

量子霍尔效应初步

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1 二维电子气的一些结果

1.1 经典霍尔效应

将电子限制在有限大小二维平面内, x 方向通上电流, z 方向加上磁场, 此时在 y 方向上出现电压, 这就是经典的霍尔效应, 电压称为霍尔电压。

在 Drude 模型下, 电子的运动方程写为:

$$m \frac{d\mathbf{v}}{dt} = -e\mathbf{E} - e\mathbf{v} \times \mathbf{B} - \frac{m\mathbf{v}}{\tau}$$

其中 τ 为弛豫时间。考虑稳态, 则有

$$\mathbf{v} + \frac{e\tau}{m} \mathbf{v} \times \mathbf{B} = -\frac{e\tau}{m} \mathbf{E}$$

设载流子(面)密度为 n 则, 电流密度为 $\mathbf{J} = -ne\mathbf{v}$, 将上式写为矩阵形式:

$$\begin{pmatrix} 1 & \omega_B \tau \\ -\omega_B \tau & 1 \end{pmatrix} \mathbf{J} = \frac{e^2 n \tau}{m} \mathbf{E} = \sigma_{DC} \mathbf{E}$$

其中回旋频率 $\omega_B = \frac{eB}{m}$ 。故电导率张量为

$$\mathbf{J} = \sigma \mathbf{E} = \frac{\sigma_{DC}}{1 + \omega_B^2 \tau^2} \begin{pmatrix} 1 & -\omega_B \tau \\ \omega_B \tau & 1 \end{pmatrix} \mathbf{E} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} \\ -\sigma_{xy} & \sigma_{xx} \end{pmatrix} \mathbf{E}$$

同样有电阻率张量

$$\rho = \sigma^{-1} = \begin{pmatrix} \rho_{xx} & \rho_{xy} \\ -\rho_{xy} & \rho_{yy} \end{pmatrix} = \frac{1}{\sigma_{DC}} \begin{pmatrix} 1 & \omega_B \tau \\ -\omega_B \tau & 1 \end{pmatrix}$$

在实际实验中, 测量 x 方向电流和 y 方向霍尔电压, 可有

$$\frac{V_y}{I_x} = -\frac{LE_y}{LI_x} = -\frac{E_y}{J_x} = \rho_{xy}$$

但要注意到 σ_{xy} 不是 ρ_{xy} 的倒数, 实际上

$$\sigma_{xx} = \frac{\rho_{xx}}{\rho_{xx}^2 + \rho_{xy}^2} \quad \sigma_{xy} = \frac{-\rho_{xy}}{\rho_{xx}^2 + \rho_{xy}^2}$$

但是后文会提到在 ρ_{xy} 呈现出量子化特点的时候, 可以发现 ρ_{xx} 为 0, 故此时确实有 $\sigma_{xy} = \rho_{xy}^{-1}$ 。经典霍尔效应的两个重要结果 $\rho - B$ 是

$$\rho_{xx} = \frac{m}{ne^2\tau} \quad \rho_{xy} = \frac{B}{ne}$$

1.2 朗道能级

二维电子气在均匀磁场中的能量是量子化的, 这一点不依赖于特定规范。写出哈密顿量:

$$H = \frac{1}{2m} (\mathbf{p} + e\mathbf{A})^2 = \frac{1}{2m} \pi^2 = \frac{1}{2m} (\pi_x^2 + \pi_y^2)$$

由于 $[x_i, p_j] = i\hbar\delta_{ij}$, 故

$$[\pi_i, \pi_j] = [p_i + eA_i, p_j + eA_j] = -ie\hbar \left(\frac{\partial A_j}{\partial x_i} - \frac{\partial A_i}{\partial x_j} \right) = -ie\hbar \epsilon_{ijk} B_k$$

也就是 $[\pi_x, \pi_y] = -ie\hbar B$ ，这里假定均匀磁场为 z 方向。

引入产生湮灭算符：

$$a = \frac{1}{\sqrt{2e\hbar B}} (\pi_x - i\pi_y) \quad a^\dagger = \frac{1}{\sqrt{2e\hbar B}} (\pi_x + i\pi_y)$$

满足 $[a, a^\dagger] = 1$ ，此时哈密顿量为

$$H = \hbar\omega_B \left(a^\dagger a + \frac{1}{2} \right)$$

显然能级是量子化的 $E_n = \hbar\omega_B \left(n + \frac{1}{2} \right)$ 。

现考虑加上 x 方向电场。将磁矢势取为朗道规范 $\mathbf{A} = xB\hat{\mathbf{y}}$ ，位置空间哈密顿写为

$$H = \frac{1}{2m} \left(p_x^2 + (p_y + eBx)^2 \right) + eEx$$

上式中只出现 p_y 而不出现 y ，故可将解写为 $\psi_k(x, y) = e^{iky} f_k(x)$ 。而此时可以看出 H 中仅包含 p_x 和 x 的最高二次项，故可以通过配分将其化为谐振子哈密顿量。波函数可解得：

$$\psi(x, y) = \psi_{n,k} \left(x + mE/eB^2, y \right)$$

其中

$$\psi_{n,k}(x, y) \sim e^{iky} H_n \left(x + kl_B^2 \right) e^{-(x+kl_B^2)^2/2l_B^2}, \quad l_B = \sqrt{\frac{\hbar}{eB}}$$

相应的能量为

$$E_{n,k} = \hbar\omega_B \left(n + \frac{1}{2} \right) - eE \left(kl_B^2 + \frac{eE}{m\omega_B^2} \right) + \frac{m}{2} \frac{E^2}{B^2}$$

y 方向的色散关系可以理解为形成霍尔电压之前的非平衡电流

$$v_y = \frac{1}{\hbar} \frac{\partial E_{n,k}}{\partial k} = -\frac{e}{\hbar} E l_B^2 = -\frac{E}{B}$$

可以发现这和经典图像下带电粒子在均匀垂直电场磁场中的漂移速度一致。

2 现象与基本解释

2.1 现象描述

最早的量子霍尔效应就是强磁场下 $\rho - B$ 关系的改变：

对于整数量子霍尔效应，电阻率 ρ_{xy} 出现量子化平台

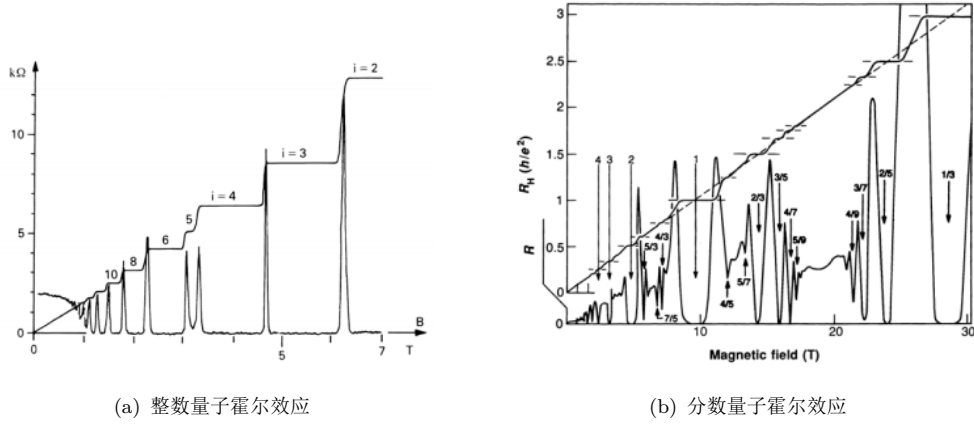
$$\rho_{xy} = \frac{2\pi\hbar}{e^2} \frac{1}{\nu} \quad \nu \in \mathbf{Z}$$

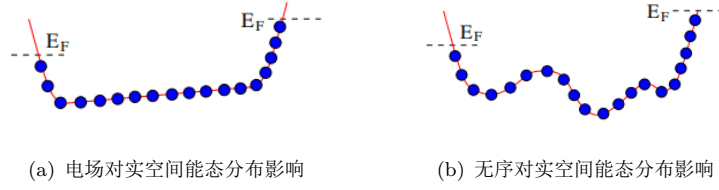
而在 ρ_{xy} 为平台时， ρ_{xx} 为 0，故如前所述此时也可以说电导 σ_{xy} 是量子化的。

实际样品中都有无序。而实验表明整数量子化平台的出现需要一定量的无序。事实上当无序逐渐减弱时，整数平台将变小，同时出现其他有理数平台，也就是分数量子霍尔效应

$$\rho_{xy} = \frac{2\pi\hbar}{e^2} \frac{1}{\nu} \quad \nu \in \mathbf{Q}$$

可以想象对于足够纯净的样品，足够多的有理数将会把 $\rho_{xy} - B$ 还原为经典测量结果。



图 3: 有限尺寸样品的势能 $V(x)$

在这种情况下, 随着磁场的改变, 应当会出现朗道能级的部分填充, 会出现一系列非平衡结果, 但实验结果表明电导量子化是在一个范围内出现的。这时需要考虑无序的影响。

事实上, 如果定义带电粒子在均匀磁场中“圆周运动”的圆心观测量 (见固体物理小结), 将可以发现圆心沿着无序势的等势线运动。无序会造成朗道能级展宽, 但展宽成局域态, 对电导没有贡献, 如图 (4) 所示:

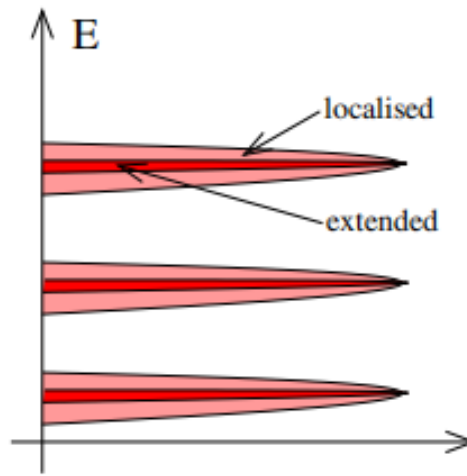


图 4: 无序对朗道能级的影响

这样电导平台就得到了解释: 连续改变磁场时, 朗道能级简并度改变, 朗道能级填充数改变, 但由于部分填充时填充的是局域态, 对电导没有贡献, 故量子化电导表现为一个平台。从图 (2) 中可以看出, 在样品的两侧, 边缘流是反向的, 即不同方向的电流分布在不同的边缘上, 从而是背散射保护的。

整数量子霍尔效应的边缘无耗散流有潜在应用价值, 但在上文的情境中有强磁场的存在。磁场是必须的吗? 后文的讨论中可以发现, 满带电导本身会表现出量子化特征, 磁场实际上让问题复杂了。

3 单电子图像的量子霍尔效应

3.1 贝利相位 & 贝利曲率

考虑缓变参数的哈密顿量, 参数的演化为一闭合曲线

$$H = H(\mathbf{R}), \quad \mathbf{R} = \mathbf{R}(t), \quad \mathbf{R}(T) = \mathbf{R}(0)$$

在每个参数下选取正交完备基

$$H(\mathbf{R})|n(\mathbf{R})\rangle = \varepsilon_n(\mathbf{R})|n(\mathbf{R})\rangle.$$

$|n(\mathbf{R})\rangle$ 的选择不是唯一的, 有相位上的自由度, 但需要在参数空间中单值。假设在这样的哈密顿量下, 态可以写为

$$|\psi_n(t)\rangle = e^{i\gamma_n(t)} \exp\left[-\frac{i}{\hbar} \int_0^t dt' \varepsilon_n(\mathbf{R}(t'))\right] |n(\mathbf{R}(t))\rangle,$$

代入 $i\hbar \frac{\partial}{\partial t} |\psi_n(t)\rangle = H(\mathbf{R}(t)) |\psi_n(t)\rangle$

可以得到

$$\gamma_n = \int_C d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R}), \quad \mathbf{A}_n(\mathbf{R}) = i \left\langle n(\mathbf{R}) \left| \frac{\partial}{\partial \mathbf{R}} \right| n(\mathbf{R}) \right\rangle.$$

其中 \mathbf{A} 称为贝利联络。若作规范变换 $|n(\mathbf{R})\rangle \rightarrow e^{i\zeta(\mathbf{R})} |n(\mathbf{R})\rangle$,

相应的 \mathbf{A} 和 γ_n 的改变量为

$$\begin{aligned} \mathbf{A}_n(\mathbf{R}) &\rightarrow \mathbf{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}} \zeta(\mathbf{R}) \\ \gamma_n &\rightarrow \gamma_n - \zeta(\mathbf{R}(T)) + \zeta(\mathbf{R}(0)) \end{aligned}$$

因为规范变换要保持单值性, 故 $e^{i\zeta(\mathbf{R})}$ 要求

$$-\zeta(\mathbf{R}(T)) + \zeta(\mathbf{R}(0)) = 2\pi k, \quad k \in \mathbf{Z}$$

所以 $e^{i\gamma_n(T)}$ 是规范不变的, 等价地说 γ_n 是有物理意义的

$$\gamma_n = \oint_C d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R})$$

γ_n 被称为几何相或贝利相位。

可以由贝利联络定义贝利曲率

$$\begin{aligned} \Omega_{\mu\nu}^n(\mathbf{R}) &= \frac{\partial}{\partial R^\mu} A_\nu^n(\mathbf{R}) - \frac{\partial}{\partial R^\nu} A_\mu^n(\mathbf{R}) \\ &= i \left[\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \left| \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \left| \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle \right] \right] \end{aligned}$$

故由 Stokes 公式, 贝利相位为

$$\gamma_n = \int_S dR^\mu \wedge dR^\nu \frac{1}{2} \Omega_{\mu\nu}^n(\mathbf{R})$$

其中 \wedge 为楔形积。三维情形下, 贝利曲率又可写为

$$\begin{aligned} \mathbf{\Omega}_n(\mathbf{R}) &= \nabla_{\mathbf{R}} \times \mathbf{A}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \langle n(\mathbf{R}) | i \nabla_{\mathbf{R}} | n(\mathbf{R}) \rangle \\ \gamma_n &= \int_S d\mathbf{S} \cdot \mathbf{\Omega}_n(\mathbf{R}) \end{aligned}$$

而事实上, 贝利曲率有一种更常用的求和形式, 由于

$$\begin{cases} \langle n|m \rangle = \delta_{mn} \\ \langle n|H|m \rangle = \epsilon_m \delta_{mn} \end{cases}$$

$$\Rightarrow \begin{cases} \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \left| m(\mathbf{R}) \right\rangle + \left\langle n(\mathbf{R}) \left| \frac{\partial m(\mathbf{R})}{\partial R^\mu} \right\rangle = 0 \\ \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \left| H(\mathbf{R}) \right| m(\mathbf{R}) \right\rangle + \left\langle n(\mathbf{R}) \left| \frac{\partial H(\mathbf{R})}{\partial R^\mu} \right| m(\mathbf{R}) \right\rangle + \left\langle n(\mathbf{R}) \left| H(\mathbf{R}) \right| \frac{\partial m(\mathbf{R})}{\partial R^\mu} \right\rangle = 0 \end{cases}$$

$$\Rightarrow \left\langle n(\mathbf{R}) \left| \frac{\partial H(\mathbf{R})}{\partial R^\mu} \right| m(\mathbf{R}) \right\rangle = (\epsilon_n - \epsilon_m) \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| m(\mathbf{R}) \right\rangle = (\epsilon_m - \epsilon_n) \left\langle n(\mathbf{R}) \left| \frac{\partial m(\mathbf{R})}{\partial R^\mu} \right\rangle \right\rangle$$

于是

$$\begin{aligned} \Omega_{\mu\nu}^n(\mathbf{R}) &= i \left[\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \middle| \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle \right] \\ &= i \sum_m \left[\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| m \right\rangle \langle m | \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \middle| m \right\rangle \langle m | \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle \right] \\ &= i \sum_{m \neq n} \left[\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| m \right\rangle \langle m | \frac{\partial n(\mathbf{R})}{\partial R^\nu} \right\rangle - \left\langle \frac{\partial n(\mathbf{R})}{\partial R^\nu} \middle| m \right\rangle \langle m | \frac{\partial n(\mathbf{R})}{\partial R^\mu} \right\rangle \right] \\ &= i \sum_{m \neq n} \frac{\left\langle n \left| \frac{\partial H(\mathbf{R})}{\partial R^\mu} \right| m \right\rangle \left\langle m \left| \frac{\partial H(\mathbf{R})}{\partial R^\nu} \right| n \right\rangle - \left\langle n \left| \frac{\partial H(\mathbf{R})}{\partial R^\nu} \right| m \right\rangle \left\langle m \left| \frac{\partial H(\mathbf{R})}{\partial R^\mu} \right| n \right\rangle}{(\epsilon_m - \epsilon_n)^2} \end{aligned}$$

其中第 3 个等号利用了 $m = n$ 项为 0 及 $\left\langle \frac{\partial n(\mathbf{R})}{\partial R^\mu} \middle| n \right\rangle + \left\langle n \left| \frac{\partial m(\mathbf{R})}{\partial R^\mu} \right\rangle = 0$ 。

这个形式和 Kubo 公式的结果很像。

3.1.1 \mathbf{T}^2 的贝利相位

$$\gamma_n = \int_S dR^\mu \wedge dR^\nu \frac{1}{2} \Omega_{\mu\nu}^n(\mathbf{R})$$

某些情况下, S 可以很特殊, 如 $S = \mathbf{T}^2$, 也即空间圆环面, 或者更一般地, 就是在两个方向上具有周期性的参数空间, 如二维布里渊区。

这里要注意的是, 单值性要求参数空间的一个点, 唯一地映射到一个态矢上。但周期性是物理上的周期性, 态矢有一个相位自由度, 所以相差一个倒格矢的两个点对应的态矢可以相差一个相位, 如布里渊区边界上的点。

考虑环路积分:

$$\gamma_n = \oint_C d\mathbf{R} \cdot \mathbf{A}_n(\mathbf{R})$$

环路取为布里渊区边界。将坐标归一化如下:

$$x = \left(k_x + \frac{\pi N_x}{L_x} \right) / \frac{2\pi N_x}{L_x}, \quad y = \left(k_y + \frac{\pi N_y}{L_y} \right) / \frac{2\pi N_y}{L_y}$$

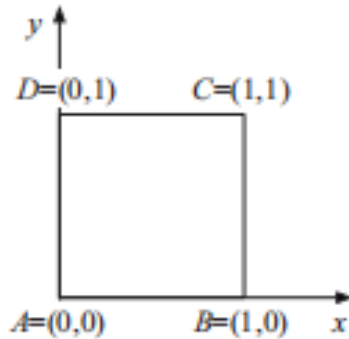


图 5: 坐标归一化的二维布里渊区

$$\begin{aligned}\frac{\gamma_n}{2\pi} &= \frac{1}{2\pi} \left\{ \int_A^B dx A_x(x, 0) + \int_B^C dy A_y(1, y) + \int_C^D dx A_x(x, 1) + \int_D^A dy A_y(0, y) \right\} \\ &= \frac{1}{2\pi} \left\{ \int_0^1 dx [A_x(x, 0) - A_x(x, 1)] - \int_0^1 dy [A_y(0, y) - A_y(1, y)] \right\}\end{aligned}$$

如上文所说，布里渊区边界上的点对应的态矢可以相差一个相位，即

$$e^{i\theta_x(x)}|u(x, 1)\rangle = |u(x, 0)\rangle, \quad e^{i\theta_y(y)}|u(1, y)\rangle = |u(0, y)\rangle$$

$$\begin{aligned}\int_0^1 dx [A_x(x, 0) - A_x(x, 1)] \\ &= i \int_0^1 dx [\langle u(x, 0) | \frac{\partial}{\partial x} | u(x, 0) \rangle - \langle u(x, 0) | e^{-i\theta_x(x)} \frac{\partial}{\partial x} (e^{i\theta_x(x)} | u(x, 0) \rangle)] \\ &= i \int_0^1 dx - i \frac{\partial \theta_x(x)}{\partial x} \\ &= \theta_x(1) - \theta_x(0)\end{aligned}$$

同理可得

$$\int_0^1 dy [A_y(0, y) - A_y(1, y)] = \theta_y(1) - \theta_y(0)$$

代入 γ_n 得

$$\frac{\gamma_n}{2\pi} = \frac{1}{2\pi} [\theta_x(1) - \theta_x(0) + \theta_y(0) - \theta_y(1)].$$

又由于在边界上有

$$\begin{aligned}e^{i\theta_x(0)}|u(0, 1)\rangle &= |u(0, 0)\rangle, \\ e^{i\theta_x(1)}|u(1, 1)\rangle &= |u(1, 0)\rangle, \\ e^{i\theta_y(0)}|u(1, 0)\rangle &= |u(0, 0)\rangle, \\ e^{i\theta_y(1)}|u(1, 1)\rangle &= |u(0, 1)\rangle,\end{aligned}$$

从而得到

$$|u(0, 0)\rangle = e^{i[\theta_x(1) - \theta_x(0) + \theta_y(0) - \theta_y(1)]} |u(0, 0)\rangle.$$

单值性要求 $[\theta_x(1) - \theta_x(0) + \theta_y(0) - \theta_y(1)]$ 是 2π 的整数倍，于是

$$\frac{\gamma_n}{2\pi} \in \mathbf{Z}$$

通常将这个整数的负值定义为能带 n 的第一陈数 C

$$C_n = -\frac{\gamma_n}{2\pi} = -\int \frac{dk^2}{2\pi} \Omega_{k_x k_y}^n$$

3.2 Kubo 公式

外场规范势 $A^\alpha = (\frac{\phi}{c}, \mathbf{A})$ ，电场磁场为

$$\begin{cases} \mathbf{E} = -\nabla\phi - \partial_t \mathbf{A} \\ \mathbf{B} = \nabla \times \mathbf{A} \end{cases}$$

取 $\phi = 0$ ，则多体哈密顿量为

$$\begin{aligned} H &= \frac{1}{2m} \sum_i (\hat{\mathbf{p}}_i - e\mathbf{A}(\hat{\mathbf{x}}_i, t))^2 \\ &= \frac{1}{2m} \sum_i \hat{\mathbf{p}}_i^2 - \frac{e}{2m} \sum_i (\hat{\mathbf{p}}_i - e\mathbf{A}(\hat{\mathbf{x}}_i, t)) \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) - \frac{e}{2m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \cdot \hat{\mathbf{p}}_i \end{aligned}$$

考虑时谐场， $\mathbf{A}(\mathbf{x}, t) = \mathbf{A}e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} = \mathbf{A}e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)}$ ，则

$$\begin{cases} \mathbf{E} = i\omega \mathbf{A}e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \\ \mathbf{B} = i\mathbf{k} \times \mathbf{A}e^{i(\mathbf{k} \cdot \mathbf{x} - \omega t)} \end{cases}$$

ϕ 和 \mathbf{A} 的选取需要满足真空中 (只考虑外场) 的麦克斯韦方程组:

$$\begin{cases} \nabla \cdot \mathbf{E} = 0 \\ \nabla \cdot \mathbf{B} = 0 \\ \nabla \times \mathbf{E} = -\partial_t \mathbf{B} \\ \nabla \times \mathbf{B} = \frac{1}{c^2} \partial_t \mathbf{E} \end{cases}$$

第二第三个方程自动满足，第一个和最后一个方程要求 $\mathbf{k} \cdot \mathbf{A} = 0$ ，即为横波。在 $\omega \rightarrow 0$ 极限下，电场磁场为匀强场稳恒场。而由 $\mathbf{k} \cdot \mathbf{A} = 0$ 可知，电场的模是磁场的模的 c 倍，对比电场力和洛伦兹力:

$$qvB \sim qv \frac{E}{c} = qE \frac{v}{c}$$

故在非相对论极限下，可以认为此时仅有匀强电场。由 $\mathbf{k} \cdot \mathbf{A} = 0$ 还可以推知

$$[\hat{\mathbf{p}}_i, \mathbf{A}_i(\hat{\mathbf{x}}, t)] = \hbar k_i \mathbf{A}_i(\hat{\mathbf{x}}, t)$$

$$\implies \hat{\mathbf{p}} \cdot \mathbf{A}(\hat{\mathbf{x}}, t) = \mathbf{A}(\hat{\mathbf{x}}, t) \cdot \hat{\mathbf{p}} + \hbar(\mathbf{k} \cdot \mathbf{A})e^{i(\mathbf{k} \cdot \hat{\mathbf{x}} - \omega t)} = \mathbf{A}(\hat{\mathbf{x}}, t) \cdot \hat{\mathbf{p}}$$

于是多体哈密顿量写为

$$\begin{aligned} H &= \frac{1}{2m} \sum_i \hat{\mathbf{p}}_i^2 - \frac{e}{m} \sum_i (\hat{\mathbf{p}}_i - e\mathbf{A}(\hat{\mathbf{x}}_i, t)) \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) - \frac{e^2}{2m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) \\ &= H_0 + \sum_i \frac{-e\pi_i}{m} \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) - \frac{e^2}{2m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) \\ &= H_0 + \mathbf{J} \cdot \mathbf{A}(\hat{\mathbf{x}}_0, t) - \frac{e^2}{2m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \cdot \mathbf{A}(\hat{\mathbf{x}}_i, t) \end{aligned}$$

最后一个等号是考虑到 $\omega \rightarrow 0$ 时， \mathbf{A} 的空间起伏很小。而上式最后一项对应 E^2 的响应，在后文中不考虑。下面进入相互作用绘景

$$|\psi(t)\rangle^I = e^{iH_0 t/\hbar} |\psi(t)\rangle, \quad \mathbf{J} \mathbf{l}^I = e^{iH_0 t/\hbar} \mathbf{J} \mathbf{l} e^{-iH_0 t/\hbar}$$

态矢会按照如下方式演化:

$$|\psi(t)\rangle^I = U(t, t_0) |\psi(t_0)\rangle^I, \quad U(t, t_0) = T \exp \left(-\frac{i}{\hbar} \int_{t_0}^t \Delta H(t') dt' \right)$$

将 U 展开到一阶，基态时电流元为

$$\begin{aligned} \langle \mathbf{J} \mathbf{l}(t) \rangle &= {}^I \langle 0(t) | \mathbf{J} \mathbf{l}^I(t) | 0(t) \rangle^I \\ &= {}^I \langle 0(-\infty) | U^{-1}(t, -\infty) \mathbf{J} \mathbf{l}^I(t) U(t, -\infty) | 0(-\infty) \rangle^I \\ &\approx {}^I \left\langle 0(-\infty) \left| \left(\mathbf{J} \mathbf{l}^I(t) + \frac{i}{\hbar} \int_{-\infty}^t dt' [\Delta H(t'), \mathbf{J} \mathbf{l}^I(t)] \right) \right| 0(-\infty) \right\rangle^I \end{aligned}$$

容易看出 $\Delta H = 0$ 时, 对应没有电场的情况, 此时电流元应为 0, 故

$$\begin{aligned} {}^I \langle 0(-\infty) | \mathbf{J}^I(t) | 0(-\infty) \rangle^I &= {}^I \left\langle 0(-\infty) \left| \mathbf{J}^I(-\infty) + \frac{e^2}{m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \right| 0(-\infty) \right\rangle^I \\ &= {}^I \left\langle 0(-\infty) \left| \frac{e^2}{m} \sum_i \mathbf{A}(\hat{\mathbf{x}}_i, t) \right| 0(-\infty) \right\rangle^I \\ &= \frac{Sn_e e^2}{m} \mathbf{A}(\hat{\mathbf{x}}_0, t) = \frac{Sn_e e^2}{m} \frac{\mathbf{E}}{i\omega} e^{-i\omega t} \end{aligned}$$

代入 ΔH , 可得

$$\begin{aligned} \langle J_i(t) \rangle &= \frac{1}{\hbar\omega} \int_{-\infty}^t dt' \langle 0 | [J_j^I(t'), J_i^I(t)] | 0 \rangle E_j e^{-i\omega t'} + \frac{Sn_e e^2}{m} \frac{E_i}{i\omega} e^{-i\omega t} \\ &= \frac{1}{\hbar\omega} \left(\int_0^\infty dt'' e^{i\omega t''} \langle 0 | [J_j^I(0), J_i^I(t'')] | 0 \rangle \right) E_j e^{-i\omega t} + \frac{Sn_e e^2}{m} \frac{E_i}{i\omega} e^{-i\omega t} \end{aligned}$$

从而电导 σ_{xy} 为

$$\sigma_{xy}(\omega) = \frac{1}{\hbar\omega} \frac{1}{L_x L_y} \int_0^\infty dt e^{i\omega t} \langle 0 | [J_y^I(0), J_x^I(t)] | 0 \rangle$$

除以 $L_x L_y$ 是因为 J_x, J_y 是电流元。回到薛定谔绘景, 利用完备性关系式:

$$\begin{aligned} \sigma_{xy}(\omega) &= \frac{1}{\hbar\omega} \int_0^\infty dt e^{i\omega t} \sum_n \left[\langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle e^{i(E_n - E_0)t/\hbar} - \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle e^{i(E_0 - E_n)t/\hbar} \right] \\ &= -\frac{i}{\omega} \frac{1}{L_x L_y} \sum_{n \neq 0} \left[\frac{\langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle}{\hbar\omega + E_n - E_0} - \frac{\langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle}{\hbar\omega + E_0 - E_n} \right] \end{aligned}$$

上式中为了收敛实际上取了 $\omega \rightarrow \omega + i\epsilon$ 。

由于 $\omega \rightarrow 0$, 故

$$\frac{1}{\hbar\omega + E_n - E_0} \approx \frac{1}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2} + O(\omega^2) \dots$$

将其代入电导的表达式中

$$\begin{aligned} \sigma_{xy}(\omega) &= -\frac{i}{\omega} \frac{1}{L_x L_y} \sum_{n \neq 0} \left[\frac{1}{E_n - E_0} - \frac{\hbar\omega}{(E_n - E_0)^2} \right] \langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle \\ &\quad + \frac{i}{\omega} \frac{1}{L_x L_y} \sum_{n \neq 0} \left[\frac{1}{E_0 - E_n} - \frac{\hbar\omega}{(E_n - E_0)^2} \right] \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle \\ &= i\hbar \frac{1}{L_x L_y} \sum_{n \neq 0} \frac{\langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle - \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle}{(E_n - E_0)^2} \\ &\quad + \frac{i}{\omega} \frac{1}{L_x L_y} \sum_{n \neq 0} \frac{\langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle + \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle}{E_0 - E_n} \end{aligned}$$

由于 σ_{xy} 应当与坐标系的选择无关, 只要都是右旋坐标系, 故在变换 $x \rightarrow y, y \rightarrow -x$ 下电导应当不变。容易验证

$$\begin{aligned} \langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle - \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle &\xrightarrow{x \rightarrow y, y \rightarrow -x} \langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle - \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle \\ \langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle + \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle &\xrightarrow{x \rightarrow y, y \rightarrow -x} -\langle 0 | J_y | n \rangle \langle n | J_x | 0 \rangle - \langle 0 | J_x | n \rangle \langle n | J_y | 0 \rangle \end{aligned}$$

从而电导公式中第二项为 0，最终结果为

$$\sigma_{xy} = i\hbar \frac{1}{L_x L_y} \sum_{n \neq 0} \frac{\langle 0 | J_{ly} | n \rangle \langle n | J_{lx} | 0 \rangle - \langle 0 | J_{lx} | n \rangle \langle n | J_{ly} | 0 \rangle}{(E_n - E_0)^2}$$

此即 Kubo 公式。

3.3 整数霍尔效应

满足平移对称性的晶格有布洛赫定理 $\langle \mathbf{x} | \psi_{\mathbf{k}} \rangle = e^{i\mathbf{k} \cdot \mathbf{x}} \langle \mathbf{x} | u_{\mathbf{k}} \rangle = \langle \mathbf{x} | e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} | u_{\mathbf{k}} \rangle$

$$\begin{aligned} H | \psi_{\mathbf{k}} \rangle &= E_{\mathbf{k}} | \psi_{\mathbf{k}} \rangle \Rightarrow (e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}} H e^{i\mathbf{k} \cdot \hat{\mathbf{x}}}) | u_{\mathbf{k}} \rangle = E_{\mathbf{k}} | u_{\mathbf{k}} \rangle \\ &\Rightarrow \tilde{H}(\mathbf{k}) | u_{\mathbf{k}} \rangle = E_{\mathbf{k}} | u_{\mathbf{k}} \rangle \end{aligned}$$

其中 $\tilde{H}(\mathbf{k}) = e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}} H e^{i\mathbf{k} \cdot \hat{\mathbf{x}}}$ 。若 $H = (\hat{\mathbf{p}} + e\mathbf{A})^2/2m$ ，则

$$\begin{aligned} \hat{\mathbf{x}}(\hat{\mathbf{p}} + e\mathbf{A}) &= (\hat{\mathbf{p}} + i\hbar + e\mathbf{A})\hat{\mathbf{x}} \\ \Rightarrow e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}}(\hat{\mathbf{p}} + e\mathbf{A}) &= (\hat{\mathbf{p}} + \hbar\mathbf{k} + e\mathbf{A})e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} \\ \tilde{H}(\mathbf{k}) &= e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}} H e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} = (\hat{\mathbf{p}} + \hbar\mathbf{k} + e\mathbf{A})^2/2m \end{aligned}$$

$| \psi_{\mathbf{k}} \rangle = e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} | u_{\mathbf{k}} \rangle$ 可以视为一种表象变换，相应可以得到算符变换。考虑速度期望：

$$\begin{aligned} \langle \dot{\mathbf{x}} \rangle &= \frac{1}{i\hbar} \langle [\mathbf{x}, H] \rangle = \frac{1}{i\hbar} \langle \psi_{\mathbf{k}} | [\mathbf{x}, H] | \psi_{\mathbf{k}} \rangle = \frac{1}{i\hbar} \langle u_{\mathbf{k}} | e^{-i\mathbf{k} \cdot \hat{\mathbf{x}}} [\mathbf{x}, H] e^{i\mathbf{k} \cdot \hat{\mathbf{x}}} | u_{\mathbf{k}} \rangle \\ &= \frac{1}{i\hbar} \langle u_{\mathbf{k}} | [\mathbf{x}, H(\mathbf{k})] | u_{\mathbf{k}} \rangle = \left\langle u_{\mathbf{k}} \left| \frac{(\hat{\mathbf{p}} + \hbar\mathbf{k} + e\mathbf{A})}{m} \right| u_{\mathbf{k}} \right\rangle = \left\langle u_{\mathbf{k}} \left| \frac{\partial H(\mathbf{k})}{\hbar \partial \mathbf{k}} \right| u_{\mathbf{k}} \right\rangle \end{aligned}$$

从而单电子贡献的电流元为

$$\langle J_l \rangle = \frac{e}{\hbar} \left\langle \frac{\partial \tilde{H}}{\partial \mathbf{k}} \right\rangle$$

可以注意到 \mathbf{k} 量子数很自然地成为哈密顿量 $\tilde{H}(\mathbf{k})$ 的参数。利用上式电流元公式和 Kubo 公式可以得到 TKNN 公式。

3.3.1 TKNN 公式

假设费米面位于带隙。Kubo 公式中的 $|0\rangle, |n\rangle$ 是多体态， J_{lx}, J_{ly} 是多体算符，也即

$$\begin{aligned} |0\rangle &= \frac{1}{\sqrt{N!}} \sum_{\sigma} \epsilon_{\sigma} | \psi_{\sigma(1)}^0 \rangle \otimes | \psi_{\sigma(2)}^0 \rangle \otimes \cdots \otimes | \psi_{\sigma(N)}^0 \rangle \\ |n\rangle &= \frac{1}{\sqrt{N!}} \sum_{\sigma} \epsilon_{\sigma} | \psi_{\sigma(1)}^n \rangle \otimes | \psi_{\sigma(2)}^n \rangle \otimes \cdots \otimes | \psi_{\sigma(N)}^n \rangle \\ J_{lx} &= J_{lx(1)} \otimes \mathbb{1}_{(2)} \otimes \cdots \otimes \mathbb{1}_{(N)} + \mathbb{1}_{(1)} \otimes J_{lx(2)} \otimes \cdots \otimes \mathbb{1}_{(N)} + \mathbb{1}_{(1)} \otimes \mathbb{1}_{(2)} \otimes \cdots \otimes J_{lx(N)} \\ J_{ly} &= J_{ly(1)} \otimes \mathbb{1}_{(2)} \otimes \cdots \otimes \mathbb{1}_{(N)} + \mathbb{1}_{(1)} \otimes J_{ly(2)} \otimes \cdots \otimes \mathbb{1}_{(N)} + \mathbb{1}_{(1)} \otimes \mathbb{1}_{(2)} \otimes \cdots \otimes J_{ly(N)} \end{aligned}$$

考察 Kubo 公式中的 $\langle 0 | J_{ly} | n \rangle$ 项，由于 J_{ly} 是对称化单体算符，故 $|0\rangle, |n\rangle$ 至多有一个单电子态不同，而 $n \neq 0$ 故两者恰好有一个单电子态不同。假设是 $| \psi_{(1)}^0 \rangle \neq | \psi_{(1)}^n \rangle$ ，则对于 $\mathbb{1}_{(1)} \otimes \cdots \otimes J_{ly(i)} \otimes \cdots \otimes \mathbb{1}_{(N)}$ 项的期望，只有形如

$$\begin{aligned} &\langle \psi_{\sigma'(2)}^0 | \otimes \langle \psi_{\sigma'(3)}^0 | \otimes \cdots \otimes \langle \psi_{(1)}^0 | \otimes \cdots \otimes \psi_{\sigma'(N)}^0 | \\ &\mathbb{1}_{(1)} \otimes \cdots \otimes J_{ly(i)} \otimes \cdots \otimes \mathbb{1}_{(N)} | \psi_{\sigma'(2)}^0 \rangle \otimes | \psi_{\sigma'(3)}^0 \rangle \otimes \cdots \otimes | \psi_{(1)}^n \rangle \otimes \cdots \otimes | \psi_{\sigma'(N)}^0 \rangle \end{aligned}$$

的项才有贡献，而这样的项一共 $N \times (N-1)! = N!$ 个，且每项结果都相同，故对于上面选定的 $|n\rangle$ ，有

$$\langle 0 | J_{Ly} | n \rangle = \langle \psi_{(1)}^0 | J_{Ly}^{single} | \psi_{(1)}^n \rangle$$

从而 Kubo 公式可以写为

$$\begin{aligned} \sigma_{xy} &= i\hbar \frac{1}{L_x L_y} \sum_{E_\alpha < E_F < E_\beta} \sum_{\mathbf{k}, \mathbf{k}'} \frac{\langle \psi_{\mathbf{k}}^\alpha | J_{Ly} | \psi_{\mathbf{k}'}^\beta \rangle \langle \psi_{\mathbf{k}'}^\beta | J_{Lx} | \psi_{\mathbf{k}}^\alpha \rangle - \langle \psi_{\mathbf{k}}^\alpha | J_{Lx} | \psi_{\mathbf{k}'}^\beta \rangle \langle \psi_{\mathbf{k}'}^\beta | J_{Ly} | \psi_{\mathbf{k}}^\alpha \rangle}{(E_\beta(\mathbf{k}') - E_\alpha(\mathbf{k}))^2} \\ &= i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_\alpha < E_F < E_\beta} \sum_{\mathbf{k}, \mathbf{k}'} \\ &\quad \frac{\left\langle u_{\mathbf{k}}^\alpha \left| \frac{\partial \tilde{H}}{\partial k_y} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \frac{\partial \tilde{H}}{\partial k_x} \right| u_{\mathbf{k}}^\alpha \right\rangle - \left\langle u_{\mathbf{k}}^\alpha \left| \frac{\partial \tilde{H}}{\partial k_x} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \frac{\partial \tilde{H}}{\partial k_y} \right| u_{\mathbf{k}}^\alpha \right\rangle}{(E_\beta(\mathbf{k}') - E_\alpha(\mathbf{k}))^2} \end{aligned}$$

这里假设费米面位于带隙中，故 \mathbf{k}, \mathbf{k}' 是在整个布里渊区求和。由于

$$\tilde{H}(\mathbf{k}) e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} = e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \tilde{H}(\mathbf{k}')$$

于是

$$\begin{aligned} \left\langle u_{\mathbf{k}}^\alpha \left| \frac{\partial \tilde{H}}{\partial k_y} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_y} \langle u_{\mathbf{k}}^\alpha | e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} | u_{\mathbf{k}'}^\beta \rangle + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \\ &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_y} \delta_{\alpha\beta} \delta_{\mathbf{k}\mathbf{k}'} + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \\ \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \frac{\partial \tilde{H}}{\partial k_x} \right| u_{\mathbf{k}}^\alpha \right\rangle &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_x} \langle u_{\mathbf{k}'}^\beta | e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} | u_{\mathbf{k}}^\alpha \rangle + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \right\rangle \\ &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_x} \delta_{\alpha\beta} \delta_{\mathbf{k}\mathbf{k}'} + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \right\rangle \\ \left\langle u_{\mathbf{k}}^\alpha \left| \frac{\partial \tilde{H}}{\partial k_x} e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_x} \langle u_{\mathbf{k}}^\alpha | e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} | u_{\mathbf{k}'}^\beta \rangle + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \\ &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_x} \delta_{\alpha\beta} \delta_{\mathbf{k}\mathbf{k}'} + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \\ \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \frac{\partial \tilde{H}}{\partial k_y} \right| u_{\mathbf{k}}^\alpha \right\rangle &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_y} \langle u_{\mathbf{k}'}^\beta | e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} | u_{\mathbf{k}}^\alpha \rangle + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \right\rangle \\ &= \frac{\partial E_\alpha(\mathbf{k})}{\partial k_y} \delta_{\alpha\beta} \delta_{\mathbf{k}\mathbf{k}'} + (E_\alpha(\mathbf{k}) - E_\beta(\mathbf{k}')) \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \right\rangle \end{aligned}$$

将上几式代入 σ_{xy} 中，得

$$\begin{aligned} \sigma_{xy} &= i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_\alpha < E_F < E_\beta} \sum_{\mathbf{k}, \mathbf{k}'} \\ &\quad \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \right\rangle \end{aligned}$$

由于 $\sum_\beta \sum_{\mathbf{k}'} |\psi_{\mathbf{k}'}^\beta\rangle \langle \psi_{\mathbf{k}'}^\beta| = \mathbb{1}$ ，故

$$\begin{aligned} \sigma_{xy} &= i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_\alpha < E_F} \sum_{\mathbf{k}} \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \left| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \left| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \right\rangle \right. \\ &\quad \left. - i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_\alpha, E_\beta < E_F} \sum_{\mathbf{k}, \mathbf{k}'} \right. \\ &\quad \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_x} \left| e^{i(\mathbf{k}' - \mathbf{k}) \cdot \hat{x}} \right| u_{\mathbf{k}'}^\beta \right\rangle \left\langle u_{\mathbf{k}'}^\beta \left| e^{i(\mathbf{k} - \mathbf{k}') \cdot \hat{x}} \right| \frac{\partial u_{\mathbf{k}}^\alpha}{\partial k_y} \right\rangle \end{aligned}$$

又由于

$$\begin{aligned}
\left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \right| u_{\mathbf{k}'}^{\beta} \right\rangle &= \left\langle \frac{\partial \psi_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \psi_{\mathbf{k}'}^{\beta} \right\rangle - \left\langle u_{\mathbf{k}}^{\alpha} \left| \frac{\partial}{\partial k_y} e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \right| u_{\mathbf{k}'}^{\beta} \right\rangle \\
&= \left\langle \frac{\partial \psi_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \psi_{\mathbf{k}'}^{\beta} \right\rangle + \left\langle u_{\mathbf{k}}^{\alpha} \left| \frac{\partial}{\partial k'_y} e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \right| u_{\mathbf{k}'}^{\beta} \right\rangle \\
&= \left\langle \frac{\partial \psi_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \psi_{\mathbf{k}'}^{\beta} \right\rangle + \left\langle \psi_{\mathbf{k}}^{\alpha} \left| \frac{\partial \psi_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle - \left\langle u_{\mathbf{k}}^{\alpha} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle \right\rangle \\
&= \frac{\partial}{\partial k_y} \langle \psi_{\mathbf{k}}^{\alpha} | \psi_{\mathbf{k}'}^{\beta} \rangle + \frac{\partial}{\partial k'_y} \langle \psi_{\mathbf{k}}^{\alpha} | \psi_{\mathbf{k}'}^{\beta} \rangle - \left\langle u_{\mathbf{k}}^{\alpha} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle \right\rangle \\
&= \delta_{\alpha\beta} \left(\frac{\partial}{\partial k_y} + \frac{\partial}{\partial k'_y} \right) \delta(\mathbf{k} - \mathbf{k}') - \left\langle u_{\mathbf{k}}^{\alpha} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle \right\rangle \\
&= - \left\langle u_{\mathbf{k}}^{\alpha} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle \right\rangle
\end{aligned}$$

第六个等号成立的原因是 δ 函数是偶函数，但 δ 函数的导数是奇函数。同理可知

$$\left\langle u_{\mathbf{k}'}^{\beta} \left| e^{i(\mathbf{k}-\mathbf{k}') \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \right\rangle \right\rangle = - \left\langle \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_x} \left| e^{i(\mathbf{k}-\mathbf{k}') \cdot \hat{\mathbf{x}}} \left| u_{\mathbf{k}}^{\alpha} \right\rangle \right\rangle$$

于是便有

$$\begin{aligned}
&-i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_{\alpha}, E_{\beta} < E_F} \sum_{\mathbf{k}, \mathbf{k}'} \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| u_{\mathbf{k}'}^{\beta} \right\rangle \right\rangle \left\langle u_{\mathbf{k}'}^{\beta} \left| e^{i(\mathbf{k}-\mathbf{k}') \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \right\rangle \right\rangle \\
&= -i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_{\alpha}, E_{\beta} < E_F} \sum_{\mathbf{k}, \mathbf{k}'} \left\langle \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_x} \left| e^{i(\mathbf{k}-\mathbf{k}') \cdot \hat{\mathbf{x}}} \left| u_{\mathbf{k}}^{\beta} \right\rangle \right\rangle \left\langle u_{\mathbf{k}}^{\alpha} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}'}^{\beta}}{\partial k'_y} \right\rangle \right\rangle \\
&= -i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_{\alpha}, E_{\beta} < E_F} \sum_{\mathbf{k}, \mathbf{k}'} (\alpha \leftrightarrow \beta) (\mathbf{k} \leftrightarrow \mathbf{k}') \\
&= -i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_{\alpha}, E_{\beta} < E_F} \sum_{\mathbf{k}, \mathbf{k}'} \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \left| e^{i(\mathbf{k}'-\mathbf{k}) \cdot \hat{\mathbf{x}}} \left| u_{\mathbf{k}'}^{\beta} \right\rangle \right\rangle \left\langle u_{\mathbf{k}'}^{\beta} \left| e^{i(\mathbf{k}-\mathbf{k}') \cdot \hat{\mathbf{x}}} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \right\rangle \right\rangle
\end{aligned}$$

也就是说， σ_{xy} 的第二个求和项等于 0，从而

$$\begin{aligned}
\sigma_{xy} &= i \frac{e^2}{\hbar} \frac{1}{L_x L_y} \sum_{E_{\alpha} < E_F} \sum_{\mathbf{k}} \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \right\rangle \right\rangle \\
&= i \frac{e^2}{\hbar} \sum_{E_{\alpha} < E_F} \int \frac{d^2 k}{(2\pi)^2} \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \right\rangle - \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \right\rangle \right\rangle \\
&= -\frac{e^2}{2\pi\hbar} \sum_{E_{\alpha} < E_F} \int \frac{d^2 k}{2\pi} i \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \right\rangle - i \left\langle \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_y} \left| \frac{\partial u_{\mathbf{k}}^{\alpha}}{\partial k_x} \right\rangle \right\rangle \\
&= -\frac{e^2}{2\pi\hbar} \sum_{E_{\alpha} < E_F} \int \frac{d^2 k}{2\pi} \Omega_{k_x k_y}^{\alpha} \\
&= \frac{e^2}{2\pi\hbar} \sum_{E_{\alpha} < E_F} C_{\alpha}
\end{aligned}$$

在 TKNN 的原始论文中对加磁场后的朗道能级 subbands 进行了讨论，不过从这里可以看到，如果只是电导量子化，并不需要磁场。

3.3.2 双带模型

\mathbf{k} 可以成为哈密顿量的参数，双带模型对应这样一个哈密顿量：

$$\tilde{H}(\mathbf{k}) = E(\mathbf{k}) \cdot \boldsymbol{\sigma}$$

其中 $\boldsymbol{\sigma}$ 是泡利矩阵。双带模型可以方便看出陈数的意义。设矢量

$$\hat{n} = \frac{\mathbf{E}(\mathbf{k})}{E(\mathbf{k})}, \quad \tilde{H}(\mathbf{k}) = E(\mathbf{k})\sigma_n$$

能量本征值为

$$\tilde{H}(\mathbf{k})|n\rangle = E(\mathbf{k})|n\rangle, \quad \tilde{H}(\mathbf{k})|-n\rangle = -E(\mathbf{k})|-n\rangle$$

计算陈数

$$\begin{aligned} C &= - \int \frac{d^2k}{2\pi} i \left\langle \frac{\partial n}{\partial k_x} \middle| \frac{\partial n}{\partial k_y} \right\rangle - i \left\langle \frac{\partial n}{\partial k_y} \middle| \frac{\partial n}{\partial k_x} \right\rangle \\ &= - \int \frac{d^2k}{2\pi} i \left\langle \frac{\partial n}{\partial k_x} \middle| n \right\rangle \langle n | \frac{\partial n}{\partial k_y} \rangle - i \left\langle \frac{\partial n}{\partial k_y} \middle| n \right\rangle \langle n | \frac{\partial n}{\partial k_x} \rangle \\ &\quad - \int \frac{d^2k}{2\pi} i \left\langle \frac{\partial n}{\partial k_x} \middle| -n \right\rangle \langle -n | \frac{\partial n}{\partial k_y} \rangle - i \left\langle \frac{\partial n}{\partial k_y} \middle| -n \right\rangle \langle -n | \frac{\partial n}{\partial k_x} \rangle \\ &= - \int \frac{d^2k}{2\pi} i \left\langle \frac{\partial n}{\partial k_x} \middle| -n \right\rangle \langle -n | \frac{\partial n}{\partial k_y} \rangle - i \left\langle \frac{\partial n}{\partial k_y} \middle| -n \right\rangle \langle -n | \frac{\partial n}{\partial k_x} \rangle \end{aligned}$$

上式最后一个等号是因为 $\left\langle \frac{\partial n}{\partial k_x} \middle| n \right\rangle = - \langle n | \frac{\partial n}{\partial k_x} \rangle$ 。由于

$$\begin{aligned} |n\rangle = \sigma_n |n\rangle &\implies \left| \frac{\partial n}{\partial k_x} \right\rangle = \frac{\partial \sigma_n}{\partial k_x} |n\rangle + \sigma_n \left| \frac{\partial n}{\partial k_x} \right\rangle \implies (\mathbb{1} - \sigma_n) \left| \frac{\partial n}{\partial k_x} \right\rangle = \frac{\partial \sigma_n}{\partial k_x} |n\rangle \\ &\implies |-n\rangle \langle -n | \left| \frac{\partial n}{\partial k_x} \right\rangle = \frac{1 - \sigma_n}{2} \left| \frac{\partial n}{\partial k_x} \right\rangle = \frac{1}{2} \frac{\partial \sigma_n}{\partial k_x} |n\rangle \end{aligned}$$

同理

$$\begin{aligned} |-n\rangle \langle -n | \left| \frac{\partial n}{\partial k_y} \right\rangle &= \frac{1 - \sigma_n}{2} \left| \frac{\partial n}{\partial k_y} \right\rangle = \frac{1}{2} \frac{\partial \sigma_n}{\partial k_y} |n\rangle \\ \left\langle \frac{\partial n}{\partial k_y} \middle| -n \right\rangle \langle -n | &= \langle n | \frac{1}{2} \frac{\partial \sigma_n}{\partial k_y} \\ \left\langle \frac{\partial n}{\partial k_x} \middle| -n \right\rangle \langle -n | &= \langle n | \frac{1}{2} \frac{\partial \sigma_n}{\partial k_x} \end{aligned}$$

又因为 $|-n\rangle \langle -n|$ 是投影算符， $|-n\rangle \langle -n| = |-n\rangle \langle -n| |-n\rangle \langle -n|$ ，故此时

$$\begin{aligned} C &= -i \int \frac{d^2k}{8\pi} \langle n | \frac{\partial \sigma_n}{\partial k_x} \frac{\partial \sigma_n}{\partial k_y} |n\rangle - \langle n | \frac{\partial \sigma_n}{\partial k_y} \frac{\partial \sigma_n}{\partial k_x} |n\rangle \\ &= -i \int \frac{d^2k}{8\pi} \langle n | \frac{\partial \sigma_n}{\partial k_x} \frac{\partial \sigma_n}{\partial k_y} |n\rangle - \langle n | \frac{\partial \sigma_n}{\partial k_y} \frac{\partial \sigma_n}{\partial k_x} |n\rangle \\ &= -i \int \frac{d^2k}{8\pi} \langle n | \left(\frac{\partial \hat{n}}{\partial k_x} \cdot \boldsymbol{\sigma} \right) \left(\frac{\partial \hat{n}}{\partial k_y} \cdot \boldsymbol{\sigma} \right) |n\rangle - \langle n | \left(\frac{\partial \hat{n}}{\partial k_y} \cdot \boldsymbol{\sigma} \right) \left(\frac{\partial \hat{n}}{\partial k_x} \cdot \boldsymbol{\sigma} \right) |n\rangle \\ &= -i \int \frac{d^2k}{8\pi} \langle n | \left(\frac{\partial \hat{n}}{\partial k_x} \cdot \frac{\partial \hat{n}}{\partial k_y} \right) |n\rangle - i \langle n | \left(\frac{\partial \hat{n}}{\partial k_y} \cdot \frac{\partial \hat{n}}{\partial k_x} \right) |n\rangle \\ &\quad - i \int \frac{d^2k}{8\pi} i \langle n | \left(\frac{\partial \hat{n}}{\partial k_x} \times \frac{\partial \hat{n}}{\partial k_y} \right) \cdot \boldsymbol{\sigma} |n\rangle - \langle n | \left(\frac{\partial \hat{n}}{\partial k_y} \times \frac{\partial \hat{n}}{\partial k_x} \right) \cdot \boldsymbol{\sigma} |n\rangle \end{aligned}$$

上式第一项显然为 0，而第二项，由于 \hat{n} 是单位球面上的法相矢量， k_x, k_y 是其参数，故 $\frac{\partial \hat{n}}{\partial k_x}, \frac{\partial \hat{n}}{\partial k_y}$ 是球面上的切矢。从而 $\left(\frac{\partial \hat{n}}{\partial k_y} \times \frac{\partial \hat{n}}{\partial k_x}\right)$ 应当平行于 \hat{n} ，故有

$$\begin{aligned} C &= \int \frac{d^2 k}{4\pi} \langle n | \left(\frac{\partial \hat{n}}{\partial k_x} \times \frac{\partial \hat{n}}{\partial k_y} \right) \cdot \sigma | n \rangle = \int \frac{d^2 k}{4\pi} \hat{n} \cdot \left(\frac{\partial \hat{n}}{\partial k_x} \times \frac{\partial \hat{n}}{\partial k_y} \right) \langle n | \sigma_n | n \rangle \\ &= \int \frac{d^2 k}{4\pi} \hat{n} \cdot \left(\frac{\partial \hat{n}}{\partial k_x} \times \frac{\partial \hat{n}}{\partial k_y} \right) \end{aligned}$$

不难看出这个公式的意义， k_x, k_y 是单位矢量 \hat{n} 的参数， C 就是 \mathbf{k} 在其范围内取值时， \hat{n} 对应的面积相对于单位球面积的倍数。

3.4 反常速度的观点

前面关于贝利曲率的讨论出发点是哈密顿量的周期性演化，其实也可以考虑非周期性演化，环路积分变为面积分，可以看到此时也会有贝利曲率的出现。

3.4.1 平行输运

还是考虑含时哈密顿量

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

将波矢展开为

$$|\psi(t)\rangle = \sum_n \exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' E_n(t')\right) a_n(t) |n(t)\rangle,$$

代入演化方程，得

$$\dot{a}_n(t) = - \sum_l a_l(t) \left\langle n(t) \left| \frac{\partial}{\partial t} \right| l(t) \right\rangle \times \exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' [E_l(t') - E_n(t')]\right)$$

态矢相位的选择存在自由度，引入平行输运条件：

$$\left\langle n(t) \left| \frac{\partial}{\partial t} \right| n(t) \right\rangle = \dot{\mathbf{R}}(t) \left\langle n(t) \left| \frac{\partial}{\partial \mathbf{R}} \right| n(t) \right\rangle = 0 \implies \mathbf{A}_n(\mathbf{R}) = 0$$

也就是说对于任意选定的 $|n(\mathbf{R})\rangle$ ，作规范变换 $e^{i\zeta(\mathbf{R}(t))}$ 使得

$$\mathbf{A}_n(\mathbf{R}) \rightarrow \mathbf{A}_n(\mathbf{R}) - \frac{\partial}{\partial \mathbf{R}} \zeta(\mathbf{R}) = 0$$

$$\gamma_n \rightarrow \gamma_n - \zeta(\mathbf{R}(T)) + \zeta(\mathbf{R}(0)) = 0$$

在 3.1 中由于是周期性演化，故 $\zeta(\mathbf{R}(t))$ 有单值性限制，而此时考虑非周期演化，故上述要求是总可以满足的。

假设开始时系统处于 $|n\rangle$ 态，则作为 0 阶近似， $a_m^{(0)} = \delta_{mn}$ 。考虑一阶近似：

$$\begin{aligned} \dot{a}_m^{(1)}(t) &= - \sum_l a_l^{(0)}(t) \left\langle m(t) \left| \frac{\partial}{\partial t} \right| l(t) \right\rangle \times \exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' [E_l(t') - E_m(t')]\right) \\ &= - \left\langle m(t) \left| \frac{\partial}{\partial t} \right| n(t) \right\rangle \times \exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' [E_n(t') - E_m(t')]\right) \end{aligned}$$

由平行输运条件可得 $a_n = 1$ 。而 $n' \neq n$ 时

$$\frac{\partial}{\partial t} a_{n'} = - \left\langle n'(t) \left| \frac{\partial}{\partial t} \right| n(t) \right\rangle \exp\left(-\frac{i}{\hbar} \int_{t_0}^t dt' [E_n(t') - E_{n'}(t')]\right)$$

假设参数变化极其缓慢, 则上式指数项的系数变化要比指数项变化慢很多, 在所考察时间范围内可近似视为常数, 故由 $a_{n'}(0) = 0$ 可积分

$$a_{n'} = -\frac{\langle \tilde{n}' | \partial / \partial t | \tilde{n} \rangle}{E_n - E_{n'}} i\hbar \times \exp \left(-\frac{i}{\hbar} \int_{t_0}^t dt' [E_n(t') - E_{n'}(t')] \right)$$

从而波矢的一阶近似为

$$|\psi(t)\rangle = \exp \left(-\frac{i}{\hbar} \int_{t_0}^t dt' E_n(t') \right) \times \left\{ |\tilde{n}\rangle - i\hbar \sum_{n \neq n'} |\tilde{n}'\rangle \frac{\langle \tilde{n}' | \partial / \partial t | \tilde{n} \rangle}{E_n - E_{n'}} \right\}$$

3.4.2 反常速度

考虑哈密顿量

$$H = \frac{(\hat{\mathbf{p}} + e\mathbf{A}(t))^2}{2m}$$

其中 $\mathbf{A}(t) = \mathbf{E}t$ 为匀强场。可以验证这样的 \mathbf{A} 是满足麦克斯韦方程的。由于匀强, 故可以保持平移对称性:

$$H(\mathbf{k}, t) = \frac{(\hbar\mathbf{k} + e\mathbf{A}(t))^2}{2m} = \frac{\hbar^2 \mathbf{q}^2}{2m}, \quad \mathbf{q} = \mathbf{k} + \frac{e}{\hbar} \mathbf{E}t, \quad \frac{\partial q_j}{\partial t} = \frac{e}{\hbar} E_j$$

由 3.3 可知

$$\langle \hat{\mathbf{x}} \rangle(t) = \left\langle u_{\mathbf{k}}(t) \left| \frac{\partial H(\mathbf{k}, t)}{\hbar \partial \mathbf{k}} \right| u_{\mathbf{k}}(t) \right\rangle$$

代入上小结中的波矢的一阶近似, 保留到一阶, 可得速度 j 分量为

$$v_{jn}(\mathbf{k}, t) = \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \sum_{n' \neq n} \left\{ \frac{\langle u_n | \partial H / \partial k_j | u_{n'} \rangle \langle u_{n'} | \partial u_n / \partial t \rangle - \langle u_{n'} | \partial H / \partial k_j | u_n \rangle \langle \partial u_n / \partial t | u_{n'} \rangle}{\varepsilon_n - \varepsilon_{n'}} \right\}$$

而与之类似有

$$\begin{aligned} \langle u_n | \partial H / \partial k_j | u_{n'} \rangle &= (\varepsilon_{n'} - \varepsilon_n) \left\langle u_n \left| \frac{\partial}{\partial k_j} u_{n'} \right. \right\rangle = (\varepsilon_n - \varepsilon_{n'}) \left\langle \frac{\partial}{\partial k_j} u_n | u_{n'} \right\rangle \\ \langle u_{n'} | \partial H / \partial k_j | u_n \rangle &= (\varepsilon_n - \varepsilon_{n'}) \left\langle u_{n'} \left| \frac{\partial}{\partial k_j} u_n \right. \right\rangle \end{aligned}$$

代入前式

$$\begin{aligned} v_{jn}(\mathbf{k}, t) &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \sum_{n' \neq n} \left\{ \left\langle \frac{\partial}{\partial k_j} u_n | u_{n'} \right\rangle \left\langle u_{n'} \left| \frac{\partial}{\partial t} u_n \right. \right\rangle - \left\langle \frac{\partial}{\partial t} u_n | u_{n'} \right\rangle \left\langle u_{n'} \left| \frac{\partial}{\partial k_j} u_n \right. \right\rangle \right\} \\ &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \sum_{n'} \left\{ \left\langle \frac{\partial}{\partial k_j} u_n | u_{n'} \right\rangle \left\langle u_{n'} \left| \frac{\partial}{\partial t} u_n \right. \right\rangle - \left\langle \frac{\partial}{\partial t} u_n | u_{n'} \right\rangle \left\langle u_{n'} \left| \frac{\partial}{\partial k_j} u_n \right. \right\rangle \right\} \\ &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \left\{ \left\langle \frac{\partial}{\partial k_j} u_n \left| \frac{\partial}{\partial t} u_n \right. \right\rangle - \left\langle \frac{\partial}{\partial t} u_n \left| \frac{\partial}{\partial k_j} u_n \right. \right\rangle \right\} \end{aligned}$$

由于

$$\frac{\partial}{\partial q_j} = \frac{\partial}{\partial k_j}, \quad \frac{\partial}{\partial t} = \sum_j \frac{\partial q_l}{\partial t} \frac{\partial}{\partial q_l}$$

$$\begin{aligned}
v_{jn}(\mathbf{k}, t) &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \frac{e}{\hbar} \sum_l E_l \left\{ \left\langle \frac{\partial}{\partial k_j} u_n \right| \frac{\partial}{\partial k_l} u_n \right\rangle - \left\langle \frac{\partial}{\partial k_l} u_n \right| \frac{\partial}{\partial k_j} u_n \right\rangle \right\} \\
&= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - i \frac{e}{\hbar} \sum_l E_l \left\{ \frac{\partial}{\partial k_j} \left\langle u_n \right| \frac{\partial}{\partial k_l} u_n \right\rangle - \frac{\partial}{\partial k_l} \left\langle u_n \right| \frac{\partial}{\partial k_j} u_n \right\rangle \right\} \\
&= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - \frac{e}{\hbar} \sum_l E_l \left\{ \frac{\partial}{\partial k_j} A_l^n - \frac{\partial}{\partial k_l} A_j^n \right\} \\
&= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial k_j} - \frac{e}{\hbar} (\nabla_{\mathbf{k}} (\mathbf{E} \cdot \mathbf{A}^n))_j + \frac{e}{\hbar} (\mathbf{E} \cdot \nabla_{\mathbf{k}}) A_j^n \\
\Rightarrow v_n(\mathbf{k}, t) &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial \mathbf{k}} - \frac{e}{\hbar} \{ \nabla_{\mathbf{k}} (\mathbf{E} \cdot \mathbf{A}^n) - (\mathbf{E} \cdot \nabla_{\mathbf{k}}) \mathbf{A}^n \} = \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial \mathbf{k}} - \frac{e}{\hbar} \mathbf{E} \times (\nabla_{\mathbf{k}} \times \mathbf{A}^n) \\
v_n(\mathbf{k}, t) &= \frac{\partial \varepsilon_n(\mathbf{k}, t)}{\hbar \partial \mathbf{k}} - \frac{e}{\hbar} \mathbf{E} \times \boldsymbol{\Omega}^n
\end{aligned}$$

上式最后一项即为反常速度。容易看出 y 方向电场对 x 方向速度贡献以及满带的电流元响应为

$$\Delta v_{xn} = -\frac{e}{\hbar} E_y \Omega_{k_x k_y}^n \Rightarrow \Delta J_{I_x} = \sum_{\mathbf{k}} e \Delta v_{xn} = \sum_{\mathbf{k}} -\frac{e^2}{\hbar} E_y \Omega_{k_x k_y}^n$$

于是得到电导

$$\sigma_{xy} = -\frac{e^2}{\hbar} \int \frac{d^2 k}{(2\pi)^2} \Omega_{k_x k_y}^n = \frac{e^2}{2\pi \hbar} C^n$$

反常速度的观点和 Kubo 公式类似，都是 y 方向的电场对 x 方向的电流的影响，不过在 Kubo 公式中用到的是时谐场 $\mathbf{A}(\hat{\mathbf{x}}, t) = \mathbf{A} e^{i(\mathbf{k} \cdot \mathbf{x} - kct)}$ ，在反常速度中用到的是均匀场 $\mathbf{A}(t) = \mathbf{E}t$ 。

3.5 量子自旋与量子反常霍尔效应简介

3.5.1 能带反转与边缘流

考虑如下参数的双带模型：

$$\begin{aligned}
H(\mathbf{k}) &= \sum_a d_a(\mathbf{k}) \sigma^a \\
\mathbf{d}(\mathbf{k}) &= (Ak_x, -Ak_y, \mathbb{M}(\mathbf{k})), \quad \mathbb{M}(\mathbf{k}) = M + B(k_x^2 + k_y^2)
\end{aligned}$$

由于陈数为

$$C = \int \frac{d^2 k}{4\pi} \hat{\mathbf{d}} \cdot \left(\frac{\partial \hat{\mathbf{d}}}{\partial k_x} \times \frac{\partial \hat{\mathbf{d}}}{\partial k_y} \right)$$

考虑连续模型，即假设晶格常数 $a \rightarrow 0$ ，则二维布里渊区为无穷大平面。容易看出 $|\mathbf{k}|$ 很大时， $\hat{\mathbf{d}} = \text{sign}(B)\hat{\mathbf{z}}$ ，故此时不会扫过球面面积，也就是说 $|\mathbf{k}|$ 很大对陈数计算没有贡献。对陈数有贡献的计及有限大区域即可，即上式积分是有意义的。

由于 $\mathbf{k} = 0$ 时， $\hat{\mathbf{d}} = \text{sign}(M)\hat{\mathbf{z}}$ ，故可以看出当 $M/B > 0$ 时， \mathbf{k} 在布里渊区取值扫过 0 个球面， $M/B < 0$ 时， \mathbf{k} 在布里渊区取值扫过 1 个球面。假定 $B > 0$ ，那么 M 的正负决定了非零量子化霍尔电导是否存在。

$\mathbf{k} = 0$ 时，显然能隙为 $2M$ ，故 M 从正到负变化对应能带的反转，大致图像如下所示：

第 3 张图中的虚线对应着边缘流。

考虑一个半无情大体系 $x > 0$ ，在 y 方向上设置周期性边界，则

$$H(\mathbf{k}) = H(-i\partial_x, k_y)$$

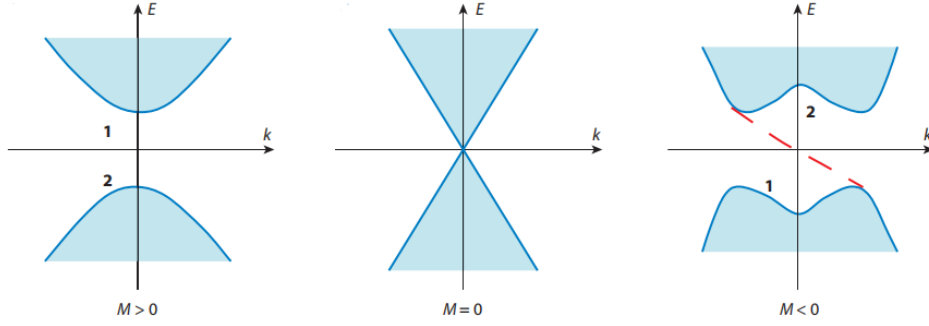


图 6: 能带反转

寻找 $k_y = 0, E = 0$ 的解, 则此时方程写为

$$[-iA\partial_x\sigma_x + (M - B\partial_x^2)\sigma_z]\psi = 0 \implies [A\partial_x\sigma_y + (M - B\partial_x^2)]\psi = 0$$

设 $\psi = C_+e^{\lambda_+x}\eta_+ + C_-e^{\lambda_-x}\eta_-$, 其中 $\sigma_y\eta_{\pm} = \pm\eta_{\pm}$, 则方程变为

$$\begin{cases} (M - B\lambda_+^2) + A\lambda_+ = 0 \\ (M - B\lambda_-^2) - A\lambda_- = 0 \end{cases} \implies \begin{cases} \lambda_+ = \frac{A \pm \sqrt{A^2 + 4BM}}{2B} \\ \lambda_- = \frac{-A \pm \sqrt{A^2 + 4BM}}{2B} \end{cases}$$

记 $\lambda_{1,2} = \frac{A \pm \sqrt{A^2 + 4BM}}{2B}$, 则解可以写为

$$\psi(x) = (c_{+1}e^{\lambda_1x} + c_{+2}e^{\lambda_2x})\eta_+ + (c_{-1}e^{-\lambda_1x} + c_{-2}e^{-\lambda_2x})\eta_-$$

体系只分布在 $x > 0$ 的区域, 由波函数连续条件, $\psi(0) = 0$, 故

$$c_{+1} + c_{+2} = 0, \quad c_{-1} + c_{-2} = 0$$

$$\psi(x) = c_{+1}(e^{\lambda_1x} - e^{\lambda_2x})\eta_+ + c_{-1}(e^{-\lambda_1x} - e^{-\lambda_2x})\eta_-$$

假设 $\lambda_{1,2}$ 一正一负, 则当 $x \rightarrow \infty$ 时, η_{\pm} 的系数均发散, 故若态存在, 必要条件是 $\lambda_1\lambda_2 > 0$, 即

$$-\frac{M}{B} > 0$$

也就是上小结非零陈数的条件。

3.5.2 磁性掺杂

目前已经看到能带反转的双带模型即可产生量子化电导, 不需要磁场, 这可以作为实现量子反常霍尔效应 (即无外磁场的整数量子霍尔效应) 的一个思路。

在现实中, 确实可以有材料通过强 SOC 作用实现能带反转。但注意到电子有自旋, 是费米子, 在时间反演对称下会有 Kramers 简并。也就是说在能带反转且满足时间反演对称的体系中, 两个自旋分量的电子各自会形成量子反常霍尔态, 但由于两个反向自旋贡献的边缘流是反向的 (时间反演), 故整体不表现出电流, 即量子自旋霍尔效应。

量子自旋霍尔效应可以通过输运实验来验证。由于一个导电通道会贡献 $\frac{e^2}{h}$ 的电导（见散射与输运小结），材料处于量子自旋霍尔态时会表现出 $\frac{2e^2}{h}$ 的电导，且应当与材料宽度无关。这会区别于与材料宽度有关的弹道输运电导。

如何在不加外磁场的情况下实现整数量子霍尔效应？一个自然的想法是先实现量子自旋霍尔效应，然后用磁性杂质破坏其中一种自旋对应的反常霍尔态，从而宏观上出现边缘流，实现量子反常霍尔效应。