

准激发模式与几何相位

物理中的几何相位（专题10）

高阳

力学

$$\vec{F} = m\vec{a}$$

$$F = -\frac{Gm_1m_2}{r^2}$$

$$\delta \int_{t_a}^{t_b} \mathcal{L}(\vec{q}, \dot{\vec{q}}, t) dt = 0$$

$$\dot{\vec{q}} = \frac{\partial H}{\partial \vec{p}}$$

$$\dot{\vec{p}} = -\frac{\partial H}{\partial \vec{q}}$$

电动

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon}$$

$$\nabla \cdot \vec{B} = 0$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$$

$$\nabla \times \vec{B} = \mu \vec{J} + \epsilon\mu \frac{\partial \vec{B}}{\partial t}$$

$$\vec{F} = q\vec{E} + q\vec{v} \times \vec{B}$$

量子

$$E = \hbar\omega$$

$$\vec{p} = \hbar\vec{k}$$

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

$$\rho(\vec{r}, t) = |\psi(\vec{r}, t)|^2$$

$$[\hat{x}, \hat{p}] = i\hbar$$

热统

$$dU = \delta Q + \delta W$$

$$\oint \frac{\delta Q}{T} \leq 0$$

$$S = k_B \ln \Omega$$

$$Z = \sum e^{-\beta H}$$

$$f = \frac{1}{e^{\beta(\epsilon - \mu)} \pm 1}$$

光与物质的耦合

单色光

$$\begin{aligned} \mathbf{E} &= -\frac{\partial A}{\partial t} \\ \mathbf{E} &= \mathbf{E}_0 e^{i\mathbf{k}\cdot\mathbf{r}-i\omega t} \\ \mathbf{B} &= \frac{\mathbf{E}}{c} \end{aligned}$$

线偏振

$$\mathbf{E} = E_0 \hat{x}$$

圆偏振

$$\mathbf{E} = E_0 (\hat{x} \pm i \hat{y})$$

速度规范, 基于薛定谔方程

$$\begin{aligned} H &= H_0 + H', \\ H_0 &= \frac{p^2}{2m} + U(r) \\ H' &= \frac{e\mathbf{p}}{m} \cdot \mathbf{A} + \frac{e^2}{2m} A^2 \end{aligned}$$

速度规范, 基于紧束缚模型

$$\begin{aligned} H &= H_0 + H', \\ H_0 &= H(k) \\ H' &= \frac{\partial H}{\partial k_i} \frac{e}{\hbar} A_i + \frac{1}{2} \frac{\partial^2 H}{\partial k_i \partial k_j} \frac{e^2}{\hbar^2} A_i A_j + \dots \end{aligned}$$

电子的响应形式

- 电流

线性阶 $J_i(\omega, q) = \sigma_{ij}(\omega, q) E_j(\omega, q)$

光场的 q 经常被忽略: $q = \frac{2\pi}{\lambda}$ $\lambda \sim 300 \text{ nm}$

相比于晶格: $k = \frac{2\pi}{a}$ $a \sim 1 - 2 \text{ \AA}$

需区分光场的动量和准激发模式的动量

等离子激元的产生 (1)

材料中的电磁场

$$\nabla \cdot \mathbf{E} = -\frac{\rho}{\epsilon_0}$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{J}_0 + \frac{1}{c^2} \frac{\partial \mathbf{E}}{\partial t}$$



只包含电场的方程

$$-\nabla \times \nabla \times \mathbf{E} = \mu_0 \frac{\partial \mathbf{J}_0}{\partial t} + \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2}$$

单色光假设

$$\nabla \rightarrow i\mathbf{q}, \quad \partial_t \rightarrow -i\omega$$

作用1: 光的传播

$$q = n\omega/c$$

折射率与本征方程

$$\mathbf{M}(n)\mathbf{E} = 0$$

3×3矩阵

列矢量

作用2: 等离子激元

等离子激元的产生 (2)

- 假定某种自发的交变电磁场可以在材料内部产生
- 首先认为电磁场在空间均匀

$$\mu_0 \frac{\partial J_0}{\partial t} + \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = (-i\omega\mu_0 \sigma_{ij}(\omega) - \omega^2 \delta_{ij}) E_j = 0$$

- 一般情况下, $\mathbf{E} = 0$, 代表交变电场不会自发产生
- 如果满足

$$\det(-i\omega_p\mu_0 \sigma_{ij}(\omega_p) - \omega_p^2 \delta_{ij}) = 0$$

则存在一个模式, 使得交变电场可以非零, 此即为等离子激元。

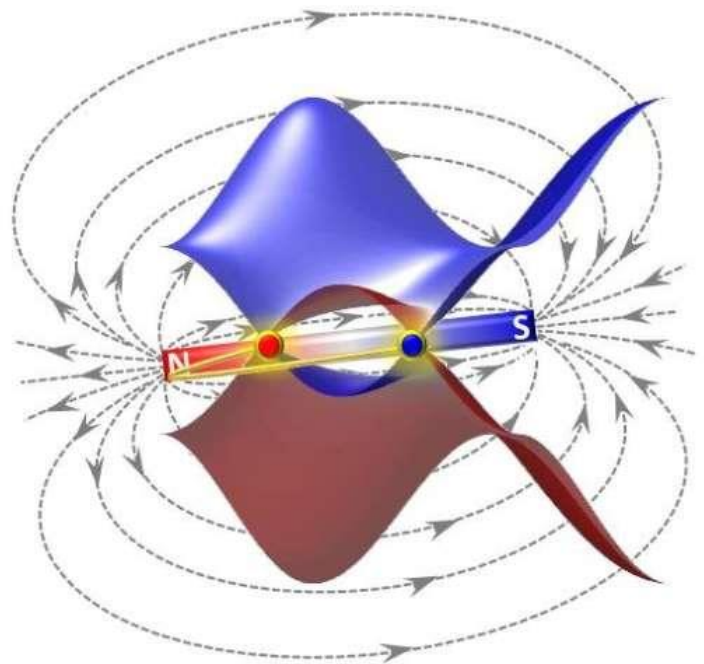
- 此结论可推广至一般的包含动量的情况

$$\det(-i\omega_p\mu_0 \sigma_{ij}(\omega_p) - \omega_p^2 \delta_{ij} + k^2 \delta_{ij}) = 0$$

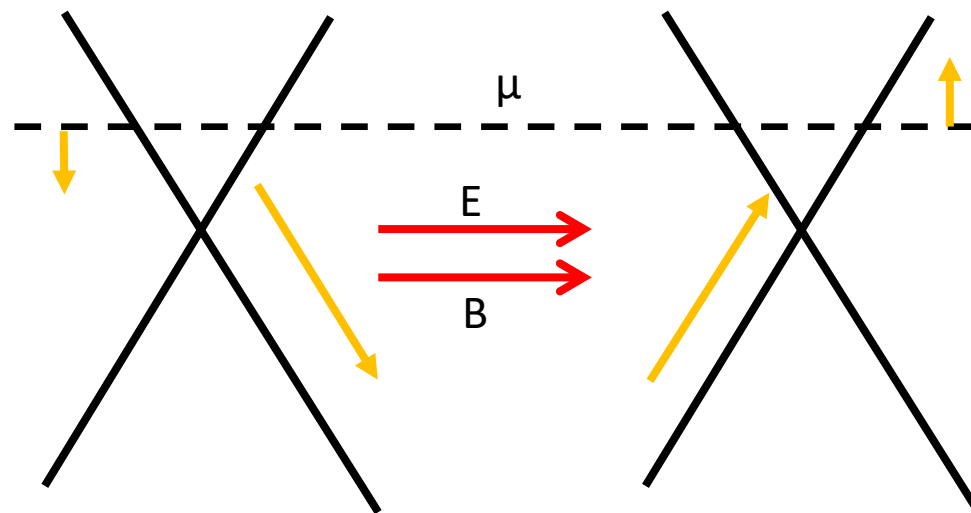
这给出了等离子激元的色散谱。

Weyl半金属中的手性反常

Weyl 点作为贝利曲率的源和漏



手性反常



$$\delta\mu_1 - \delta\mu_2 = -\frac{e^2\tau}{2\pi^2\hbar^2g(\mu)}\mathbf{E} \cdot \mathbf{B}$$

Weyl半金属中的手性磁电流

- 半经典运动方程

$$\dot{\mathbf{r}} = \frac{\partial \varepsilon}{\hbar \partial \mathbf{k}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}$$
$$\hbar \dot{\mathbf{k}} = -e\mathbf{E} - e\dot{\mathbf{r}} \times \mathbf{B}$$

- 态密度: $D = 1 + \frac{e}{\hbar} \mathbf{B} \cdot \boldsymbol{\Omega}$
- 获得 $D\dot{\mathbf{r}} = \frac{\partial \varepsilon}{\hbar \partial \mathbf{k}} + \frac{e}{\hbar} \mathbf{E} \times \boldsymbol{\Omega} + \frac{e}{\hbar} \left(\frac{\partial \varepsilon}{\hbar \partial \mathbf{k}} \cdot \boldsymbol{\Omega} \right) \mathbf{B}$
- 手性磁电流

$$J = -e \int \frac{d\mathbf{k}}{(2\pi)^3} D\dot{\mathbf{r}} f = -\frac{e^2}{\hbar} \int \frac{d\mathbf{k}}{(2\pi)^3} (\mathbf{v} \cdot \boldsymbol{\Omega}) \mathbf{B} f$$

↑
贝利曲率的通量

Weyl半金属中的特征磁阻

单个Weyl点的手性磁电流

$$\begin{aligned} J_1 &= -\frac{e^2}{\hbar^2} \mathbf{B} \int \frac{d\mathbf{k}}{(2\pi)^3} \frac{v\mathbf{k}}{k} \cdot \frac{\mathbf{k}}{2k^3} \Theta(\mu_1 - \varepsilon) \\ &= -\frac{e^2}{\hbar^2} \mathbf{B} \int \frac{k^2 dk}{2\pi^2} \frac{v}{2k^2} \\ &= -\frac{e^2}{\hbar^2} \frac{\mu_1}{4\pi^2} \mathbf{B} \end{aligned}$$

Weyl点总是成对，手性相反，故

$$J = -\frac{e^2}{\hbar^2} \frac{\mu_1 - \mu_2}{4\pi^2} \mathbf{B}$$

手性反常 $\delta\mu_1 - \delta\mu_2 = -\frac{e^2\tau}{2\pi^2\hbar^2 g(\mu)} \mathbf{E} \cdot \mathbf{B}$

特征磁阻 $J = \frac{e^4\tau}{8\pi^4\hbar^4 g(\mu)} (\mathbf{E} \cdot \mathbf{B}) \mathbf{B}$ 磁场增大，电导增强

Weyl半金属中的特征磁阻的频率依赖

含时的玻尔兹曼方程

$$\frac{\partial N}{\partial t} + D \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = -\frac{N - N_0}{\tau}$$

$$D \dot{\mathbf{k}} \cdot \frac{\partial f}{\partial \mathbf{k}} = \left(i\omega - \frac{1}{\tau} \right) \delta N = \left(i\omega - \frac{1}{\tau} \right) g(\mu) \delta \mu$$

静态解到含时解的替换

$$\tau \rightarrow \frac{\tau}{1 - i\omega\tau}$$

磁场下的电流

$$\mathbf{J} = \frac{e^4 \tau}{8\pi^4 \hbar^4 g(\mu) (1 - i\omega\tau)} (\mathbf{E} \cdot \mathbf{B}) \mathbf{B}$$

Weyl半金属中的特殊等离子激元

假设电磁场沿z方向，则普通电导部分

$$\sigma_{zz} = \frac{ne^2\tau}{m} \rightarrow \frac{ne^2\tau}{m(1-i\omega\tau)}$$

由于手性反常的磁电导部分

$$\sigma_{zz}^B = \frac{e^4\tau}{8\pi^4\hbar^4g(\mu)(1-i\omega\tau)} B^2$$

考虑如下情况:

- (1) 费米能靠近Weyl点，使得 n 很小
- (2) 频率很高使得 $\omega\tau \gg 1$

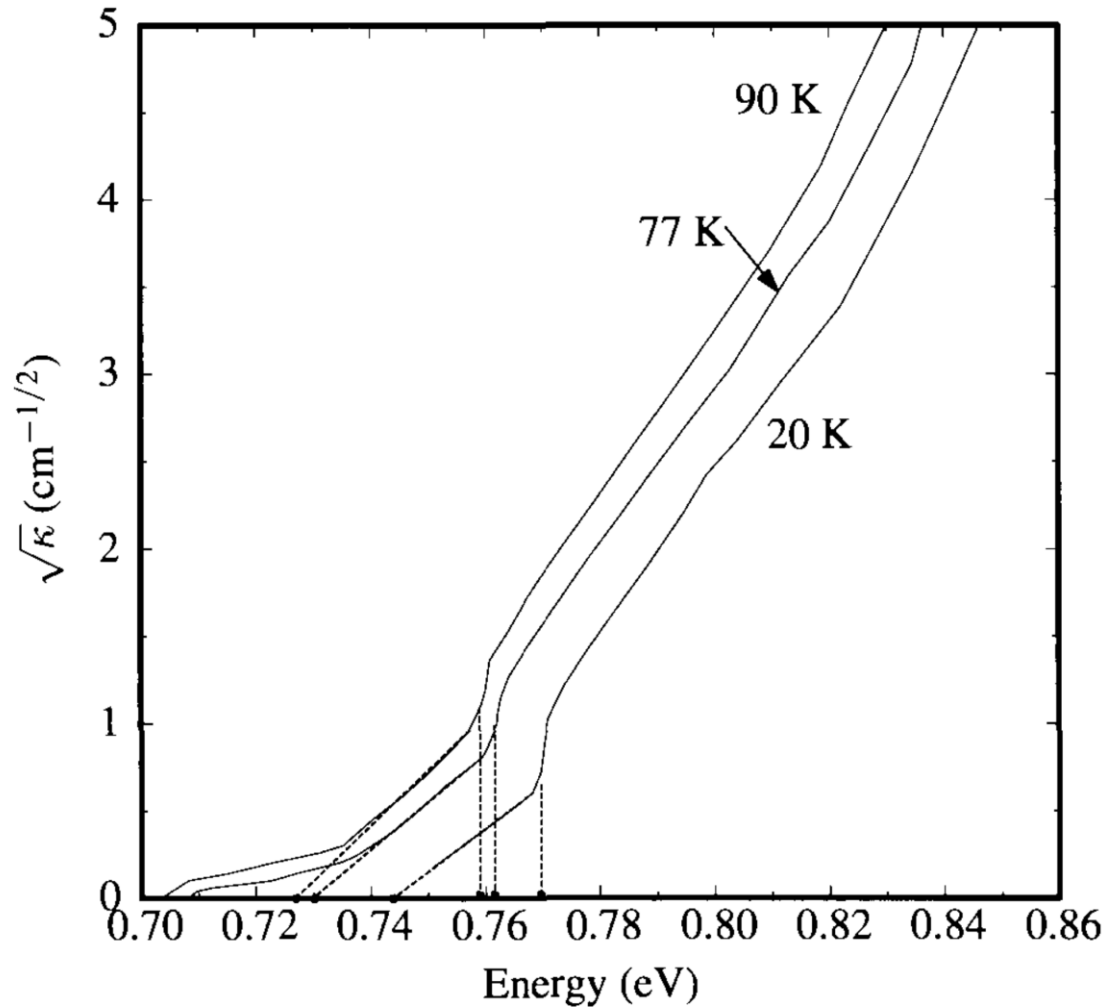
则手性反常部分占主导

代入等离子体频率的方程

$$-i\omega\mu_0 \sigma_{zz}^B - \omega^2 = 0$$

获得 $\omega_p = B \sqrt{\frac{e^4}{8\pi^4\hbar^4g(\mu)}}$

半导体的光吸收



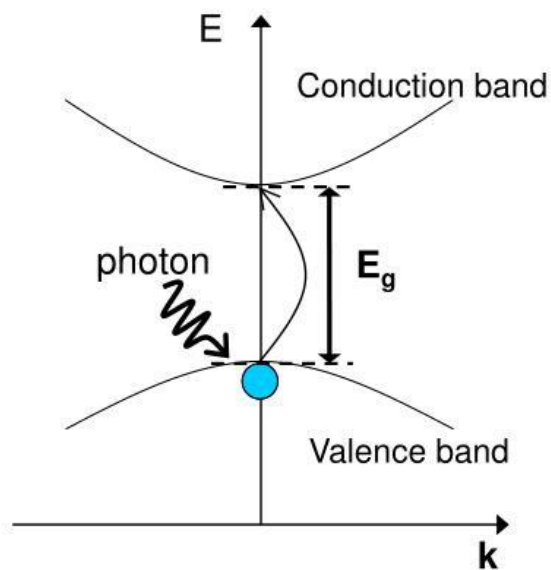
摘自M. Marder, Condensed Matter Physics

$$\kappa \propto (\hbar\omega \mp \hbar\omega_{ph} - E_g)^2 \Theta(\hbar\omega \mp \hbar\omega_{ph} - E_g)$$

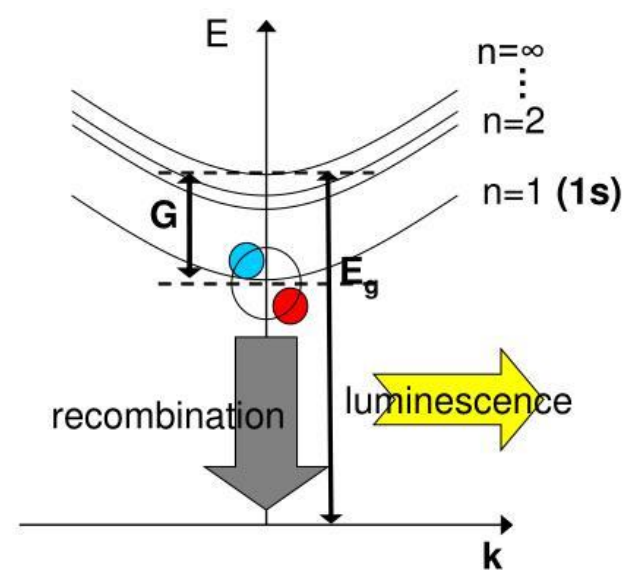
激子的产生：电子-空穴对

Exciton

Band structure of semiconductor



Exciton energy diagram



● electron
● hole

摘自Itoh Lab的ppt

激子的波函数与能谱

激子波函数：电子-空穴对的线性组合

$$|\phi_{ex}\rangle = \sum_k f(k) c_{ck}^+ c_{vk} |\Phi_0\rangle$$

固体中电子的哈密顿量：

$$\hat{H} = \frac{p_1^2 + p_2^2}{2m} - \frac{e^2}{|\mathbf{r}_1 - \mathbf{r}_2|} + U(\mathbf{r}_1) + U(\mathbf{r}_2)$$

平均场近似下：

$$\hat{H}_{eff} |\phi_{ex}\rangle = E_{ex} |\phi_{ex}\rangle$$

$$\hat{H}_{eff} = -\frac{p_h^2}{2m_h} + \frac{p_e^2}{2m_e} - \frac{e^2}{|r_e - r_h|}$$

类比于氢原子模型

激子能谱与几何相位(1)

平均场近似下（一般情况）：

$$\hat{H}|\phi_{ex}\rangle = E_{ex}|\phi_{ex}\rangle$$

$$E_{ex}f(k) = (E_{ck} - E_{vk})f(k) - \frac{1}{S} \sum_{k_2} \frac{2\pi e^2}{|k-k_2|} s_{kk_2}^c s_{k_2k}^v f(k_2)$$

$$s_{kk_2}^c = \langle ck|ck_2\rangle, s_{k_2k}^v = \langle vk_2|vk\rangle$$

几何相位的作用：

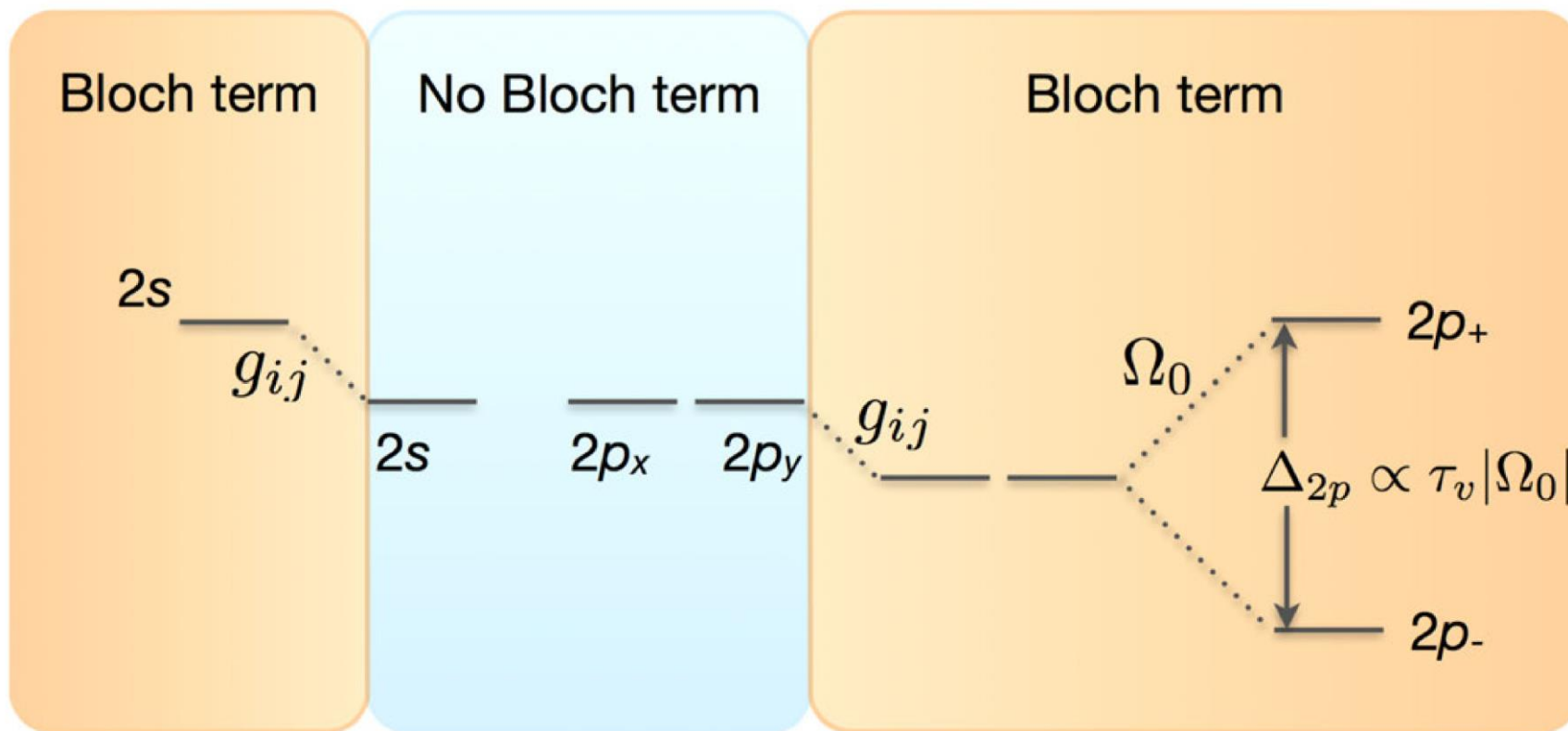
$$s_{k,k+dk}^c = 1 + \langle ck|\partial_{k_i}|ck\rangle dk_i + \frac{1}{2} \langle ck|\partial_{k_i}\partial_{k_j}|ck\rangle dk_i dk_j + \dots$$

几何因子：

$$s_{kk_2}^c s_{k_2k}^v = 1 + \frac{|\Omega_0|}{2} \left(i\tau(\mathbf{k}_2 \times \mathbf{k})_z - \frac{1}{2} |\mathbf{k} - \mathbf{k}_2|^2 \right)$$

激子能谱与几何相位(2)

几何相位的效果



激子动力学与几何相位

激子波函数（质心动量不为0）：

$$|\phi_{ex}(\mathbf{q})\rangle = \sum_{\mathbf{k}} f(\mathbf{k}, \mathbf{q}) c_{c\mathbf{k} + \frac{m_e}{M}\mathbf{q}}^+ c_{v\mathbf{k} - \frac{m_h}{M}\mathbf{q}} |\Phi_0\rangle$$

激子能谱：

$$E_{ex} = \varepsilon_{ex}(\mathbf{q})$$

激子的波包

$$|W\rangle = \int d\mathbf{q} C(\mathbf{q}) e^{i\mathbf{q}\cdot\mathbf{R}} |\phi_{ex}(\mathbf{q})\rangle$$

贝利曲率

$$\boldsymbol{\Omega}_{ex} = \nabla_{\mathbf{q}} \times \langle \phi_{ex}(\mathbf{q}) | i\partial_{\mathbf{q}} | \phi_{ex}(\mathbf{q}) \rangle$$

运动方程

$$\dot{\mathbf{R}} = \frac{\partial \varepsilon}{\hbar \partial \mathbf{q}} - \dot{\mathbf{q}} \times \boldsymbol{\Omega}_{ex}$$

$$\hbar \dot{\mathbf{q}} = -\frac{\partial \varepsilon}{\partial \mathbf{R}} - \dot{\mathbf{R}} \times \mathbf{D} \quad \mathbf{D} = ed \frac{\partial B_z}{\partial z} \hat{z}$$