本次课内容在 Mahan 多体物理 3.8 节

计算输运问题
- ① Drude 公式（经典，缺乏统计）
- ② 玻尔兹曼方程（半经典）
- ③ Kubo（久保）公式 → 线性输运

可以看作线性响应的条件
- ① 外场强度不大
- ② 空间变化不大 → 统计上宏观小，微观大
- ③ 频率不大

线性响应需要外场
- 加磁场（测磁矩）
- 加温度场（测能流）
- 加压力场（测电极化，杨氏模量）
- 加电场（测电导率）
- 加光场（光吸收）

在线性响应条件下，电流

$$J_\alpha(\vec r,t)=\sum_\beta\int d\vec r'\int_{-\infty}^{t}dt'\,\sigma_{\alpha\beta}(\vec r-\vec r',t-t')\,E_\beta(\vec r',t') \qquad ①$$

E_β 指系统总电场的 β 分量，$\beta=x,y,z$。

设外加电场的形式为

$$\vec E(\vec r,t)=\vec\Xi\, e^{i\vec k\cdot\vec r-i\omega t} \qquad ②$$

一般情况下，总电场并不等于外加场，但我们忽略这些微小的差异，

则把②代入①，得

$$J_\alpha(\vec r,t)=\sum_\beta \Xi_\beta\int d\vec r'\int_{-\infty}^{t}dt'\,\sigma_{\alpha\beta}(\vec r-\vec r',t-t')\,e^{i\vec k\cdot\vec r'-i\omega t'}$$

$$=\sum_\beta \Xi_\beta\left[\int d\vec r'\int_{-\infty}^{t}dt'\,\sigma_{\alpha\beta}(\vec r-\vec r',t-t')\,e^{i\vec k\cdot(\vec r'-\vec r)-i\omega(t'-t)}\right]e^{i\vec k\cdot\vec r-}$$

$$=\sum_\beta \Xi_\beta\,\sigma_{\alpha\beta}(-\vec k,\omega)\,e^{i\vec k\cdot\vec r-i\omega t}$$

电流的表达式

$$J_\alpha(\vec{r}) = e\langle \sum_i \hat{v}_{i\alpha}\delta(\vec{r}-\vec{r}_i)\rangle \qquad ①$$

速度算符 $\hat{\vec{v}} = \frac{\partial \vec{r}}{\partial t} = \frac{1}{i\hbar}[\vec{r}, \hat{H}]$

哈密顿量 $\hat{H} = \frac{1}{2m}(\vec{p} - \frac{e}{c}\vec{A}(\vec{r}))^2$

由于 $[\vec{r}, f(\hat{\vec{p}})] = i\hbar \frac{\partial f(\vec{p})}{\partial \vec{p}}$，因此

$$\hat{v} = \frac{1}{m}[\vec{p} - \frac{e}{c}\vec{A}(\vec{r})]$$

代入①，得

$$J_\alpha(\vec{r}) = \frac{e}{m}\langle \sum_i \hat{P}_{i\alpha}\delta(\vec{r}-\vec{r}_i)\rangle - \frac{e}{mc}\langle \sum_i A_{i\alpha}(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\rangle$$

$$= J_\alpha^{(2)}(\vec{r}) + J_\alpha^{(1)}(\vec{r})$$

$$J_\alpha^{(1)}(\vec{r}) = -\frac{e}{mc}\langle \int \psi^+(\vec{r}_i)A_{i\alpha}(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)\,d\vec{r}_i\rangle$$

$$= -\frac{e}{mc}\langle A_{i\alpha}(\vec{r})\psi^+(\vec{r})\psi(r)\rangle$$

$$= -\frac{e}{mc}A_{i\alpha}(\vec{r})\langle \psi^+(\vec{r})\psi(r)\rangle$$

$$= -\frac{en_0}{mc}A_{i\alpha}(\vec{r})$$

由于 $\frac{1}{c}A_\alpha = \frac{-i}{\omega}E_\alpha$（电动力学）

$$J_\alpha^{(1)}(\vec{r}) = i\frac{en_0}{m\omega}E_\alpha(\vec{r})$$

定义流算符

$$\hat{j}_\alpha(\vec{r}) = \frac{1}{2m}e\sum_i[\hat{P}_{i\alpha}\delta(\vec{r}-\vec{r}_i) + \delta(\vec{r}-\vec{r}_i)\hat{P}_{i\alpha}] \xrightarrow{\text{作出}} \text{二次量子化}$$

$$J_\alpha^{(2)}(\vec{r}) = \langle \hat{j}_\alpha(\vec{r}) \rangle$$

在前面我们已提到，对于物理可观测量

$$\langle B(t) \rangle = Tr(\rho \hat{B})$$

$$= B_0 - \frac{i}{\hbar} \int_{-\infty}^{t} \langle\langle [\hat{B}(t), H_I'(t')] \rangle\rangle_0 \, dt'$$

在这里

$$H'(t) = \sum_\beta -\frac{1}{c} \int d\vec{r} \, \hat{j}_\beta(\vec{r}) A_\beta(\vec{r}, t)$$

$$A_\beta(\vec{r}, t) = A_\beta e^{i\vec{q}\cdot\vec{r} - i\omega t}$$

则 $$H'(t) = \sum_\beta -\frac{1}{c} \int d\vec{r} \, \hat{j}_\beta(\vec{r}) A_\beta e^{i\vec{q}\cdot\vec{r} - i\omega t}$$

$$= \sum_\beta -\frac{1}{c} \hat{j}_\beta(-\vec{q}) A_\beta e^{-i\omega t}$$

$$= \frac{i}{\omega} \sum_\beta E_\beta(\vec{r}, t) e^{-i\vec{q}\cdot\vec{r}} \hat{j}_\beta(-\vec{q})$$

由于加外场前是没有电流的，所以 $\hat{J}_0 = 0$

则 $$J_\alpha^{(2)}(\vec{r}, t) = \langle \hat{j}_\alpha(\vec{r}, t) \rangle = -\frac{i}{\hbar} \int_{-\infty}^{t} \langle\langle [\hat{J}_\alpha(\vec{r}, t), H_I'(t')] \rangle\rangle_0$$

$$= \frac{1}{\hbar\omega} \sum_\beta \int_{-\infty}^{t} E_\beta(\vec{r}, t') e^{-i\vec{q}\cdot\vec{r}} \langle\langle [\hat{j}_\alpha(\vec{r}, t), \hat{j}_\beta(-\vec{q}, t')] \rangle\rangle_0$$

$$= \frac{1}{\hbar\omega} \sum_\beta E_\beta(\vec{r}, t) e^{-i\vec{q}\cdot\vec{r}} \int_{-\infty}^{t} e^{i\omega(t-t')} \langle\langle [\hat{j}_\alpha(\vec{r}, t), \hat{j}_\beta(-\vec{q}, t')] \rangle\rangle_0$$

由于 $$J_\alpha(\vec{r}, t) = \sum_\beta E_\beta(\vec{r}, t) \sigma_{\alpha\beta}(\vec{q}, \omega)$$

则

$$G_{\alpha\beta}(-\vec{q},w)=\frac{1}{\hbar w}e^{-i\vec{q}\cdot\vec{r}}\int_{-\infty}^{t}e^{iw(t-t')}\langle\langle[\hat{j}_\alpha(\vec{r},t),\hat{j}_\beta(-\vec{q},t')]\rangle\rangle_0\,dt'$$

最后一步，对空间作平均

$$\frac{1}{V}\int G_{\alpha\beta}(-\vec{q},w)\,d\vec{r}=\frac{1}{V}\int d\vec{r}\,\frac{1}{\hbar w}e^{-i\vec{q}\cdot\vec{r}}\int_{-\infty}^{t}e^{iw(t-t')}\langle\langle[\hat{j}_\alpha(\vec{r},t),\hat{j}_\beta(-\vec{q},t')]\rangle\rangle_0\,dt'$$

$$G_{\alpha\beta}(-\vec{q},w)=\frac{1}{\hbar w}\int_{-\infty}^{t}e^{iw(t-t')}\langle\langle[j_\alpha(\vec{q},t),j_\beta(-\vec{q},t')]\rangle\rangle_0\,dt'$$

作业：二次量子化流算符

$$\vec{j}(\vec{r})=\frac{1}{2m}e\sum_i[\hat{P}_i\delta(\vec{r}-\vec{r}_i)+\delta(\vec{r}-\vec{r}_i)\hat{P}_i]$$

$$\vec{j}(\vec{r})=\frac{e}{2m}\int\psi^+(\vec{r}_i)[\hat{P}_i\delta(\vec{r}-\vec{r}_i)+\delta(\vec{r}-\vec{r}_i)\hat{P}_i]\psi(\vec{r}_i)\,d\vec{r}_i$$

$$=\frac{e}{2m}\int\psi^+(\vec{r}_i)\hat{P}_i[\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)]\,d\vec{r}_i+\frac{e}{2m}\int\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\hat{P}_i\psi(\vec{r}_i)\,d\vec{r}_i$$

$$=\frac{e}{2m}\int\hat{P}_i[\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)]-\hat{P}_i[\psi^+(\vec{r}_i)]\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)\,d\vec{r}_i$$

$$+\frac{e}{2m}\int\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\hat{P}_i\psi(\vec{r}_i)\,d\vec{r}_i$$

第一项 $-i\hbar\int\frac{\partial}{\partial\vec{r}_i}[\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)]\,d\vec{r}_i=-i\hbar[\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)]\Big|_{-\infty}^{+\infty}$

$$=0$$

因此

$$\vec{j}(\vec{r})=\frac{e}{2m}i\hbar\int\left(\frac{\partial}{\partial\vec{r}_i}\psi^+(\vec{r}_i)\right)\delta(\vec{r}-\vec{r}_i)\psi(\vec{r}_i)-\psi^+(\vec{r}_i)\delta(\vec{r}-\vec{r}_i)\left(\frac{\partial}{\partial\vec{r}_i}\psi(\vec{r}_i)\right)d\vec{r}_i$$

$$=\frac{i\hbar e}{2m}\left[\frac{\partial\psi^+(r)}{\partial r}\psi(r)-\psi^+(r)\frac{\partial\psi(r)}{\partial r}\right]$$

由于 $\psi(\vec{r})=\frac{1}{\sqrt{V}}\sum_{k}a_k e^{i\vec{k}\cdot\vec{r}}$ $\quad\psi^{+}(\vec{r})=\frac{1}{\sqrt{V}}\sum_{k}a_k^{+} e^{-i\vec{k}\cdot\vec{r}}$

则

$$\vec{J}(\vec{r})=\frac{i\hbar e}{2m}\frac{1}{V}\sum_{k,k'}\left[-i\vec{k}'a_{k'}^{+}a_k e^{i(\vec{k}-\vec{k}')\cdot r}-i\vec{k}a_{k'}^{+}a_k e^{i(\vec{k}-\vec{k}')\cdot r}\right]$$

$$=\frac{\hbar e}{2m}\frac{1}{V}\sum_{k,k'}(\vec{k}'+\vec{k})a_{k'}^{+}a_k e^{i(\vec{k}-\vec{k}')\cdot r}$$

$$=\frac{1}{V}\sum_{q}\vec{J}(\vec{q})e^{i\vec{q}\cdot\vec{r}}\qquad(\vec{k}-\vec{k}'=\vec{q})$$