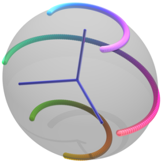


☞ 这个 bundle 等价于三维球面 S^3：Hopf fibration

Hopf fibration







- 四维空间中的三维球面（$x_1^2 + x_2^2 + x_3^2 + x_4^2 = 1$）在三维空间中的投影 $\Rightarrow$ 在二维平面上的显示

https://vlad0007.github.io/Hopf-fibration-quantum-rotations/

- “Hopf fibration —- seven times in physics”, Urbantke, J. Geom. Phys. **46**, 125 (2003)

“磁单极” /“Magnetic” monopole

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

$$4\pi = \oiint_{\boldsymbol{Q}} \boldsymbol{\Omega}_+ \cdot d\boldsymbol{S}_{\boldsymbol{B}} = \iiint \nabla_{\boldsymbol{B}} \cdot \boldsymbol{\Omega}_+ dV_{\boldsymbol{B}} = 4\pi \iiint \delta(\boldsymbol{B}) dV_{\boldsymbol{B}}$$

$\Rightarrow$ 点“磁荷”产生的有效“磁场”

$\Rightarrow \boldsymbol{B} \to 0 \longrightarrow \Omega_+(\boldsymbol{B}) \to \infty$

$\Rightarrow \mathcal{A}_+ = \frac{\sin\theta/2}{2B^2\cos\theta/2}\mathbf{e}_\phi \xrightarrow{\theta\to\pi} \infty$

$\Rightarrow$ 一般情况下 $\nabla_{\boldsymbol{Q}} \cdot \boldsymbol{\Omega} = \nabla_{\boldsymbol{Q}} \cdot [\nabla_{\boldsymbol{Q}} \times \mathcal{A}] = 0$

$\Rightarrow$ 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

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

$\Omega_n(\boldsymbol{Q}) \to \infty \Leftarrow \mathcal{E}_n(\boldsymbol{Q}) = \mathcal{E}_m(\boldsymbol{Q})$

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

More than 3D

$$
\begin{aligned}
\boldsymbol{Q} &= (Q_1, Q_2, Q_3, \cdots, Q_p) \\
\gamma(C) &= \oint_C \mathcal{A}(\boldsymbol{Q}) \cdot d\boldsymbol{Q} = \sum_{\mu=1}^{p} \oint_C \mathcal{A}_i(\boldsymbol{Q}) d\boldsymbol{Q}_i \\
&= \int \int_S \boldsymbol{\Omega}_{\mu\nu}(\boldsymbol{Q}) \cdot d\boldsymbol{S}_{\mu\nu} \\
\boldsymbol{\Omega}_{\mu\nu} &= \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu \\
d\boldsymbol{S}_{\mu\nu} &= dQ_\mu \wedge dQ_\nu = -dQ_\nu \wedge dQ_\mu
\end{aligned}
$$

几何相位的应用：晶体的电极化理论

“Theory of Polarization: A Modern Approach”, R. Resta and D. Vanderbilt, Chap. 2 of “Physics of Ferroelectrics: A Modern Perspective”, Springer (2007)

“A beginner’s guide to the modern theory of polarization”, N. A. Spaldin, J. Sol. Stat. Chem. **195**, 2 (2012)

- 分子/原子团（有限体系）的电极化

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

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- 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

$$\mathbf{P} = \sum_{li} q_i \boldsymbol{r}_{li} = \sum_{li} q_i(\boldsymbol{R}_l + \boldsymbol{r}_i) = \sum_l \sum_i (q_i \boldsymbol{r}_i) + \sum_l \boldsymbol{R}_l \Big(\sum_i q_i\Big) = 0$$

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

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

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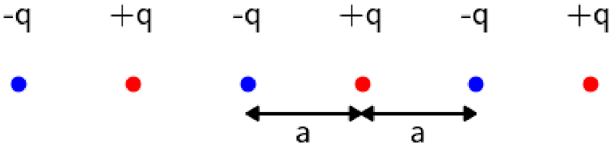

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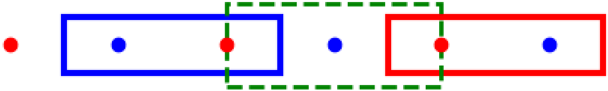

$$\boldsymbol{p}_0 = [(+q) * (-a)/2 + (+q) * (+a)/2 + (-q) * (0)]/(2a) = 0$$

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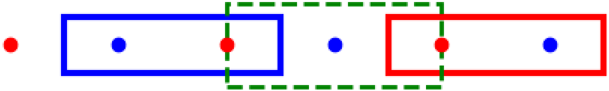

$$\boldsymbol{p}_0 = [(+q)*(-a)/2 + (+q)*(+a)/2 + (-q)*(0)]/(2a) = 0$$

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

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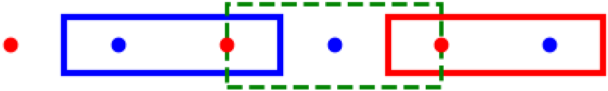

$$\boldsymbol{p}_0 = [(+q) * (-a)/2 + (+q) * (+a)/2 + (-q) * (0)]/(2a) = 0$$

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

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

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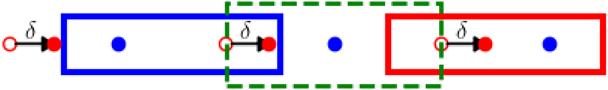


$$\boldsymbol{p}_0 = [(+q)*(-a)/2 + (+q)*(+a)/2 + (-q)*(0)]/(2a) = 0$$

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

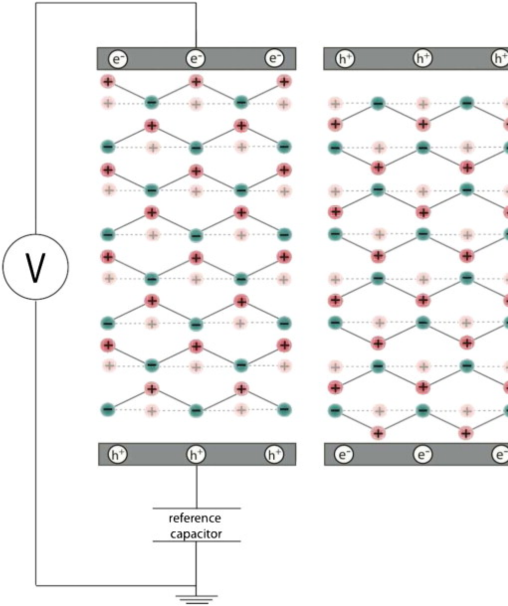
$$\boldsymbol{p}_2 = [(-q)*(-a/2) + (q)*(a/2)]/(2a) = q/2$$

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

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

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 $\boldsymbol{R}_j \Rightarrow \boldsymbol{R}_j(\lambda)$， $|\psi_n(\boldsymbol{k})\rangle \rightarrow |\psi_n(\boldsymbol{k},\lambda)\rangle$

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

$$\mathbf{p}_{el}(\lambda) = \frac{1}{N}\int \rho_{el}(\boldsymbol{r})\boldsymbol{r}\, d\boldsymbol{r} = -\frac{e}{N}\sum_n \int d\boldsymbol{k}\, \langle\psi_n(\boldsymbol{k},\lambda)|\boldsymbol{r}|\psi_n(\boldsymbol{k},\lambda)\rangle$$

$$= -\frac{e}{N}\sum_n\sum_l \boldsymbol{R}_l - ei\sum_{n\boldsymbol{k}}\langle u_n(\boldsymbol{k},\lambda)|\partial_{\boldsymbol{k}} u_n(\boldsymbol{k},\lambda)\rangle$$

$$= -\frac{e}{N}\sum_n\sum_l \boldsymbol{R}_l - e\sum_n \int d\boldsymbol{k}\, \boldsymbol{\Omega}_n(\boldsymbol{k},\lambda) \Rightarrow \gamma_n(\lambda)$$

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

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

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

Zak phase：晶体里的 Berry phase

J. Zak, “Berry’s phase for energy bands in solids”, PRL **62**, 2747 (1989)

$$\mathcal{H} = \frac{(-i\hbar\nabla)^2}{2m} + V(\boldsymbol{r})$$

$$|\psi_n(\boldsymbol{k})\rangle = e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}|u_n(\boldsymbol{k})\rangle$$

$$\Rightarrow \mathcal{H}(\boldsymbol{k}) = e^{-i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}}\mathcal{H}e^{i\boldsymbol{k}\cdot\hat{\boldsymbol{r}}} = \frac{(\hbar\boldsymbol{k} - i\nabla)^2}{2m} + V(\boldsymbol{r})$$

$$\Rightarrow \mathcal{H}(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle = E_n(\boldsymbol{k})|u_n(\boldsymbol{k})\rangle$$

- 参数空间: $\boldsymbol{k}$, 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：$\mathcal{A}_{n\mu}(\boldsymbol{k}) = i\langle u_n(\boldsymbol{k})|\partial_{k_\mu} u_n(\boldsymbol{k})\rangle$
- Berry curvature：$\boldsymbol{\Omega}_{\mu\nu}(\boldsymbol{k}) = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu$

  $\Rightarrow$ k-空间里的“磁场”

$$\dot{\boldsymbol{r}} = \nabla_{\boldsymbol{k}}\varepsilon(\boldsymbol{k}) - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}(\boldsymbol{k})$$

$$\dot{\boldsymbol{k}} = \boldsymbol{F} = -e(\boldsymbol{E} + \boldsymbol{v} \times \boldsymbol{B}) = \nabla_{\boldsymbol{r}}\phi(\boldsymbol{r}) + \dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r})$$