凝聚态中的二次量子化方法

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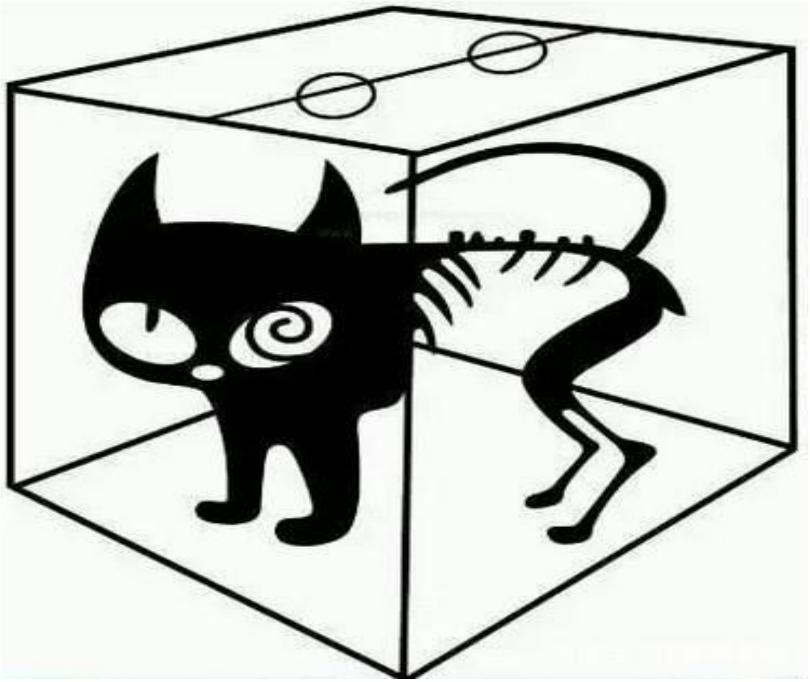
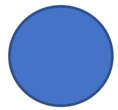
目录

“一次”量子化

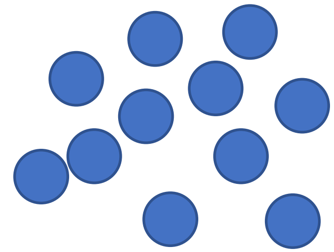
- “一次”量子化是把经典理论加以改变，使之成为量子理论的手续。



二次量子化的原因



N=1



$N \sim 10^{23}$

- 一次量子化关注单体运动，重点计算波函数，计算一个粒子出现在哪里的概率。
- 二次量子化则关注多体系统，重点计算体系的状态，采用粒子在不同态的占据数来表示系统，计算系统处于不同粒子占据态的概率。

目录

二次量子化的具体步骤

（1） 建立全同粒子体系的基矢

设有一个由n个全同粒子构成的系统，这个系统的希尔伯特空间和本征矢分别为：

$$R_{\mathrm{n}} = R^{(1)} \otimes R^{(2)} \otimes \cdots \otimes R^{(n)}$$

$$|b> = |b^{\alpha}>_1 |b^{\beta}>_2 \ldots |b^{\gamma}>_n$$

式中$R^{(i)}$为第i个粒子的希尔伯特空间，$|b^{\alpha}>_{\mathrm{i}}$为第i个粒子的α态

二次量子化的具体步骤

由于量子力学基本原理的限制，体系的波函数写为：

$$|n; b^{\alpha}\, b^{\beta} \ldots\, b^{\gamma} >= \frac{1}{n!} \sum_P \varepsilon^p P |b^{\alpha} >_1 |b^{\beta} >_2 \ldots |b^{\gamma} >_n$$

式中P算符的作用是对粒子编号取一个排列，p表示置换次数，ε=1(玻色子)或-1(费米子)。

(2) 写出粒子的产生湮灭算符

- 位置表象

$$\hat{\psi}^{\dagger}(\mathrm{x})|n; x^{\alpha}\, x^{\beta} \ldots x^{\gamma} > = \sqrt{n+1}|n+1; x\, x^{\alpha}\, x^{\beta} \ldots x^{\gamma} >$$

$$\begin{aligned}\hat{\psi}(\mathrm{x})|n;\ x^{\alpha}\, x^{\beta} \ldots x^{\gamma} > = \frac{1}{\sqrt{n!}} & [\delta(x-x^{\alpha})\ |n-1;\ x^{\beta} \ldots x^{\gamma} > \\ & +\varepsilon\delta\left(x-x^{\beta}\right)\ |n-1;\ x^{\alpha} \ldots x^{\gamma} > \\ & + \cdots \\ & +\varepsilon^{n-1}\delta(x-x^{\gamma})|n-1; x^{\alpha}\, x^{\beta} \ldots >]\end{aligned}$$

二次量子化的具体步骤

- 不同表象之间产生湮灭算符的关系

$$\hat{\Psi}^{\dagger}(x)=\sum_{b}\hat{C}^{\dagger}(b)<b|x>，\quad \hat{\Psi}(x)=\sum_{b}\hat{C}(b)<x|b>$$

例如：

布洛赫表象 $\hat{\Psi}(x)=\sum_{k}\sum_{\sigma}\hat{C}_{k,\sigma}\cdot\psi_{k,\sigma}(x)$

瓦尼尔表象 $\hat{\Psi}(\vec{r})=\sum_{l}\sum_{\sigma}\hat{C}_{l,\sigma}\cdot a_{\sigma}\left(\vec{r}-\vec{R}_{l}\right)$

二次量子化的具体步骤

（3）用这些算符去表示哈密顿算符

- 位置表象

$$\widehat{H} = \sum_i \widehat{h}(\vec{r}_i) + \sum_{i \neq j} \widehat{U}(\vec{r}_i - \vec{r}_j) = \widehat{H}^{(1)} + \widehat{H}^{(2)}$$

二次量子化的具体步骤

- 单体算符

$$\widehat{H}^{(1)} = \sum_i \widehat{h}(x_i)$$
$$= \int \widehat{\psi}^\dagger(x)\widehat{h}(x)\widehat{\psi}(x)dx$$

- 两体算符

$$\widehat{H}^{(2)} = \sum_{i,j} \widehat{U}(x_i - x_j)$$
$$= \frac{1}{2}\iint \widehat{\psi}^\dagger(x)\widehat{\psi}^\dagger(x')\widehat{U}(x - x')\widehat{\psi}(x')\widehat{\psi}(x)dxdx'$$

二次量子化的具体步骤

- 位置表象下全同粒子体系的哈密顿量的二次量子化表示

$$\boxed{\begin{aligned}\widehat{H} = &\int \widehat{\psi}^\dagger(x)\widehat{h}(x)\widehat{\psi}(x)dx \\ &+ \frac{1}{2}\iint \widehat{\psi}^\dagger(x)\widehat{\psi}^\dagger(x')\widehat{U}(x-x')\widehat{\psi}(x')\widehat{\psi}(x)dxdx'\end{aligned}}$$

二次量子化的具体步骤

- 根据研究的物理过程以及物理量，选择合适的表象，并利用产生湮灭算符的表象变换规则得到对应表象下全同粒子体系的哈密顿量的二次量子化表示

  例如：
  倒空间：布洛赫表象
  实空间：瓦尼尔表象

二次量子化的范式

1. 确定全同粒子系统哈密顿量

$$\hat{H}=\sum_i \hat{h}(\vec{r}_i)+\sum_{i\neq j}\hat{U}(\vec{r}_i-\vec{r}_j)$$

2. 带入坐标表象下哈密顿量的二次量子化公式

$$\hat{H}=\int \hat{\Psi}^\dagger(\vec{r})\hat{h}(\vec{r})\hat{\Psi}(\vec{r})d\vec{r}$$
$$+\frac{1}{2}\iint \hat{\Psi}^\dagger(\vec{r})\hat{\Psi}^\dagger(\vec{r}')\hat{U}(\vec{r}-\vec{r}')\hat{\Psi}(\vec{r}')\hat{\Psi}(\vec{r})d\vec{r}d\vec{r}'$$

3. 选择合适的表象，将$\hat{\psi}(\vec{r})$和$\hat{\psi}^\dagger(\vec{r})$展开
4. 考虑限制条件
5. 计算得到哈密顿量的二次量子化表示

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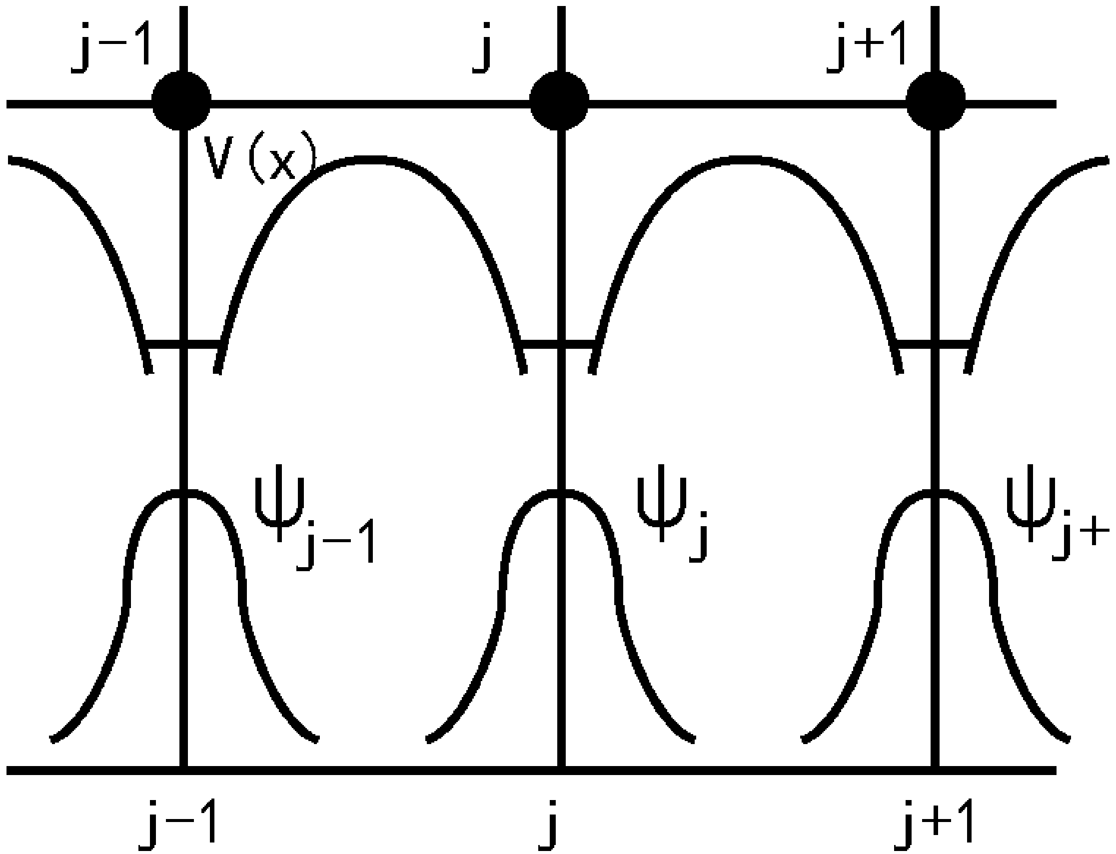
Tight-binding模型

物理模型：

晶体势场

原子波函数



Tight-bonding模型

1. 系统哈密顿量

$$\hat{H} = \sum_i \hat{h}(\vec{r}_i) = \sum_i \left[-\frac{\hbar^2}{2m} \nabla_i^2 + V(\vec{r}_i) \right]$$

2. 带入坐标表象下哈密顿量的二次量子化公式

$$\hat{H} = \int \hat{\Psi}^\dagger(\vec{r}) \hat{h}(\vec{r}) \hat{\Psi}(\vec{r}) d\vec{r}$$

Tight-bonding模型

3. 选取瓦尼尔表象 $\hat{\Psi}(\vec{r})=\sum_{l}\hat{C}_{l}a\left(\vec{r}-\vec{R}_{l}\right)$

$$\hat{H}=\int\hat{\Psi}^{\dagger}(\vec{r})\hat{h}(\vec{r})\hat{\Psi}(\vec{r})d\vec{r}$$

$$=\int\sum_{l,l'}\hat{C}_{l}^{\dagger}a^{*}\left(\vec{r}-\vec{R}_{l}\right)\hat{h}(\vec{r})\hat{C}_{l'}a\left(\vec{r}-\vec{R}_{l}{}'\right)d\vec{r}$$

$$=\sum_{l,l'}\hat{C}_{l}^{\dagger}\hat{C}_{l'}J_{ll'}$$

式中 $J_{ll'}=\int a^{*}\left(\vec{r}-\vec{R}_{l}\right)\hat{h}(\vec{r})a\left(\vec{r}-\vec{R}_{l}{}'\right)d\vec{r}$

4. 只考虑最近邻（限制条件：$\vec{l}=\vec{l}'$或$\vec{l}+\vec{\rho}=\vec{l}'$）

$$\hat{H}=\varepsilon(0)\sum_{l}\hat{n}_{l}-J\sum_{l,\rho}\hat{C}_{l}^{\dagger}\hat{C}_{l+\rho}$$

Tight-bonding模型

计算色散关系，转换为布洛赫表象

$$\hat{C}_l = \frac{1}{\sqrt{N}} \sum_k e^{i\vec{k}\cdot\vec{l}} \hat{C}_k$$

$$\hat{H} = \varepsilon(0) \sum_l \hat{n}_l - J \sum_k \sum_\rho e^{i\vec{k}\cdot\vec{\rho}} \hat{C}_k^\dagger \hat{C}_k$$

$$= \sum_k \left(\varepsilon(0) - J \sum_\rho e^{i\vec{k}\cdot\vec{\rho}} \right) \hat{C}_k^\dagger \hat{C}_k$$

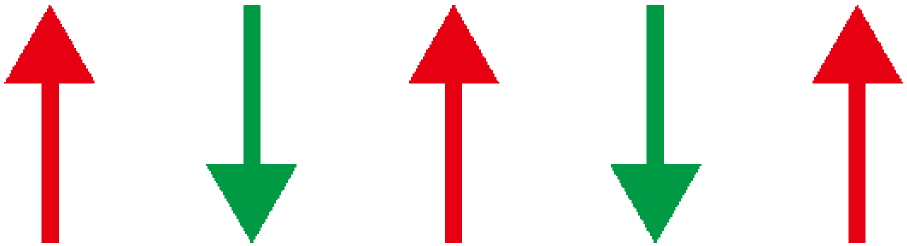
$$= \sum_k E\left(\vec{k}\right) \cdot \hat{n}_k$$

$$E\left(\vec{k}\right) = \varepsilon(0) - J \sum_\rho e^{i\vec{k}\cdot\vec{\rho}}$$

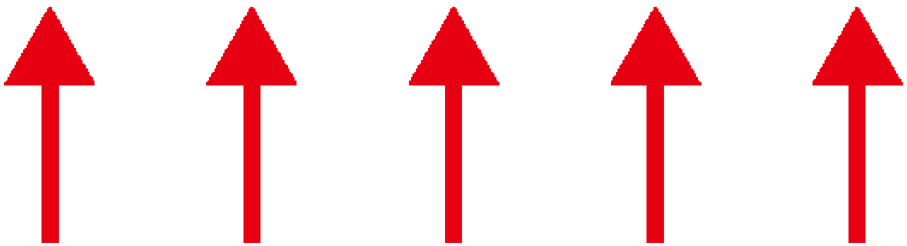
Heisenberg模型

物理模型：

交换积分<0:



交换积分>0:



Heisenberg模型

1. 电子之间的库伦势

$$\widehat{H}_c = \sum_{i,j} \widehat{U}(\vec{r}_i, \vec{r}_j) = \sum_{i,j} \frac{e^2}{|\vec{r}_i - \vec{r}_j|}$$

2. 带入坐标表象下哈密顿量的二次量子化公式

$$\widehat{H}_c = \frac{1}{2} \sum_{s,s'} \iint \widehat{\Psi}^\dagger(\vec{r}, s) \widehat{\Psi}^\dagger(\vec{r}', s') \frac{e^2}{|\vec{r} - \vec{r}'|} \widehat{\Psi}(\vec{r}', s') \widehat{\Psi}(\vec{r}, s) d\vec{r} d\vec{r}'$$

3. 选取瓦尼尔表象

$$\widehat{\Psi}(\vec{r},s)=\sum_{l}\sum_{\sigma}a\left(\vec{r}-\vec{R}_l\right)\chi_\sigma(s)\widehat{C}_{l,\sigma}$$

$$\widehat{H}_c=\frac{1}{2}\sum_{l_1l_2l_3l_4}\sum_{\sigma_1\sigma_2}\iint a^*\left(\vec{r}-\vec{R}_{l_1}\right)a^*\left(\vec{r}-\vec{R}_{l_2}\right)\widehat{U}(\vec{r}-\vec{r}\,')$$

$$\cdot a\left(\vec{r}\,'-\vec{R}_{l_3}\right)a\left(\vec{r}-\vec{R}_{l_4}\right)d\vec{r}d\vec{r}\,'\widehat{C}^\dagger_{l_1,\sigma_1}\widehat{C}^\dagger_{l_2,\sigma_2}\widehat{C}_{l_3,\sigma_2}\widehat{C}_{l_4,\sigma_1}$$

$$=\frac{1}{2}\sum_{l_1l_2l_3l_4}\sum_{\sigma_1\sigma_2}<l_1l_2|\widehat{U}|l_3l_4>\widehat{C}^\dagger_{l_1,\sigma_1}\widehat{C}^\dagger_{l_2,\sigma_2}\widehat{C}_{l_3,\sigma_2}\widehat{C}_{l_4,\sigma_1}$$

$$<l_1l_2|\widehat{U}|l_3l_4>=\iint a^*\left(\vec{r}-\vec{R}_{l_1}\right)a^*\left(\vec{r}-\vec{R}_{l_2}\right)\widehat{U}(\vec{r}-\vec{r}\,')a\left(\vec{r}\,'-\vec{R}_{l_3}\right)a\left(\vec{r}-\vec{R}_{l_4}\right)d\vec{r}d\vec{r}\,'$$

Heisenberg模型

$$\frac{1}{2}\sum_{l_1 l_2 l_3 l_4}\sum_{\sigma_1\sigma_2} < l_1 l_2|\widehat{U}|l_3 l_4 > \widehat{C}^{\dagger}_{l_1,\sigma_1}\widehat{C}^{\dagger}_{l_2,\sigma_2}\widehat{C}_{l_3,\sigma_2}\widehat{C}_{l_4,\sigma_1}$$

$-e,\vec{R}_{l_1}$

$-e,\vec{R}_{l_2}$

$\widehat{C}^{\dagger}_{l_1,\sigma_1}$ $\widehat{C}_{l_2,\sigma_1}$

$\widehat{C}_{l_1,\sigma_2}$ $\widehat{C}^{\dagger}_{l_2,\sigma_2}$

Heisenberg模型

4. 限制条件：只考虑电子的交换($\vec{l}_1=\vec{l}_3, \vec{l}_2=\vec{l}_4$)

$$\hat{H}_c=\frac{1}{2}\sum_{l_1 l_2}{}'\sum_{\sigma_1\sigma_2}<l_1 l_2|\hat{U}|l_1 l_2>\hat{C}^\dagger_{l_1,\sigma_1}\hat{C}^\dagger_{l_2,\sigma_2}\hat{C}_{l_1,\sigma_2}\hat{C}_{l_2,\sigma_1}$$

$$=-\frac{1}{2}\sum_{ll'}{}'\sum_{\sigma\sigma'}U_{ll'}\cdot\hat{C}^\dagger_{l\sigma}\hat{C}_{l\sigma'}\cdot\hat{C}^\dagger_{l'\sigma'}\hat{C}_{l'\sigma}$$

$$=-\frac{1}{2}\sum_{ll'}{}'U_{ll'}\cdot\Big(\hat{C}^\dagger_{l\uparrow}\hat{C}_{l\uparrow}\cdot\hat{C}^\dagger_{l'\uparrow}\hat{C}_{l'\uparrow}+\hat{C}^\dagger_{l\uparrow}\hat{C}_{l\downarrow}\cdot\hat{C}^\dagger_{l'\downarrow}\hat{C}_{l'\uparrow}$$

$$+\hat{C}^\dagger_{l\downarrow}\hat{C}_{l\uparrow}\cdot\hat{C}^\dagger_{l'\uparrow}\hat{C}_{l'\downarrow}+\hat{C}^\dagger_{l\downarrow}\hat{C}_{l\downarrow}\cdot\hat{C}^\dagger_{l'\downarrow}\hat{C}_{l'\downarrow}\Big)$$

Heisenberg模型

记自旋朝上对应态为$\begin{pmatrix}1\\0\end{pmatrix}$，自旋朝下对应态为$\begin{pmatrix}0\\1\end{pmatrix}$

$$\hat{C}_\uparrow^\dagger\hat{C}_\uparrow=\begin{pmatrix}1&0\\0&0\end{pmatrix},\hat{C}_\uparrow^\dagger\hat{C}_\downarrow=\begin{pmatrix}0&1\\0&0\end{pmatrix},\hat{C}_\downarrow^\dagger\hat{C}_\uparrow=\begin{pmatrix}0&0\\1&0\end{pmatrix},\hat{C}_\downarrow^\dagger\hat{C}_\downarrow=\begin{pmatrix}0&0\\0&1\end{pmatrix}$$

$$\hat{\sigma}_x=\begin{pmatrix}0&1\\1&0\end{pmatrix},\hat{\sigma}_y=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\hat{\sigma}_z=\begin{pmatrix}1&0\\0&-1\end{pmatrix}$$

$$\hat{C}_\uparrow^\dagger\hat{C}_\uparrow=\frac{1+\hat{\sigma}_z}{2},\hat{C}_\uparrow^\dagger\hat{C}_\downarrow=\frac{\hat{\sigma}_x+i\hat{\sigma}_y}{2},\hat{C}_\downarrow^\dagger\hat{C}_\uparrow=\frac{\hat{\sigma}_x-i\hat{\sigma}_y}{2},\hat{C}_\downarrow^\dagger\hat{C}_\downarrow=\frac{1-\hat{\sigma}_z}{2}$$

Heisenberg模型

$$\widehat{H}_c = -\frac{1}{2}\sum_{ll'}{}'\sum_{\sigma\sigma'} U_{ll'}\cdot \widehat{C}^{\dagger}_{l\sigma}\cdot \widehat{C}_{l\sigma'}\cdot \widehat{C}^{\dagger}_{l'\sigma'}\cdot \widehat{C}^{\dagger}_{l'\sigma}$$

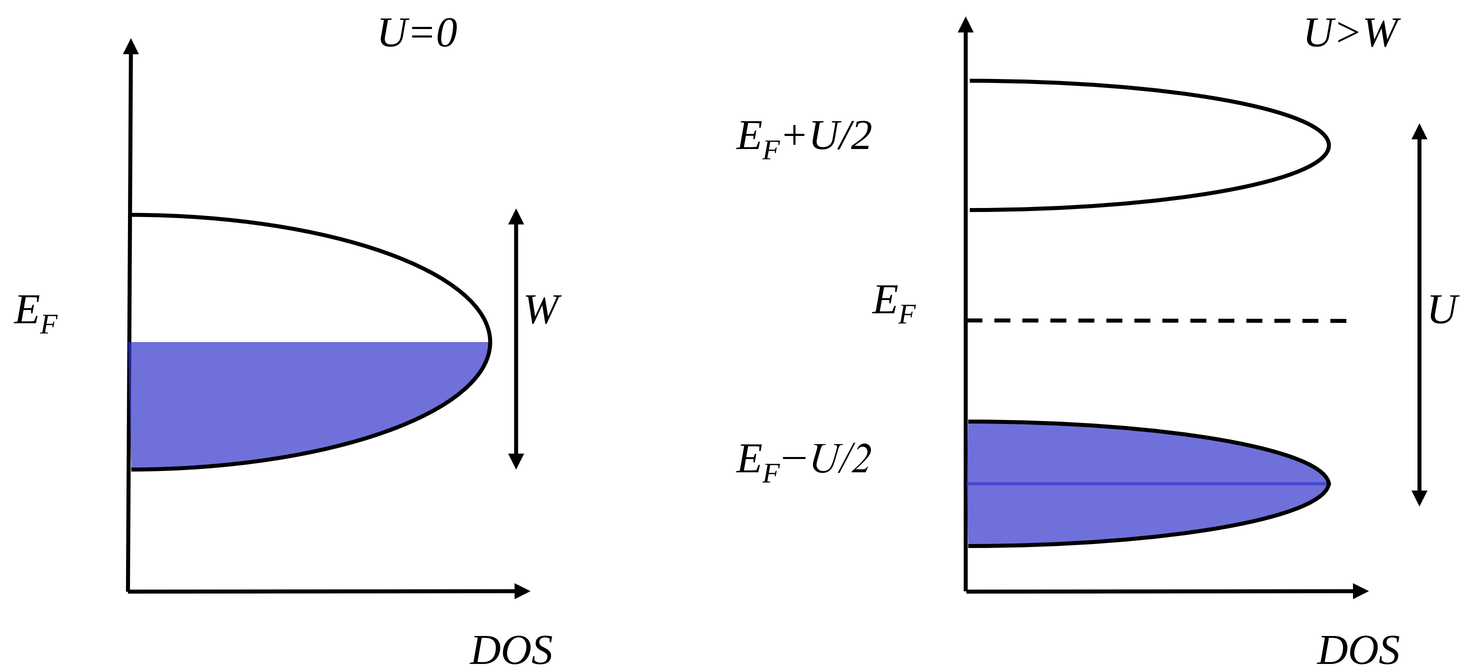
$$= -\frac{1}{2}\sum_{ll'}{}' U_{ll'}\left(\frac{1+\widehat{\sigma}_{lz}}{2}\cdot\frac{1+\widehat{\sigma}_{l'z}}{2}+\frac{\widehat{\sigma}_{lx}+i\widehat{\sigma}_{ly}}{2}\cdot\frac{\widehat{\sigma}_{l'x}-i\widehat{\sigma}_{l'y}}{2}\right.$$

$$\left.+\frac{\widehat{\sigma}_{lx}-i\widehat{\sigma}_{ly}}{2}\cdot\frac{\widehat{\sigma}_{l'x}+i\widehat{\sigma}_{l'y}}{2}+\frac{1-\widehat{\sigma}_{lz}}{2}\cdot\frac{1-\widehat{\sigma}_{l'z}}{2}\right)$$

$$= -\frac{1}{4}\sum_{ll'}{}' U_{ll'}(\widehat{\sigma}_l\cdot\widehat{\sigma}_{l'}+1)$$

Hubbard模型

物理模型：



Hubbard模型

1. 系统哈密顿量

$$\hat{H}=\sum_{i}\hat{h}(\vec{r}_i)+\sum_{<i,j>}U(\vec{r}_i,\vec{r}_j)=\sum_{i}\hat{h}(\vec{r}_i)+\sum_{<i,j>}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}$$

2. 带入坐标表象下哈密顿量的二次量子化公式

$$\hat{H}=\int\hat{\Psi}^{\dagger}(\vec{r})\hat{h}(\vec{r})\hat{\Psi}(\vec{r})d\vec{r}$$

$$+\frac{1}{2}\iint\hat{\Psi}^{\dagger}(\vec{r})\hat{\Psi}^{\dagger}(\vec{r}')\hat{U}(\vec{r}-\vec{r}')\hat{\Psi}(\vec{r}')\hat{\Psi}(\vec{r})d\vec{r}d\vec{r}'$$

3. 选取瓦尼尔表象 $\hat{\Psi}(\vec{r},s)=\sum_{l}\sum_{\sigma}a_l(\vec{r})\chi_\sigma(s)\hat{C}_{l\sigma}$

Hubbard模型

- 单体项

$$\hat{H}^{(1)} = \sum_{l,l'} \sum_{\sigma} \hat{C}^{\dagger}_{l\sigma} \hat{C}_{l'\sigma} J_{ll'}$$

$$J_{ll'} = \int a^*\left(\vec{r} - \vec{l}\,\right) \hat{h}(\vec{r})\, a\left(\vec{r} - \vec{l}\,'\right) d\vec{r}$$

- 两体项

$$\hat{H}^{(2)} = \frac{1}{2} \sum_{l_1 l_2 l_3 l_4} \sum_{\sigma_1 \sigma_2} < l_1 l_2 |\hat{U}| l_3 l_4 > \hat{C}^{\dagger}_{l_1\sigma_1} \hat{C}^{\dagger}_{l_2\sigma_2} \hat{C}_{l_3\sigma_2} \hat{C}_{l_4\sigma_1}$$

$$< l_1 l_2 |\hat{U}| l_3 l_4 > = \iint a^*\left(\vec{r} - \vec{R}_{l_1}\right) a^*\left(\vec{r} - \vec{R}_{l_2}\right) \hat{U}(\vec{r} - \vec{r}\,')\, a\left(\vec{r}\,' - \vec{R}_{l_3}\right) a\left(\vec{r} - \vec{R}_{l_4}\right) d\vec{r} d\vec{r}\,'$$

4. 限制条件

(1) 对单体项的近似（只记最近邻格点间的电子跃迁）

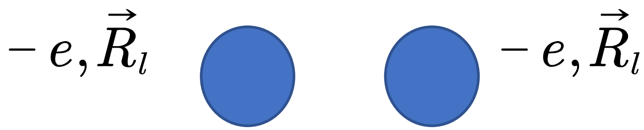
$$\hat{H}^{(1)} = \sum_{l,l'} \sum_{\sigma} \hat{C}^{\dagger}_{l,\sigma} \hat{C}_{l',\sigma} J_{l,l'}$$

$$= \varepsilon(0) \sum_{l} \sum_{\sigma} \hat{C}^{\dagger}_{l,\sigma} \hat{C}_{l,\sigma} - J \sum_{l,\rho} \sum_{\sigma} \hat{C}^{\dagger}_{l,\sigma} \hat{C}_{l+\rho,\sigma}$$

$\vec{\rho}$：最近邻格点矢量差，$\varepsilon(0) = J_{l,l}$，$J_{l,l+\rho} = -J$

Hubbard模型

$$\frac{1}{2}\sum_{l_1 l_2 l_3 l_4}\sum_{\sigma_1\sigma_2} < l_1 l_2|\hat{U}|l_3 l_4 > \hat{C}^{\dagger}_{l_1,\sigma_1}\hat{C}^{\dagger}_{l_2,\sigma_2}\hat{C}_{l_3,\sigma_2}\hat{C}_{l_4,\sigma_1}$$



$$\hat{C}^{\dagger}_{l,\sigma_1} \quad \hat{C}_{l,\sigma_1}$$

$$\hat{C}^{\dagger}_{l,\sigma_2} \quad \hat{C}_{l,\sigma_2}$$

Hubbard模型

(2) 对二体项的近似（只记单中心积分的贡献）

$$\widehat{H}^{(2)}=\frac{1}{2}\sum_{l_1l_2l_3l_4}\sum_{\sigma_1\sigma_2}<l_1l_2|\widehat{U}|l_3l_4>\widehat{C}^{\dagger}_{l_1,\sigma_1}\widehat{C}^{\dagger}_{l_2,\sigma_2}\widehat{C}_{l_3,\sigma_3}\widehat{C}_{l_4,\sigma_4}$$

$$=\frac{U}{2}\sum_{l}\sum_{\sigma\sigma'}\widehat{C}^{\dagger}_{l,\sigma}\widehat{C}^{\dagger}_{l,\sigma'}\widehat{C}_{l,\sigma'}\widehat{C}_{l,\sigma}$$

$$=\frac{U}{2}\sum_{l}\sum_{\sigma}\widehat{C}^{\dagger}_{l,\sigma}\widehat{C}^{\dagger}_{l,-\sigma}\widehat{C}_{l,-\sigma}\widehat{C}_{l,\sigma}$$

$$=U\sum_{l}\widehat{C}^{\dagger}_{l,\uparrow}\widehat{C}^{\dagger}_{l,\downarrow}\widehat{C}_{l,\downarrow}\widehat{C}_{l,\uparrow}$$

$$=U\sum_{l}\widehat{n}_{l,\uparrow}\widehat{n}_{l,\downarrow}$$

$$U=\iint a^*\left(\vec{r}-\vec{R}_l\right)a^*\left(\vec{r}-\vec{R}_l\right)U\left(\vec{r}-\vec{r}'\right)a\left(\vec{r}'-\vec{R}_l\right)a\left(\vec{r}-\vec{R}_l\right)d\vec{r}d\vec{r}'$$

Hubbard模型

$$\widehat{H}=\varepsilon(0)\sum_{l}\sum_{\sigma}\widehat{C}_{l,\sigma}^{\dagger}\widehat{C}_{l,\sigma}-J\sum_{l}\sum_{\rho}\sum_{\sigma}\widehat{C}_{l,\sigma}^{\dagger}\widehat{C}_{l+\rho,\sigma}+U\sum_{l}\widehat{n}_{l,\uparrow}\widehat{n}_{l,\downarrow}$$

主要物理状态取决于U和t的比值。

U>>t→金属绝缘体相变

总结

1. 二次量子化是研究全同粒子体系的量子理论

2. 二次量子化计算的范式:
   (1) 确定全同粒子系统哈密顿量
   (2) 带入坐标表象二次量子化公式
   (3) 选择合适的表象
   (4) 考虑限制条件
   (5) 计算哈密顿量的二次量子化表示

谢谢！

讲义下载地址：
https://zhangtianyi030.github.io/JiangYi/second_quantization_in_condensed_matter.pdf