极化算符

$$\vec{P} = \int d^3r \, \vec{r} \, \hat{\rho}(\vec{r})$$

$$\frac{\partial \vec{P}}{\partial t} = \int d^3r \, \vec{r} \, \frac{\partial \hat{\rho}(\vec{r})}{\partial t}$$

由于 $\frac{\partial \hat{\rho}(\vec{r})}{\partial t} = -\nabla \cdot \vec{J}$

因此

$$\frac{\partial \vec{P}}{\partial t} = -\int d^3r \, \vec{r} \, \nabla \cdot \vec{J}$$

由于 $\nabla \cdot (\vec{J}\vec{r}) = (\nabla \cdot \vec{J})\vec{r} + \vec{J} \cdot \nabla \vec{r}$

因此 $\frac{\partial \vec{P}}{\partial t} = -\int d^3r \, \nabla \cdot (\vec{r}\vec{J}) + \int d^3r \, \vec{J} \cdot \nabla \vec{r}$

由于无穷远处电流为0

则 $\int d^3r \, \nabla \cdot (\vec{r}\vec{J}) = 0$

$$\frac{\partial \vec{P}}{\partial t} = \int d^3r \, \vec{J} \cdot \nabla \vec{r} = \int d^3r \, \vec{J}$$

极化算符离散化

由于 $\hat{\rho}(r) = \sum_i \delta(\vec{r} - \vec{r}_i)$，二次量子化后

$\hat{\rho}(r) = \psi^{+}(r)\psi(r)$ 是粒子数密度算符

离散化 $\hat{\rho}(r) \Rightarrow \hat{n}_i = a_i^{+} a_i$

$$\vec{r} \Rightarrow \vec{R}_i$$

$$\vec{P} = \sum_i \vec{R}_i \hat{n}_i$$

由于 $\dfrac{\partial \vec{P}}{\partial t} = i[\hat{H}, \vec{P}]$

$$\hat{H} = \underbrace{\sum_j \varepsilon_j C_j^+ C_j}_{\text{在位项}} + \underbrace{\sum_{j\delta} W C_{j+\delta}^+ C_j}_{\text{跃迁项}} + \underbrace{\frac{1}{2} \sum_{ij} \hat{n}_i \hat{n}_j V_{ij}}_{\text{相互作用项}}$$

$$\hat{n}_i = C_i^+ C_i$$

$$[\hat{H}, \vec{P}] = \overset{①}{\sum_j \sum_i} \varepsilon_j \vec{R}_i [C_j^+ C_j, C_i^+ C_i] + \overset{②}{\sum_{j\delta}} \sum_i W \vec{R}_i [C_{j+\delta}^+ C_j, C_i^+ C_i]$$

$$+ \overset{③}{\sum_{ij}} \frac{1}{2} V_{ij} [\hat{n}_i \hat{n}_j, \hat{n}_i]$$

注意到，费米子满足反对易关系

$$[C_i, C_j^+]_+ = \delta_{ij}, \quad [C_i, C_j]_+ = 0, \quad [C_i^+, C_j^+]_+ = 0$$

$$[C_j^+ C_j, C_i^+ C_i] = C_j^+ [C_j, C_i^+ C_i] + [C_j^+, C_i^+ C_i] C_j$$

$$= C_j^+ \underbrace{[C_j, C_i^+]_+}_{\delta_{ji}} C_i - C_i^+ \underbrace{[C_j^+, C_i]_+}_{\delta_{ji}} C_j$$

$$= C_i^+ C_i - C_i^+ C_i$$

$$= 0$$

因此，第①项为0

由于 $[c_j^+ c_j, c_i^+ c_i] = [\hat{n}_j, \hat{n}_i]$

所以第③项也为0

第②项：$[c_{j+\delta}^+ c_j, c_i^+ c_i] = c_{j+\delta}^+ [c_j, c_i^+ c_i] + [c_{j+\delta}^+, c_i^+ c_i] c_j$

$$= c_{j+\delta}^+ c_i \delta_{ij} - c_i^+ c_j \delta_{i,j+\delta}$$

因此 $[\hat{H}, \hat{P}] = \sum_{j\delta} W(\vec{R}_j - \vec{R}_{j+\delta}) c_{j+\delta}^+ c_j$

$$= -\sum_{j\delta} W \vec{\delta} c_{j+\delta}^+ c_j$$

$$\frac{\partial \vec{P}}{\partial t} = i[\hat{H}, \vec{P}] = -i \sum_{j\delta} W \vec{\delta} c_{j+\delta}^+ c_j$$

所以 $\vec{J} = -iW \sum_{j\delta} \vec{\delta} c_{j+\delta}^+ c_j$