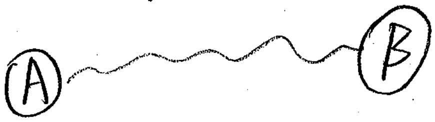
电-声相互作用

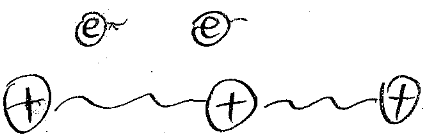
若有两个系统



对于单独的A，B系统，已知其性质

→ 研究其相互作用

→ 电子-声子相互作用



声子：晶格振动 → 改变周围势场 → 改变电子运动

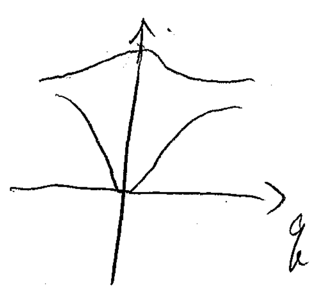
波恩-奥本海默近似：电子速度远大于原子核，电子感受原子核的势场无延迟

把系统哈密顿量写出来：

$$\hat{H} = \hat{H}_p + \hat{H}_e + \hat{H}_{ei}$$

$$\hat{H}_p = \sum_{\vec{q},\lambda} \omega_{\vec{q},\lambda} a^+_{\vec{q},\lambda} a_{\vec{q},\lambda}$$ ~ 声子哈密顿

↳ 支

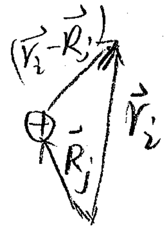


$$\hat{H}_e = \sum_i \Big[\frac{p_i^2}{2m} + \frac{e}{2} \sum_{j \neq i} \frac{1}{r_{ij}} \Big]$$ 电子哈密顿

动量

↳ 电子-电子相互作用

$$H_{ei} = \underbrace{\sum_i}_{\text{把电子加起来}} \underbrace{\sum_j}_{\text{把所有核加起来}} V(\vec{r}_i - \vec{R}_j)$$



$V(\vec{r}_i - \vec{R}_j)$ → 电子感受到原子核的势（只是坐标的函数）

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① 若 $\vec{R}_j = \vec{R}_j^{(0)}$ 原子核在平衡位置

$\underline{H_e + H_{ei}}$ —— 电子能带 $[\varepsilon_{k\alpha} C_{k\alpha}^{+} C_{k\alpha}]$ α ↳ 支

② $\vec{R}_j \neq \vec{R}_j^{(0)}$ 偏离平衡位置 电声相互作用

压电效应

$\Rightarrow \vec{R}_j = \vec{R}_j^{(0)} + \vec{Q}_j$ → 位移场 (displacement field)

把 $V(\vec{r}_i - \vec{R}_j)$ 作展开

$$V(\vec{r}_i - \vec{R}_j^{(0)} - \vec{Q}_j)$$

$$= \underbrace{V(\vec{r}_i - \vec{R}_j^{(0)})}_{\text{周期势场}} - \vec{Q}_j \cdot \nabla V(\vec{r}_i - \vec{R}_j^{(0)}) + \frac{1}{2} Q_{j\mu} Q_{j\nu} \frac{\partial^2}{\partial R_\mu R_\nu} V(\vec{r}_i - \vec{R}_j^{(0)}) + O(Q^3)$$

主要看第二项

$$\hat{H}_{ep} = \sum_i \sum_j -\vec{Q}_j \cdot \nabla V(\vec{r}_i - \vec{R}_j^{(0)})$$

$$= \sum_i H_{ep}^{(i)} = -\sum_i V_{ep}(\vec{r}_i)$$

$$V_{ep}(\vec{r}) = \sum_j \vec{Q}_j \cdot \nabla V(\vec{r} - \vec{R}_j^{(0)})$$

二次量子化它!

$$\to \int d\vec{r}\ \psi^\dagger(\vec{r})\, V_{ep}(\vec{r})\, \psi(\vec{r})$$

$\to$ 博立叶展开 $V_{ep}(\vec{r})$

$$V(\vec{r} - \vec{R}_j^{(0)}) = \frac{1}{N} \sum_{\vec{q}} V(\vec{q})\, e^{i\vec{q}\cdot(\vec{r} - \vec{R}_j^{(0)})}$$

$$\to \nabla V(\vec{r} - \vec{R}_j^{(0)}) = \frac{i}{N} \sum_{\vec{q}} V(\vec{q})\, e^{i\vec{q}\cdot(\vec{r} - \vec{R}_j^{(0)})}$$

$$V_{ep}(\vec{r}) = \sum_j \vec{Q}_j \cdot \frac{i}{N} \sum_{\vec{q}} \vec{q}\, V(\vec{q})\, e^{i\vec{q}\cdot(\vec{r} - \vec{R}_j)}$$

$$= \frac{i}{N} \sum_{\vec{q}} V(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}\quad \vec{q}\cdot\left(\sum_j \vec{Q}_j\, e^{-i\vec{q}\cdot\vec{R}_j^{(0)}}\right)$$

$$\vec{Q}_j \xrightarrow{\text{声子量子化}} i \sum_{k,\lambda} \sqrt{\frac{\hbar}{2MN\omega_{k,\lambda}}}\ \varepsilon_{k,\lambda}\left(a_{k,\lambda} + a^\dagger_{-k,\lambda}\right) e^{ik\cdot\vec{R}_j^{(0)}}$$

代入上式

$$\sum_j \vec{Q}_j e^{-i\vec{q}\cdot\vec{R}_j^{(0)}} = \sum_j \sum_{k,\lambda} i \sqrt{\frac{\hbar}{2MN\omega_{k,\lambda}}}\ \varepsilon_{k,\lambda}\left(a_{k,\lambda} + a^\dagger_{-k,\lambda}\right) e^{i(k - \vec{q})\vec{R}_j}$$

$$= i \sum_{G,\lambda} N \sqrt{\frac{\hbar}{2MN\omega_{\vec{q},\lambda}}}\ \varepsilon_{\vec{q}+G,\lambda}\left(a_{\vec{q}+G,\lambda} + a^\dagger_{-(\vec{q}+G),\lambda}\right)$$

$$\Rightarrow V_{ep}(\vec{r}) = -\sum_{\vec{q},G} \sum_\lambda V(\vec{q})\, e^{i\vec{q}\cdot\vec{r}}\, \vec{q} \sqrt{\frac{\hbar}{2MN\omega_{\vec{q}}}}\ \varepsilon_{\vec{q}+\vec{G},\lambda}\left(a_{\vec{q}+\vec{G},\lambda} + \hat{a}^\dagger_{-(\vec{q}+\vec{G}),\lambda}\right)$$

$$= -\sum_{\vec{q},\vec{G}} \sum_{\lambda} V(\vec{q}+\vec{G}) e^{i(\vec{q}+\vec{G})\cdot\vec{r}} (\vec{q}+\vec{G}) \varepsilon_{\vec{q},\lambda} \sqrt{\frac{\hbar}{2MN\omega_{\vec{q},\lambda}}} (\hat{a}_{\vec{q},\lambda} + \hat{a}^{+}_{-\vec{q},\lambda})$$

代入二次量子化的哈密顿中

$$H_{ep} = \int d\vec{r}_i \ \psi^{+}(\vec{r}_i) V_{ep}(\vec{r}_i) \psi(\vec{r}_i)$$

$$= \int d\vec{r}_i \ \rho(\vec{r}_i) V_{ep}(\vec{r}_i) \qquad \rho(\vec{r}_i) = C$$

其中 $\int d\vec{r}_i \ \rho(\vec{r}_i) e^{i(\vec{q}+\vec{G})\cdot\vec{r}_i} = \rho(\vec{q}+\vec{G})$

$$\Rightarrow \sum_{\vec{q},\vec{G}} \sum_{\lambda} \rho(\vec{q}+\vec{G}) V(\vec{q}+\vec{G}) (\vec{q}+\vec{G}) \varepsilon_{\vec{q},\lambda} \sqrt{\frac{\hbar}{2MN\omega_{\vec{q},\lambda}}} (\hat{a}_{\vec{q},\lambda} + \hat{a}^{+}_{-\vec{q},\lambda})$$

其中: $\rho(\vec{q}) = \sum_{k} C^{+}_{k} C_{k+\vec{q}}$

$$\sum_{k} \hat{C}^{+}_{\vec{q}+\vec{G}} C_{\vec{q}+\vec{G}+\vec{k}}$$

若 $M_\lambda(\vec{q}+\vec{G}) = -V(\vec{q}+\vec{G})(\vec{q}+\vec{G}) \cdot \varepsilon_{\vec{q},\lambda} \sqrt{\frac{\hbar}{2MN\omega_{\vec{q},\lambda}}}$

$$H_{ep} = \sum_{\vec{q},\vec{G},\lambda} M_\lambda(\vec{q}+\vec{G}) \rho(\vec{q}+\vec{G}) (\hat{a}_{\vec{q}} + \hat{a}^{+}_{-\vec{q}})$$

作业. 证明. $\sum_{j} e^{i(\vec{k}-\vec{q})\cdot\vec{R}^{(0)}_j} = N\delta_{\vec{k}-\vec{q},\vec{G}}$

解 $\vec{G}$为倒格矢, 满足 $\vec{G}\cdot\vec{R}^{(0)}_j = 2\pi N \Rightarrow 1 = e^{i\vec{G}\cdot\vec{R}_j}$

$$\sum_{j} e^{i(\vec{k}-\vec{q})\cdot\vec{R}^{(0)}_j} \times 1 = \sum_{j} e^{i(\vec{k}-\vec{q}-\vec{G})\cdot\vec{R}^{(0)}_j}$$

$$= N\delta_{\vec{k}-\vec{q},\vec{G}} \begin{cases} \vec{k}-\vec{q}=\vec{G} \rightarrow N\text{个粒子} \\ \vec{k}-\vec{q}\neq\vec{G} \rightarrow \text{求和为零} \end{cases}$$