线性响应 （凝聚态系统）

一般情况很难，但当激发较小，可以准确计算

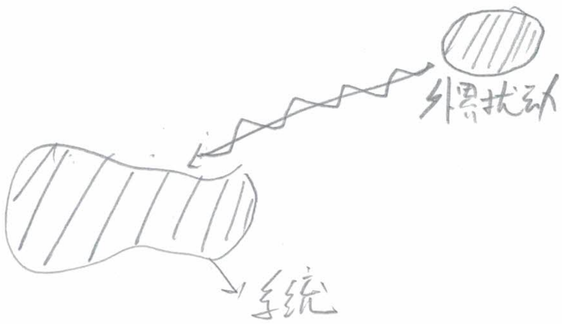
从密度矩阵出发（量子统计）

$$\hat{\rho} = |\psi\rangle\langle\psi|$$

$$i\frac{\partial\hat{\rho}}{\partial t} = [\hat{H}, \hat{\rho}]$$

$\hat{H}$ → 体系的Hamiltonian

多电子系： $\sum_i \frac{\hat{p}_i^2}{2m} + V(\vec{r}_i)$



$$\hat{H} = \hat{H}_0 + \hat{H}'$$

$\hat{H}'$ → 驱动项

由外界系统导致

① 零温密度矩阵

$\hat{\rho} = |\psi(t)\rangle\langle\psi(t)|$ ，Schrödinger表象中

② 有限温

$\psi_1(t)$ $\psi_2(t)$ $\psi_3(t)$ …… $\psi_N(t)$

由 $e^{-\frac{\hbar\omega}{k_B T}}$ 分布

$$\hat{\rho} = \sum_i P_i |\psi_i\rangle\langle\psi_i|$$

作业：利用Schrödinger方程推出该式

求大学量（物理可观测量）

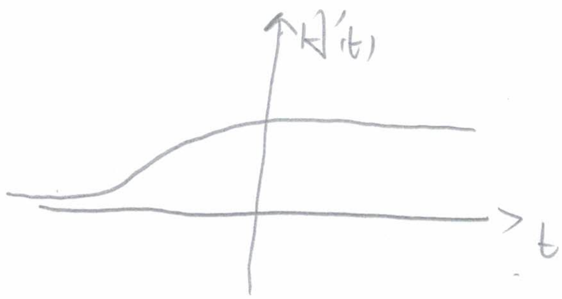
$$\bar{F} = tr(\hat{\rho}(t)\hat{F})$$

① 零温：$\langle\psi|\hat{F}|\psi\rangle = tr(|\psi\rangle\langle\psi|\hat{F})$

② 有限温：$\bar{F} = \sum_i P_i \langle\psi_i|\hat{F}|\psi_i\rangle = tr(P_i|\psi_i\rangle\langle\psi_i|\hat{F})$

$\boxed{\text{在 } H' \ll H_0 \text{ 时，} H' \text{ 对体系做一个扰动}}$

$H'(t)$ 绝热引入：$t \to -\infty$，$H'(t) = 0$



无限缓慢引入扰动 H'

$t \to -\infty$ 时，体系处于平衡态

$$\boxed{\hat{\rho}(-\infty) = \frac{e^{-\beta\hat{H}_0}}{Z} = \hat{\rho}_0}$$

作业：证明对自由 $\begin{cases}\text{电子}\\\text{玻色}\end{cases}$ 气，成立

证明 $tr(\hat{\rho}\hat{n}_i) = f_i$

由 $\hat{H}_0 = \sum_i \varepsilon_i |\psi_i\rangle\langle\psi_i|$

$$\frac{e^{-\beta\sum_i \varepsilon_i|\psi_i\rangle\langle\psi_i|}}{Z} = \sum_i e^{-\beta\varepsilon_i}|\psi_i\rangle\langle\psi_i|$$

$$Z = tr(e^{-\beta\hat{H}_0})$$

用相互作用表象处理

$$\hat{\rho}_I(t) = e^{i\hat{H}_0 t}\,\hat{\rho}(t)\,e^{-i\hat{H}_0 t}$$

$$\hat{A}_I(t) = e^{i\hat{H}_0 t}\,\hat{A}\,e^{-i\hat{H}_0 t}$$

$$\Rightarrow i\,\frac{\partial \hat{\rho}_I(t)}{\partial t} = [H_I'(t), \hat{\rho}_I(t)]$$

作微扰解：（级数解）

$$\rho_I(t) = \rho_I(-\infty) - i\int_{-\infty}^{t} d\tau\,[H_I'(\tau), \rho_I(\tau)]$$

$$= \rho_0(0) + \frac{1}{i}\int_{-\infty}^{t} d\tau\,[H_I'(t), \rho_0]$$

$$+ \left(\frac{1}{i}\right)^2 \int_{-\infty}^{t} d\tau_1 \int_{-\infty}^{\tau_1} d\tau_2\,[H_I'(\tau_1), [H_I'(\tau_2), \rho_0]]$$

$$+ \cdots\cdots$$

线性响应（只保留一阶项）

$$\underline{\rho_I(t) \approx \rho_0 + \frac{1}{i}\int_{-\infty}^{t} d\tau\,[H_I'(t), \rho_0]}$$

力学量： $\bar{F} = tr(\hat{\rho}(t)\hat{F}) = \langle\langle \hat{F} \rangle\rangle$ （统计平均）

$$= tr\left(e^{-iH_0 t}\hat{\rho}_I(t)e^{iH_0 t}\hat{F}\right)$$

$$= tr\left(\hat{\rho}_I(t)\,\underline{e^{iH_0 t}\hat{F}e^{-iH_0 t}}\right)$$

$$= tr\left(\hat{\rho}_I(t)\,\hat{F}_I(t)\right)$$

$$\bar F = \langle\langle \hat F \rangle\rangle$$

$$= tr(\hat\rho_I(t)\hat F_I(t))$$

$$= tr(\hat\rho_0 \hat F_I(t)) + \frac{1}{i}\int_{-\infty}^{t} d\tau\, tr([\hat H_I'(\tau), \hat\rho_0]\hat F_I(t))$$

其中 $tr(\hat H_I'(\tau)\hat\rho_0 \hat F_I(t) - \hat\rho_0 \hat H_I'(\tau)\hat F_I(t))$

$$= tr(\hat\rho_0(\hat F_I(t)\hat H_I'(\tau) - \hat H_I'(\tau)\hat F_I(t)))$$

$$= tr(\hat\rho_0[\hat F_I(t), \hat H_I'(\tau)])$$

$$\Rightarrow \bar F = tr(\hat\rho_0 \hat F_I(t)) + \frac{1}{i}\int_{-\infty}^{t} d\tau\, tr(\hat\rho_0[\hat F_I(t), \hat H_I'(\tau)])$$

例子：电子的自旋密度响应

（外加一个含时小磁场）

$$\hat S(\vec r) = \boxed{\frac{1}{2}\sum_i \hat\sigma_i\, \delta(\vec r - \vec r_i)}$$ → 作业：二次量子化

自旋密度

磁矩密度：$\hat m(\vec r) = \gamma\hbar \hat S(\vec r)$

动量空间:

$$\hat{S}(\vec{r}) = \int \frac{d\vec{q}}{(2\pi)^3}\, \hat{S}(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}$$

$$\hat{S}(\vec{q}) = \sum_i \frac{1}{2} \hat{\sigma}_i\, e^{i\vec{q}\cdot\vec{r}_i}$$

$$\hat{S}(\vec{q}) = \int d\vec{r}\, \hat{\Psi}^{\dagger}(\vec{r})\, \frac{1}{2}\vec{\sigma}\, e^{-i\vec{q}\cdot\vec{r}}\, \hat{\Psi}(\vec{r})$$

$$\hat{\Psi}(\vec{r}) = \frac{1}{\sqrt{V}} \sum_{k,\sigma} \hat{a}_{k,\sigma}\, e^{i\vec{k}\cdot\vec{r}}\, \chi_\sigma$$

$$\hat{S}(\vec{q}) = \sum_{k} \frac{1}{2} \sigma_{\alpha\beta}\, \hat{a}^{\dagger}_{\vec{k}+\vec{q},\alpha}\, \hat{a}_{\vec{k},\beta}$$

$$H' = -\int d\vec{r}\, \underset{\text{Zeeman coupling}}{\vec{m}(\vec{r})} \cdot \underbrace{\vec{H}(\vec{r},t)}_{\text{外加磁场}}$$

$$M_i(\vec{r},t) = \langle \underbrace{\rho_0\, m_i(\vec{r},t)}_{\text{无磁化, } 0} \rangle + \frac{1}{i}\int_{-\infty}^{t} tr\left(\rho_0 [m_i^I(t), H_I'(\tau)]\right) d\tau$$

$$= \underbrace{-\frac{1}{i}\int_{-\infty}^{t} dt' \int d\vec{r}'\, tr\left(\hat{\rho}_0 [m_i^I(\vec{r},t), m_j^I(\vec{r}',t')]\right)}_{\text{推迟Green Function}} H_j(\vec{r}',t')$$

Mahan: 168–170

Kittel 11章: M S S 关系