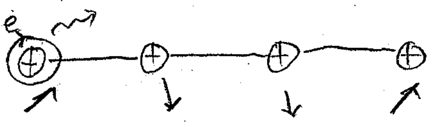
凝聚态系统 (固体, 液体)

↓

原子核 + 电子 (+电磁波)



交换相互作用 (磁性基本起源)

基态 (原子核排布, 电子的状态) → 量子物态

波函数 {轨道, 自旋}

激发态 {magnon, Bogolivbov particle, 费米面激发, 声子, 光子, 激子} → 相互作用

磁性

超导

金属 (能带, 费米

铁电 (dipole

研究系统的哈密顿量: $H = H_0 + V$

A —V— B 温度 非平衡

第一节: 复习二次量子化

$$\hat{H} = \sum_i \hat{h}_i$$ 总哈密顿 = 所有粒子能量之和

对每个粒子: $$\hat{h}_i = \int \hat{\Psi}^\dagger(\vec{r})\, \hat{h}_i\, \hat{\Psi}(\vec{r})\, d\vec{r}$$

重要的几个算符: [作业: 定义自旋密度算符]

① 密度算符

$$\rho(\vec{r}) = \sum_j \delta(\vec{r}-\vec{r}_j) = \sum_j \rho_j(\vec{r})$$

用场算符表示:

$$\rho(\vec{r}) = \sum_j \rho_j(\vec{r}) = \sum_j \hat{\Psi}^\dagger(\vec{r}_j)\hat{\Psi}(\vec{r}_j)\delta(\vec{r}-\vec{r}_j) = \int \hat{\Psi}^\dagger(\vec{r}_j)\hat{\Psi}(\vec{r}_j)\delta(\vec{r}-\vec{r}_j)\, d\vec{r}_j$$

$$\rho(\vec{r}) = \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}(\vec{r})$$

$\Psi(\vec r)$用产生湮灭算符表示：

$$\Psi(\vec r) = \sum_l \hat a_l \boxed{\phi_l(\vec r)}$$

波函数

正交完备基

典型例子

①紧束缚模型　l = 格点　ϕ_l为原子波函数

②平面波　l = 波矢$\vec k$　ϕ_l为Bloch波函数 $u_{\vec k} e^{i\vec k\cdot\vec r}$

$$\Psi(\vec r) = \frac{1}{\sqrt V}\sum_{\vec k} \hat a_{\vec k} e^{i\vec k\cdot\vec r}$$

$$\begin{cases} \Psi(\vec r) = \frac{1}{\sqrt V}\sum_{\vec k} \hat a_{\vec k} e^{i\vec k\cdot\vec r} \\ \Psi^+(\vec r) = \frac{1}{\sqrt V}\sum_{\vec k} \hat a^+_{\vec k} e^{-i\vec k\cdot\vec r} \end{cases}$$

$$\hat \rho(\vec q) = \frac{1}{V}\int \sum_{\vec k}\sum_{\vec k'} \hat a^+_{\vec k} e^{-i\vec k\cdot\vec r} \hat a_{\vec k'} e^{i\vec k'\cdot\vec r} \underbrace{e^{-i\vec q\cdot\vec r}}_{\vec k'=\vec k+\vec q} d\vec r$$

$$= \sum_{\vec q}\sum_{\vec k} \hat a^+_{\vec k} \hat a_{\vec k+\vec q}$$

$$\hat \rho(\vec r) = \hat \rho(\vec q) e^{i\vec q\cdot\vec r}$$

$$= \frac{1}{V}\sum_{\vec q}\left(\sum_{\vec k} \hat a^+_{\vec k} \hat a_{\vec k+\vec q}\right) e^{i\vec q\cdot\vec r}$$

②流算符
（电荷流）

[作业：自旋流算符]

$$\vec j_j = e_j \dot{\vec r}_j \delta(\vec r-\vec r_j) \qquad \boxed{\vec j = \rho \vec v}$$

$$\boxed{\begin{aligned} AB &\Rightarrow \frac{1}{2}\{\hat A, \hat B\} \\ ABC &\Rightarrow \{\hat A \hat B \hat C\} \end{aligned}}$$

从经典到量子化需要对称性处理
（A, B, C不对易的情况下）

$$\vec j(\vec r) = \sum_j \frac{e}{2}[\dot{\vec r}_j \delta(\vec r-\vec r_j) + \delta(\vec r-\vec r_j)\dot{\vec r}_j]\vec r_j$$

$$\hat{\dot{\vec r}}_j = \dot{\hat{\vec r}}_j = \frac{i}{\hbar}[\hat H, \hat r_j] = \frac{i}{2m\hbar}[\hat p^2, \hat r_j]$$

$$= 2\hat p_j \cdot \frac{i}{2m\hbar}(-i\hbar) = \frac{\hat p_j}{m}$$

对 $\hat H_j = \frac{\hat p_j^2}{2m} + V(\vec r_j)$ 而言

$$\vec{j}(\vec{r}) = \frac{e}{2m}\sum_j [\hat{\vec{p}}_j \delta(\hat{\vec{r}}-\vec{r}_j) + \delta(\hat{\vec{r}}-\vec{r}_j)\hat{\vec{p}}_j] = \sum_j \vec{j}_j(\vec{r})$$

二次量子化：

$$\vec{j}(\vec{r}) = \frac{e}{2m}\int d\vec{r}_j\, \hat{\Psi}^+(\vec{r}_j)\left((-i\hbar\nabla_j)\delta(\vec{r}-\vec{r}_j) + \delta(\vec{r}-\vec{r}_j)(-i\hbar\nabla_j)\right)\hat{\Psi}(\vec{r}_j)$$

$$= \frac{e}{2m}\int d\vec{r}_j\, \hat{\Psi}^+(\vec{r}_j)[\underbrace{(-i\hbar\nabla_j)\delta(\vec{r}-\vec{r}_j)\hat{\Psi}(\vec{r}_j)}_{\text{分部积分}}^{\text{I}} + \overbrace{\delta(\vec{r}-\vec{r}_j)(-i\hbar\nabla_j)\hat{\Psi}(\vec{r}_j)}^{\text{II}}]$$

$$\boxed{\hat{\Psi}^+(\vec{r}_j)\delta(\vec{r}-\vec{r}_j)\hat{\Psi}(\vec{r}_j)\Big|_{-\infty}^{\infty} = 0}$$

$$\text{I}: \underbrace{-i\hbar\int \nabla_j\left(\hat{\Psi}^+(\vec{r}_j)\delta(\vec{r}-\vec{r}_j)\hat{\Psi}(\vec{r}_j)\right)d\vec{r}_j}_{} + i\hbar\int (\nabla_j\hat{\Psi}^+(\vec{r}_j))\delta(\vec{r}-\vec{r}_j)\hat{\Psi}(\vec{r}_j)\,d\vec{r}_j$$

(分部积分)

$$= i\hbar\,(\nabla\hat{\Psi}^+(\vec{r}))\hat{\Psi}(\vec{r})$$

$$\text{II}: \quad -i\hbar\,\hat{\Psi}^+(\vec{r})(\nabla\hat{\Psi}(\vec{r}))$$

$$\Rightarrow \vec{j}(\vec{r}) = \frac{\hbar e}{2mi}[\hat{\Psi}^+(\vec{r})\nabla\hat{\Psi}(\vec{r}) - \nabla\hat{\Psi}^+(\vec{r})\hat{\Psi}(\vec{r})]$$

$$j(\vec{r}) = \sum_{\vec{q}} e^{i\vec{q}\cdot\vec{r}}\,\vec{j}(\vec{q})$$

$\boxed{\text{作业3：} j(\vec{q})}$

$$j(\vec{q}) = \frac{\hbar}{m}\sum_{\vec{k}}\left(\vec{k}+\frac{\vec{q}}{2}\right)\hat{C}^+_{\vec{k}}\hat{C}_{\vec{k}+\vec{q}}$$

③ polarization operator

[作业4]

提示：经典中 $\vec{P} = e\int \rho(\vec{r})(\vec{r})\,d\vec{r}$

作业1：定义自旋密度算符

解：$\rho_s(\vec{r}) = \sum_j \delta(\vec{r}-\vec{r}_j)\vec{s}_j$

$$\hat{\rho}_s(\vec{r}) = \sum_j \hat{\rho}_s^j(\vec{r}) = \sum_j \Phi^+(\vec{r}_j)\Phi(\vec{r}_j)\delta(\vec{r}-\vec{r}_j)\vec{s}_j$$

$$= \int d\vec{r}_j \frac{\hbar}{2}\Phi_\alpha^+(\vec{r}_j)\Phi_{\alpha'}(\vec{r}_j)\sigma_{\alpha\alpha'}\delta(\vec{r}-\vec{r}_j)$$

$$= \frac{\hbar}{2}\Phi_\alpha^+(\vec{r})\sigma_{\alpha\alpha'}\Phi_{\alpha'}(\vec{r})$$

作业2：定义自旋流算符

$$\vec{J}_s^a(\vec{r}) = \sum_j \vec{v}_j\delta(\vec{r}-\vec{r}_j)S_j^a$$

$$= \frac{1}{2}\sum_j S_j^a[\vec{v}_j\delta(\vec{r}-\vec{r}_j) + \delta(\vec{r}-\vec{r}_j)\vec{v}_j]$$

对 $\hat{H} = \sum_j\left(\frac{\hat{P}_j^2}{2m} + V(\vec{r}_j)\right)$

速度 $\hat{v}_j = \dot{\hat{r}}_j = \frac{i}{\hbar}[\hat{H}, \hat{r}_j] = \frac{\hat{P}_j}{m}$

则 $\vec{J}_s(\vec{r})$ 二次量子化后为：

$$\hat{J}_s^a(\vec{r}) = \sum_j \frac{\hbar}{4m}\sigma_{\delta\varepsilon}^a\Phi_\delta^+(\vec{r}_j)[(-i\hbar\nabla_j)\delta(\vec{r}-\vec{r}_j) + \delta(\vec{r}-\vec{r}_j)(-i\hbar\nabla_j)]\Phi_\varepsilon(\vec{r}_j)$$

$$= \int\frac{\hbar d\vec{r}_j}{4m}\sigma_{\delta\varepsilon}^a\{\underbrace{\Phi_\delta^+(\vec{r}_j)[-i\hbar\nabla_j\delta(\vec{r}-\vec{r}_j)\Phi_\varepsilon(\vec{r}_j)]}_{\mathrm{I}} + \underbrace{\Phi_\delta^+(\vec{r}_j)\delta(\vec{r}-\vec{r}_j)[-i\hbar\nabla_j\Phi_\varepsilon(\vec{r}_j)]}_{\mathrm{II}}\}$$

$$I = \frac{\hbar \sigma^{\alpha}_{s\varepsilon}}{4m} \int d\vec{r}_j \, (-i\hbar \nabla_j) \left[\hat{\Phi}^{+}_{s}(\vec{r}_j) \hat{\Phi}_{\varepsilon}(\vec{r}_j) \delta(\vec{r}-\vec{r}_j) \right]$$

$$+ \frac{\hbar \sigma^{\alpha}_{s\varepsilon}}{4m} \int d\vec{r}_j \left(i\hbar \nabla_j \hat{\Phi}^{+}_{s}(\vec{r}_j) \right) \hat{\Phi}_{\varepsilon}(\vec{r}_j) \, \delta(\vec{r}-\vec{r}_j)$$

第一项：$\int d\vec{r}_j \, -i\hbar \nabla_j \left[\hat{\Phi}^{+}_{s}(\vec{r}_j) \hat{\Phi}_{\varepsilon}(\vec{r}_j) \delta(\vec{r}-\vec{r}_j) \right]$

考虑a分量：$\int d\vec{r}_j \, -i\hbar \nabla_j|_a \left[\hat{\Phi}^{+}_{s}(\vec{r}_j) \hat{\Phi}_{\varepsilon}(\vec{r}_j) \delta(\vec{r}-\vec{r}_j) \right]$

$$= \int dr_j|_b \int dr_j|_c \left\{ -i\hbar \underbrace{\hat{\Phi}^{+}_{s}(\vec{r}_j) \hat{\Phi}_{\varepsilon}(\vec{r}_j) \delta(\vec{r}-\vec{r}_j) \Big|_{-\infty}^{\infty}}_{=0} \right\}$$

$$= 0$$

所以第一项 a, b, c 三分量均为0，第一项 = 0

第二项 = $\frac{\hbar \sigma^{\alpha}_{s\varepsilon}}{4m} \, i\hbar \left(\nabla \hat{\Phi}^{+}_{s}(\vec{r}) \right) \hat{\Phi}_{\varepsilon}(\vec{r})$

$$II = \frac{\hbar \sigma^{\alpha}_{s\varepsilon}}{4m} (-i\hbar) \, \hat{\Phi}^{+}_{s}(\vec{r}) \left(\nabla \hat{\Phi}_{\varepsilon}(\vec{r}) \right)$$

$$I + II = \frac{\hbar^2 \sigma^{\alpha}_{s\varepsilon}}{4mi} \left[\hat{\Phi}^{+}_{s}(\vec{r}) \left(\nabla \hat{\Phi}_{\varepsilon}(\vec{r}) \right) - \left(\nabla \hat{\Phi}^{+}_{s}(\vec{r}) \right) \hat{\Phi}_{\varepsilon}(\vec{r}) \right]$$

$$\hat{J}^{\alpha}_{s}(\vec{r}) = \frac{\hbar^2}{4mi} \hat{\Phi}^{+}_{s}(\vec{r}) \, \sigma^{\alpha}_{s\varepsilon} \left(\nabla \hat{\Phi}_{\varepsilon}(\vec{r}) \right) + H.c.$$

作业3：电荷流 $\vec{j}(\vec{r}) = \frac{\hbar e}{2mi}[\hat{\Phi}^{+}(\vec{r})\nabla\hat{\Phi}(\vec{r}) - \nabla\hat{\Phi}^{+}(\vec{r})\hat{\Phi}(\vec{r})]$，
求 $\vec{j}(\vec{q})$

解：$\hat{\Phi}(\vec{r}) = \frac{1}{\sqrt{V}}\sum_{\vec{k}} \hat{C}_{\vec{k}} e^{i\vec{k}\cdot\vec{r}}$ 用平面波展开

$$\vec{j}(\vec{r}) = \frac{\hbar e}{2miV}\left[\sum_{\vec{k}\vec{k}'} \hat{C}^{+}_{\vec{k}'}\hat{C}_{\vec{k}}(i\vec{k})e^{i(\vec{k}-\vec{k}')\cdot\vec{r}} - \hat{C}^{+}_{\vec{k}'}\hat{C}_{\vec{k}}(-i\vec{k}')e^{i(\vec{k}-\vec{k}')\cdot\vec{r}}\right]$$

$$\vec{j}(\vec{q}) = \int \vec{j}(\vec{r}) e^{-i\vec{q}\cdot\vec{r}} d\vec{r}$$

$$= \int \frac{\hbar e}{2mV}\sum_{\vec{k}\vec{k}'} \hat{C}^{+}_{\vec{k}'}\hat{C}_{\vec{k}}(\vec{k}'+\vec{k}) e^{i(\vec{k}-\vec{k}'-\vec{q})\cdot\vec{r}} d\vec{r}$$

$$= \frac{\hbar e}{2m}\sum_{\vec{k}} \hat{C}^{+}_{\vec{k}}\hat{C}_{\vec{k}+\vec{q}}(2\vec{k}+\vec{q})$$

$$= \frac{\hbar e}{m}\sum_{\vec{k}}\left(\vec{k}+\frac{\vec{q}}{2}\right)\hat{C}^{+}_{\vec{k}}\hat{C}_{\vec{k}+\vec{q}}$$

作业4：计算 polarization operator：$\vec{P} = e\int \rho(\vec{r})\,\vec{r}\,d\vec{r}$
的二次量子化形式

解：$\vec{P}(\vec{r}) = \sum_{j} e\,\vec{r}_j\,\delta(\vec{r}-\vec{r}_j)$

$$\hat{P}(\vec{r}) = \int d\vec{r}_j\, e\,\hat{\Phi}^{+}(\vec{r}_j)\,\vec{r}_j\,\delta(\vec{r}-\vec{r}_j)\,\hat{\Phi}(\vec{r}_j)$$

$$= e\,\vec{r}\,\hat{\Phi}^{+}(\vec{r})\hat{\Phi}(\vec{r})$$

用平面波展开：

$$\hat\Phi(\vec r)=\frac{1}{\sqrt V}\sum_{\vec k}\hat c_{\vec k}e^{i\vec k\cdot\vec r}$$

$$\hat P(\vec r)=\frac{e}{V}\sum_{\vec k\vec k'}\vec r\,\hat c^+_{\vec k}\hat c_{\vec k'}e^{i(\vec k'-\vec k)\cdot\vec r}$$

由 $\hat P(\vec q)=\int\hat P(\vec r)e^{-i\vec q\cdot\vec r}d\vec r$ 得：

$$\hat P(\vec q)=\int\frac{e}{V}\sum_{\vec k\vec k'}\vec r\,\hat c^+_{\vec k}\hat c_{\vec k'}e^{i(\vec k'-\vec k-\vec q)\cdot\vec r}d\vec r$$

$$=\frac{e}{V}\sum_{\vec k\vec k'}\hat c^+_{\vec k}\hat c_{\vec k'}\int(-i\partial_{\vec k'})e^{i(\vec k'-\vec k-\vec q)\cdot\vec r}d\vec r$$

$$=e\sum_{\vec k\vec k'}\hat c^+_{\vec k}\hat c_{\vec k'}(-i\partial_{\vec k'})\delta_{\vec k',\vec k+\vec q}$$

$$=e\sum_{\vec k}\int\hat c^+_{\vec k}\hat c_{\vec k'}\left[(-i\partial_{\vec k'})\delta(\vec k'-\vec k-\vec q)\right]d\vec k'$$

$$=e\sum_{\vec k}\underbrace{\hat c^+_{\vec k}\hat c_{\vec k'}\delta(\vec k'-\vec k-\vec q)\Big|_{\vec k'=-\infty}^{\vec k'=\infty}}_{0}+e\sum_{\vec k}\int\left[(i\partial_{\vec k'})\hat c^+_{\vec k}\hat c_{\vec k'}\right]\delta(\vec k'-\vec k-\vec q)d\vec k'$$

$$=e\sum_{\vec k}(i\partial_{\vec k+\vec q})\hat c^+_{\vec k}\hat c_{\vec k+\vec q}=e\sum_{\vec k}(i\partial_{\vec q})\hat c^+_{\vec k}\hat c_{\vec k+\vec q}$$