ADVANCED QUANTUM MECHANICS

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1.4.1　置换对称性

考虑两粒子体系, 一个粒子用 $|k'\rangle$ 描述. 两粒子体系所处的态为 $|k'\rangle_1 \otimes |k''\rangle_2$ 描述. 若 $k' \neq k''$, 则 $|k'\rangle_1 \otimes |k''\rangle_2 \neq |k''\rangle_1 \otimes |k'\rangle_2$. 约定总是以编号顺序直积各态, 便可省去下标与直积符号. 线性组合 $c_1|k'\rangle|k''\rangle + c_2|k''\rangle|k'\rangle$ 会给出等价的本征值.

引入置换算符 P_{12}, 作用为 $P_{12}|k'\rangle|k''\rangle = |k''\rangle|k'\rangle$, 显然有 $P_{12} = P_{21}$ 与 $P_{12}^2 = \mathbb{I}$. 所以 P_{12} 本征值为 ± 1.

写出全同两粒子体系的哈密顿量. 坐标 x_i 和动量 p_i 等量对于 $i = 1, 2$ 对称, 如

$$H = \sum_i^2 \frac{\vec{p}_i^2}{2m} + V_{\text{pair}}(|\vec{x}_1 - \vec{x}_2|) + \sum_i^2 V_{\text{ext}}(\vec{x}_i)$$

通过构造 $P_{12}HP_{12} = H$ 证明 $[P_{12}, H] = 0$. 则 P_{12} 的本征态为 $|k'k''\rangle_\pm = \dfrac{1}{\sqrt{2}}(|k'\rangle|k''\rangle \pm |k''\rangle|k'\rangle)$, 即要么完全对称, 要么完全反对称. 推广到 N 个全同粒子, 引入置换算符 P_{ij}, 作用是

$$P_{ij}|k'\rangle_1|k''\rangle_2 \cdots |k^{(i)}\rangle_i|k^{(i+1)}\rangle_{i+1} \cdots |k^{(j)}\rangle_j \cdots = |k'\rangle_1|k''\rangle_2 \cdots |k^{(j)}\rangle_i|k^{(i+1)}\rangle_{i+1} \cdots |k^{(i)}\rangle_j \cdots$$

完全对称态满足玻色-爱因斯坦统计, 完全反对称态满足费米-狄拉克统计.

1.4.2　两电子系统

电子具有自旋, 因此系统波函数除了空间波函数, 还有旋量. 通过对 $\left|\frac{1}{2}, \frac{1}{2}\right\rangle \left|\frac{1}{2}, \frac{1}{2}\right\rangle = |\uparrow\uparrow\rangle$ 使用 $S^- = S^-_{(1)} + S^-_{(2)}$ 可以得到三重态和单态:

$$\begin{aligned}
\psi(\vec{x}_1, \vec{x}_2; s, m) &= \phi(\vec{x}_1, \vec{x}_2)|s, m\rangle \\
|1, 1\rangle &= |\uparrow\uparrow\rangle, \\
|1, 0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle), \\
|1, -1\rangle &= |\downarrow\downarrow\rangle, \\
|0, 0\rangle &= \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)
\end{aligned}$$

因为空间波函数和旋量直乘, 而费米-狄拉克要求总函数反对称, 若旋量对称, 对应空间波函数反对称, 反之亦然. 观察可知, 三重态对称, 而单态反对称.

1.4.3 多电子系统

1.4.3.1 多电子系统的哈密顿量

对于大量电子和原子核构成的系统, 其哈密顿量一般为

$$
\begin{aligned}
H=&-\sum_i \frac{\hbar^2}{2m_e}\nabla_i^2+\sum_{i,I}\frac{1}{4\pi\epsilon_0}\frac{Z_Ie^2}{|\vec{r}_i-\vec{R}_I|}+\frac{1}{2}\sum_{i\neq j}\frac{1}{4\pi\epsilon_0}\frac{e^2}{|\vec{r}_i-\vec{r}_j|}\\
&-\sum\frac{\hbar^2}{2M_I}\nabla_I^2+\frac{1}{2}\sum_{I\neq J}\frac{1}{4\pi\epsilon_0}\frac{Z_IZ_Je^2}{|\vec{R}_I-\vec{R}_J|}
\end{aligned}
$$

电子使用小写, 原子核使用大写. 采用波恩-奥本海默近似/绝热近似, 即因原子核质量远大于电子质量, 而近似忽略原子核的动能项, 且视原子核相对静止, 从而认为原子核之间的互能为常数. 采用 Hartree 原子单位制, 多电子哈密顿量可简化为

$$
\begin{aligned}
H&=T+V_{ne}+V_{ee}\\
&=\sum_i\left(-\frac{1}{2}\nabla_i^2\right)+\sum_i v\left(\vec{r}_i\right)+\sum_{i<j}\frac{1}{r_{ij}}\\
v\left(\vec{r}_i\right)&=-\sum_I\frac{Z_I}{r_{iI}}
\end{aligned}
$$

1.4.3.2 变分原理

$$
\begin{aligned}
\psi&=\sum_i c_i\psi_i,\\
E&=\frac{\sum_i||c_i||^2E_i}{\sum_i||c_i||^2}\geq\frac{\sum_i||c_i||^2E_0}{\sum_i||c_i||^2}=E_0,\quad E=E_0\iff\psi=\psi_0\\
\delta\big[\langle\psi|H|\psi\rangle&-E(\langle\psi|\psi\rangle-1)\big]=0,\quad\delta(\langle\psi|):\langle\delta\psi|H-E|\psi\rangle=0
\end{aligned}
$$

1.4.3.3 Hatree-Fock 近似

设系统波函数可由 Slater 行列式近似, 即 $\Psi=\frac{1}{\sqrt{N!}}\det[\psi_{q(1)}\psi_{q(2)}\cdots\psi_{q(N)}]$, $\psi_q(\vec{x})$ 表示单个电子的波函数(空间直乘自旋), q 标记所有量子数. Hartree-Fock 近似认为, 使得 E 最小化的波函数仍然维持行列式形式, 只是需要通过变分法确定各量子数 q. 通过这样的方法求得的 E_0 被标记为

$$
\begin{aligned}
E_{\text{HF}}&=\langle\Psi_{\text{HF}}|H|\Psi_{\text{HF}}\rangle=\sum_i H_i+\frac{1}{2}\sum_{i,j}(J_{ij}-K_{ij})\\
H_i&=\int\psi_i^*(\vec{x})\left[-\frac{1}{2}\nabla^2+v(\vec{x})\right]\psi_i(\vec{x})\mathrm{d}\vec{x}\\
J_{ij}&=\iint\psi_i^*(\vec{x}_1)\psi_j^*(\vec{x}_2)\frac{1}{r_{12}}\psi_i(\vec{x}_1)\psi_j(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2,\quad\text{Coulomb integrals}\\
K_{ij}&=\iint\psi_i^*(\vec{x}_1)\psi_j^*(\vec{x}_2)\frac{1}{r_{12}}\psi_j(\vec{x}_1)\psi_i(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2,\quad\text{exchange integrals}
\end{aligned}
$$

省去分母是因为 Slater 行列式的系数已经确保波函数可以归一化.

$$
\begin{aligned}
&\left\langle \Psi_{\mathrm{HF}} \left| \frac{1}{r_{ij}} \right| \Psi_{\mathrm{HF}} \right\rangle \\
=&\int \frac{1}{N!}\sum_{PP'}\eta_P\eta_{P'}\left(\psi^*_{P(1)}(\vec{x}_1)\cdots\psi^*_{P(N)}(\vec{x}_N)\right)\frac{1}{r_{ij}}\left(\psi_{P(1)}(\vec{x}_1)\cdots\psi_{P(N)}(\vec{x}_N)\right)\mathrm{d}\vec{x}^N \\
=&\int \frac{1}{N!}\sum_{PP'}\eta_P\eta_{P'}\prod_{k\neq i,j}\delta_{P(k),P'(k)}\psi^*_{P(i)}(\vec{x}_i)\psi^*_{P(j)}(\vec{x}_j)\frac{1}{r_{12}}\psi_{P(i)}(\vec{x}_i)\psi_{P(j)}(\vec{x}_j)\mathrm{d}\vec{x}_i\mathrm{d}\vec{x}_j \\
=&\int \frac{1}{N!}\sum_{PP'}\eta_P\eta_{P'}\left(\delta_{P',P}+\delta_{P',PP_{ij}}\right)\psi^*_{P(i)}(\vec{x}_1)\psi^*_{P(j)}(\vec{x}_2)\frac{1}{r_{12}}\psi_{P'(i)}\psi_{P'(j)}(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \\
=&\int \frac{1}{N!}\sum_{P}\psi^*_{P(i)}(\vec{x}_1)\psi^*_{P(j)}(\vec{x}_2)\frac{1}{r_{12}}\psi_{P(i)}(\vec{x}_1)\psi_{P(j)}(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \\
&-\int \frac{1}{N!}\sum_{P}\psi_{P(i)}(\vec{x}_1)^*\psi^*_{P(j)}(\vec{x}_2)\frac{1}{r_{12}}\psi_{P(j)}(\vec{x}_1)\psi_{P(i)}(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \\
=&\int \frac{1}{N(N-1)}\sum_{i\neq j}\psi^*_i(\vec{x}_1)\psi^*_j(\vec{x}_2)\frac{1}{r_{12}}\psi_i(\vec{x}_1)\psi_j(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \\
&-\int \frac{1}{N(N-1)}\sum_{i\neq j}\psi^*_i(\vec{x}_1)\psi^*_j(\vec{x}_2)\frac{1}{r_{12}}\psi_j(\vec{x}_1)\psi_i(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2
\end{aligned}
$$

系数 $\frac{1}{N(N-1)}$ 可以通过对 i,j 求和消去. 对 E_{HF} 求 $\delta\psi_i^*$ 变分, 且使用 $\int\psi_i^*(\vec{x})\psi_j(\vec{x})\mathrm{d}\vec{x}=\delta_{ij}$ 正交条件, 得到 Hatree-Fock 微分方程:

$$
\begin{aligned}
\left[-\frac{1}{2}\nabla^2+v+\hat{j}-\hat{k}\right]\psi_i(\vec{x})&=\sum_j\varepsilon_{ij}\psi_j(\vec{x}) \\
\Rightarrow\int\psi_i^*(\vec{x})\left[-\frac{1}{2}\nabla^2+v+\hat{j}-\hat{k}\right]\psi_i(\vec{x})\mathrm{d}\vec{x}&=\int\psi_i^*(\vec{x})\sum_j\varepsilon_{ij}\psi_j(\vec{x})\mathrm{d}\vec{x}=\varepsilon_{ii}\equiv\varepsilon_i \\
\hat{j}(\vec{x}_1)f(\vec{x}_1)&=\sum_{k=1}^N\int\psi_k^*(\vec{x}_2)\psi_k(\vec{x}_2)\frac{1}{r_{12}}f(\vec{x}_1)\mathrm{d}\vec{x}_2 \\
\hat{k}(\vec{x}_1)f(\vec{x}_1)&=\sum_{k=1}^N\int\psi_k^*(\vec{x}_2)f(\vec{x}_2)\frac{1}{r_{12}}\psi_k(\vec{x}_1)\mathrm{d}\vec{x}_2
\end{aligned}
$$

将轨道能量 ε_i 对 i 求和, 与 E_{HF} 比较可知

$$
\begin{aligned}
E_{\mathrm{HF}}&=\sum_{i=1}^N\varepsilon_i-V_{ee} \\
V_{ee}&=\int\Psi^*_{\mathrm{HF}}(\vec{x}^N)\left(\sum_{i<j}\frac{1}{r_{ij}}\right)\Psi_{\mathrm{HF}}(\vec{x}^N)\mathrm{d}\vec{x}^N=\frac{1}{2}\sum_{i,j=1}^N(J_{ij}-K_{ij})
\end{aligned}
$$

1.4.3.4 均匀电子气

无相互作用的电子气哈密顿量为 $H_0=\sum_i\left(-\frac{1}{2}\nabla_i^2\right)$, 因为 $[p_i,H_0]=[p_i,p_j]=0$, 所以具有共同本征态. 动量本征态在 $\vec{x}$ 表象下是平面波 $\psi_{\vec{k}}(\vec{r})=\frac{1}{\sqrt{V}}e^{i\vec{k}\cdot\vec{r}}$, 使用 Slater 行列式将 N 电子气体波函数写为 $\Psi_0=\frac{1}{\sqrt{N!}}\det[\psi_{\vec{k}_j,s_j}(\vec{x}_i)]$, 其中 $\psi_{\vec{k},s}=\psi_{\vec{k}}\chi(s)$. 系统能量为 $E=\sum_i\frac{|k_i|^2}{2}$. 求解能量和粒子数密度可参见 5a, 此处略过.

接下来考虑加入电子相互作用的修正. 首先是 Coulomb 能:

$$E_{\text{Coulomb}} = \frac{1}{2}\sum_{i,j}\iint \psi^*_{\vec{k}_i}(\vec{x}_1)\psi^*_{\vec{k}_j}(\vec{x}_2)\frac{1}{r_{12}}\psi_{\vec{k}_i}(\vec{x}_1)\psi_{\vec{k}_j}(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2$$

这部分积分会产生发散. 一般是通过引入正电荷背景以进行抵消. 而 eXchange 能对于修正更具有意义, 它是

$$E_{\text{eXchange}} = -\frac{1}{2}\sum_{i,j}\iint \psi^*_{\vec{k}_i}(\vec{x}_1)\psi^*_{\vec{k}_j}(\vec{x}_2)\frac{\delta_{s_i,s_j}}{r_{12}}\psi_{\vec{k}_j}(\vec{x}_1)\psi_{\vec{k}_i}(\vec{x}_2)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2$$

为了便于计算, 将势能写作动量空间的形式. 由于傅里叶变化形式众说纷纭, 所以约定

$$\begin{cases} F(\vec{k}) = \displaystyle\int f(\vec{x})e^{-i\vec{k}\cdot\vec{x}}\mathrm{d}\vec{x} \\ f(\vec{x}) = \left(\dfrac{1}{2\pi}\right)^3\displaystyle\int F(\vec{k})e^{i\vec{k}\cdot\vec{x}}\mathrm{d}\vec{q} \end{cases}$$

于是汤川势有

$$\mathcal{F}\left[\frac{e^{-ar}}{r}\right] = \int\frac{e^{-ar}}{r}e^{-i\vec{q}\cdot\vec{r}}\mathrm{d}\vec{r} = \frac{4\pi}{q^2+a^2}$$

库伦势是汤川势 $a=0$ 的特例: $\displaystyle\int\frac{1}{r}e^{-i\vec{q}\cdot\vec{r}}\mathrm{d}\vec{r} = \frac{4\pi}{q^2}$, 所以其逆变换为

$$\frac{1}{r_{12}} = \left(\frac{1}{2\pi}\right)^3\int\frac{4\pi}{q^2}e^{i\vec{q}\cdot(\vec{x}_1-\vec{x}_2)}\mathrm{d}\vec{q}$$

将其代入于 E_{eXchange} 中, 且使用普朗克尔定理 $\displaystyle\int\mathrm{d}^3\vec{x}e^{i\vec{k}\cdot\vec{x}} = (2\pi)^3\delta^{(3)}(\vec{k},\vec{0})$:

$$\begin{aligned}
E_{\text{eXchange}} &= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\iint\frac{1}{\sqrt{V}}e^{-i\vec{k}_i\cdot\vec{x}_1}\frac{1}{\sqrt{V}}e^{-i\vec{k}_j\cdot\vec{x}_2}\left[\left(\frac{1}{2\pi}\right)^3\frac{4\pi}{q^2}e^{i\vec{q}\cdot(\vec{x}_1-\vec{x}_2)}\mathrm{d}\vec{q}\right]\frac{1}{\sqrt{V}}e^{i\vec{k}_j\cdot\vec{x}_1}\frac{1}{\sqrt{V}}e^{i\vec{k}_i\cdot\vec{x}_2}\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2 \\
&= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\int\left[\frac{1}{V^2}\left(\int e^{-i\vec{k}_i\cdot\vec{x}_1}e^{i\vec{q}\cdot\vec{x}_1}e^{i\vec{k}_j\cdot\vec{x}_1}\mathrm{d}\vec{x}_1\right)\left(\int e^{-i\vec{k}_j\cdot\vec{x}_2}e^{-i\vec{q}\cdot\vec{x}_2}e^{i\vec{k}_i\cdot\vec{x}_2}\mathrm{d}\vec{x}_2\right)\right]\frac{4\pi}{q^2}\frac{\mathrm{d}\vec{q}}{(2\pi)^3} \\
&= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\int\left[\frac{1}{V^2}\left(\iint e^{i(\vec{k}_i-\vec{k}_j)\cdot(\vec{x}_1-\vec{x}_2)}e^{-i\vec{q}\cdot(\vec{x}_1-\vec{x}_2)}\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2\right)\right]\frac{4\pi}{q^2}\frac{\mathrm{d}\vec{q}}{(2\pi)^3} \\
&= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\int\left[\frac{1}{V^2}\left(\iint e^{i(\vec{k}_i-\vec{k}_j)\cdot\vec{r}}e^{-i\vec{q}\cdot\vec{r}}\mathrm{d}\vec{r}\mathrm{d}\vec{x}_1\right)\right]\frac{4\pi}{q^2}\frac{\mathrm{d}\vec{q}}{(2\pi)^3} \\
&= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\int\left[\frac{1}{V^2}(2\pi)^{(3)}\delta^{(3)}(\vec{k}_i-\vec{k}_j,\vec{q})\cdot V\right]\frac{4\pi}{q^2}\frac{\mathrm{d}\vec{q}}{(2\pi)^3} \\
&= -\frac{\delta_{s_i,s_j}}{2}\sum_{i,j}\left[\frac{1}{V}\right]\frac{4\pi}{|\vec{k}_i-k_j|^2} \\
&= -\frac{1}{2V}\sum_{i,j}\frac{4\pi\delta_{s_i,s_j}}{|\vec{k}_i-\vec{k}_j|^2}
\end{aligned}$$

每个波矢 $\vec{k}$ 可提供两个自旋态, 所以将其移出 $\vec{k}_i$, 从而只对波矢求和:

$$
\begin{aligned}
E_{\text{eXchange}} &= -\frac{1}{V}\sum_{\vec{k}_m,\vec{k}_n}\frac{4\pi}{|\vec{k}_m-\vec{k}_n|^2} \\
&= -4\pi\sum_{\vec{k}_m}\int_{k_n\le k_F}\frac{\mathrm{d}\vec{k}_n}{(2\pi)^3}\frac{1}{|\vec{k}_m-\vec{k}_n|^2} \\
&= -4\pi\sum_{\vec{k}_m}\frac{k_F F\left(\dfrac{k_m}{k_F}\right)}{2\pi^2}
\end{aligned}
$$

其中 $F(x)=\dfrac{1}{2}+\dfrac{1-x^2}{4x}\ln\left|\dfrac{1+x}{1-x}\right|$. 进一步使用技巧 $\sum_{\vec{k}_m}=\dfrac{V}{(2\pi)^3}\int\mathrm{d}\vec{k}_m$, 且使用结论 $k_F=\left(3\pi^2 n\right)^{1/3}$, 即有

$$
E_{\text{eXchange}}=\boxed{-\frac{k_F^4 V}{4\pi^3}}=-\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}n^{\frac{4}{3}}V
$$

1.4.4 二次量子化

1.4.4.1 一次量子化和二次量子化

$$
E=\frac{p^2}{2m}+V(\vec{x},t)\Rightarrow\hat{H}=\frac{1}{2m}\hat{p}^2+\hat{V}\Rightarrow\hat{H}=\sum_{i,j}\hat{a}_i^\dagger\hat{a}_j
$$

一次量子化引入算符和波函数, 二次量子化引入场算符.

1.4.4.1.1 一次量子化态 一般性地, 设单粒子的 Hilbert 空间维度为 D, 且基矢为 $\{|\psi\rangle\},\psi=\psi_1,\psi_2,\cdots\psi_D$. 那么 N 粒子体系的 Hilbert 空间维度将是 D^N, 基矢为各粒子基矢的直积 $|[\psi]\rangle=|\psi\rangle_{(1)}\otimes|\psi\rangle_{(2)}\otimes\cdots\otimes|\psi\rangle_{(N)}$, $|\psi\rangle_{(j)}=|\psi_1\rangle,|\psi_2\rangle,\cdots,|\psi_D\rangle$

1. 一次量子化中的一般态: $|\Psi\rangle=\sum_{[\psi]}C[\psi]|[\psi]\rangle$, $C[\psi]$ 是多体波函数的系数.
2. 全同玻色子: $\mathcal{S}|[\psi]=\sum_{P\in S_N}\prod_{i=1}^{N}|\psi\rangle_{P(i)}$
3. 全同费米子: $\mathcal{A}|[\psi]\rangle=\sum_{P\in S_N}\eta_P\prod_{i=1}^{N}|\psi\rangle_{P(i)}$

通过组合数计算可知, 全同玻色/费米子在总 Hilbert 空间中占据极少, 所以使用一次量子化的表述总是不方便的. 而二次量子化使用的 Fock 空间将自动考虑粒子全同性, 即在 Fock 空间中任意态都是满足粒子全同性的.

1.4.4.1.2 二次量子化态 二次量子化的观点是占据数表象, 即定义单个粒子态 $|\psi_\alpha\rangle$ 占据数为 n_α, 那么 N 粒子态波函数可以写为 Fock 态: $|[n]\rangle=|n_1,n_2,\cdots,n_\alpha,\cdots,n_D\rangle$. 玻色子可以有任意多个粒子占据同一态, 即 $n_\alpha\in\mathbb{N}$; 费米子至多有一个, 即 $n_\alpha=0,1$. 由于粒子数守恒, 有 $\sum_\alpha n_\alpha=N$. 使用上述定义的 Fock 态作为基矢, 张成的空间即为 Fock 空间. 如果使用 $\mathcal{F}$ 表示 Fock 空间, 那么

$$
\begin{aligned}
\mathcal{F}&=\mathcal{F}^0\oplus\mathcal{F}^1\oplus\mathcal{F}^2\oplus\cdots \\
\mathcal{F}^{N_j}&=\text{span}\left\{|n_1,n_2,\cdots,n_D\rangle|\sum_{i=1}^{D}n_i=N_j\right\}
\end{aligned}
$$

二次量子化下的多体态函数是 Fock 态的线性组合 $|\Psi\rangle=\sum_{[n]}C[n]|[n]\rangle$, 每个 Fock 态都有其一次量子化表示.

1.4.4.1.3 Fock 态的表示 引入下标 B 表示玻色统计, F 表示费米统计. 占据数均为 0 ($n_i = 0, \forall i$) 的 Fock 态被称为真空态 $|0\rangle = |\cdots, 0\cdots\rangle$, 所以 $|0\rangle_B = |0\rangle_F$. 仅有一个占据数 $n_\psi \neq 0$ 的 Fock 态被称为单模(single-mode) Fock 态.

$$
\begin{aligned}
|n_\psi\rangle &= |\cdots, 0, n_\psi, 0, \cdots\rangle \\
|1_\psi\rangle_B &= |1_\psi\rangle_F = |\psi\rangle \\
|n_\psi\rangle_B &= \prod_{i=1}^{n_\psi} |\psi\rangle \equiv |\psi\rangle^{\otimes n_\psi}
\end{aligned}
$$

对于多模(multi-mode) Fock 态, 则涉及多个粒子态(比如 $|\psi_i\rangle$, $|\psi_j\rangle$). 在一次量子化中已经学习过如何根据交换对称/反对称构造其波函数:

$$
\begin{aligned}
|1_{\psi_i}, 1_{\psi_j}\rangle_B &= \frac{1}{\sqrt{2}}(|\psi_i\rangle \otimes |\psi_j\rangle + |\psi_j\rangle \otimes |\psi_i\rangle) \\
|1_{\psi_i}, 1_{\psi_j}\rangle_F &= \frac{1}{\sqrt{2}}(|\psi_i\rangle \otimes |\psi_j\rangle - |\psi_j\rangle \otimes |\psi_i\rangle) \\
|2_{\psi_i}, 1_{\psi_j}\rangle_B &= \frac{1}{\sqrt{3}}(|\psi_i\rangle \otimes |\psi_i\rangle \otimes |\psi_j\rangle + |\psi_i\rangle \otimes |\psi_j\rangle \otimes |\psi_i\rangle + |\psi_j\rangle \otimes |\psi_i\rangle \otimes |\psi_i\rangle) \\
|1_{\psi_i}, 1_{\psi_j}, 1_{\psi_k}\rangle &= \frac{1}{\sqrt{6}}(|\psi_i\rangle \otimes |\psi_j\rangle \otimes |\psi_k\rangle + |\psi_j\rangle \otimes |\psi_k\rangle \otimes |\psi_i\rangle + |\psi_k\rangle \otimes |\psi_i\rangle \otimes |\psi_j\rangle \\
&\quad - |\psi_k\rangle \otimes |\psi_j\rangle \otimes |\psi_i\rangle - |\psi_j\rangle \otimes |\psi_i\rangle \otimes |\psi_k\rangle - |\psi_i\rangle \otimes |\psi_k\rangle \otimes |\psi_j\rangle)
\end{aligned}
$$

1. 玻色子:

$$
|[n]\rangle_B = \left(\frac{1}{N!\prod_\psi n_\psi!}\right)^{\frac{1}{2}} \mathcal{S} \bigotimes_\psi |\psi\rangle^{\otimes n_\psi}
$$

2. 费米子:

$$
|[n]\rangle_F = \left(\frac{1}{N!}\right)^{\frac{1}{2}} \mathcal{A} \bigotimes_\psi |\psi\rangle^{\otimes n_\psi}
$$

1.4.5 产生湮灭算符

1.4.6 态的产生和湮灭

下面介绍如何引入产生/湮灭算符, 即在量子多体系统中产生/湮灭一个粒子. 准备单粒子态 $|\psi_i\rangle$, $|\psi_j\rangle$; 单位张量 $|0\rangle = \mathbb{I}$, 一次量子化的态函数 $|\Psi\rangle$, $|\Phi\rangle$. 定义添加(Add)算符 $\hat{A}_\pm$ 和删除(Delete)算符 $\hat{D}_\pm$, 下标 $\pm$ 表示添加/删除后的态需要对称化/反对称化. 比如, $|\psi_i\rangle\hat{A}_+|\Psi\rangle$ 表示在已有的态函数 $|\Psi\rangle$ 中添加一个粒子且该粒子态为 $|\psi_i\rangle$, 且要求增加后的态函数对称化. 可以总结出 $\hat{A}_\pm$ 和 $\hat{D}_\pm$ 将具有

1. 线性性: $\begin{cases} |\psi_i\rangle\hat{A}_\pm(a|\Psi\rangle + b|\Phi\rangle) = a|\psi_i\rangle\hat{A}_\pm|\Psi\rangle + b|\psi_i\rangle\hat{A}_\pm|\Phi\rangle \\ |\psi_i\rangle\hat{D}_\pm(a|\Psi\rangle + b|\Phi\rangle) = a|\psi_i\rangle\hat{D}_\pm|\Psi\rangle + b|\psi_i\rangle\hat{D}_\pm|\Phi\rangle \end{cases}$

2. 真空态: $|\psi_i\rangle\hat{A}_\pm|0\rangle = |\psi_i\rangle, \quad |\psi_i\rangle\hat{D}_\pm|0\rangle = 0$

3. 直积展开: $\begin{cases} |\psi_i\rangle\hat{A}_\pm|\psi_j\rangle \otimes |\Psi\rangle = |\psi_i\rangle \otimes |\psi_j\rangle \otimes |\Psi\rangle \pm |\psi_j\rangle \otimes (|\psi_i\rangle\hat{A}_\pm|\Psi\rangle) \\ |\psi_i\rangle\hat{D}_\pm|\psi_j\rangle \otimes |\Psi\rangle = \langle\psi_i|\psi_j\rangle|\Psi\rangle \pm |\psi_j\rangle \otimes (|\psi_i\rangle\hat{D}_\pm|\Psi\rangle) \end{cases}$

1.4.7 玻色子的产生湮灭算符

1. 玻色产生算符 $b_\alpha^\dagger$, 即在 $|\alpha\rangle$ 上添加一个玻色子, 占据数 $n_\alpha \to n_\alpha + 1$. 因为在 $N+1$ 个位置对称添加 $|\alpha\rangle$, 所以有
$$b_\alpha^\dagger|\Psi\rangle = \frac{1}{\sqrt{N+1}}|\alpha\rangle\hat{A}_+|\Psi\rangle$$
2. 玻色湮灭算符 b_α, 即在 $|\alpha\rangle$ 上移除一个玻色子, 占据数 $n_\alpha \to n_\alpha - 1$. 因为在 N 个位置对称移除 $|\alpha\rangle$, 所以有
$$b_\alpha|\Psi\rangle = \frac{1}{\sqrt{N}}|\alpha\rangle\hat{D}_-|\Psi\rangle$$

玻色产生湮灭算符对 Fock 态的作用:

1. 单模 Fock 态:
$$\begin{aligned}
b_\alpha^\dagger|n_\alpha\rangle &= \frac{1}{\sqrt{n_\alpha+1}}|\alpha\rangle\hat{A}_+|\alpha\rangle^{\otimes n_\alpha} = \frac{n_\alpha+1}{\sqrt{n_\alpha+1}}|\alpha\rangle^{\otimes(n_\alpha+1)} = \sqrt{n_\alpha+1}|n_\alpha+1\rangle \\
b_\alpha|n_\alpha\rangle &= \frac{1}{\sqrt{n_\alpha}}|\alpha\rangle\hat{D}_+|\alpha\rangle^{\otimes n_\alpha} = \frac{n_\alpha}{\sqrt{n_\alpha}}|\alpha\rangle^{\otimes(n_\alpha-1)} = \sqrt{n_\alpha}|n_\alpha-1\rangle
\end{aligned}$$
   对于真空态即有 $b_\alpha^\dagger|0_\alpha\rangle = |1_\alpha\rangle, b_\alpha|0_\alpha\rangle = 0$. 观察到玻色子的粒子数算符 $b_\alpha^\dagger b_\alpha|\alpha\rangle = n_\alpha|n_\alpha\rangle$

   单模 Fock 态可以用产生算符 $b_\alpha^\dagger$ 作用于真空态得到: $|n_\alpha\rangle = \frac{1}{\sqrt{n_\alpha!}}\left(b_\alpha^\dagger\right)^{n_\alpha}|0_\alpha\rangle$
2. 一般 Fock 态:
$$\begin{aligned}
b_\alpha^\dagger|\cdots,n_\beta,n_\alpha,n_\gamma,\cdots\rangle_B &= \sqrt{n_\alpha+1}|\cdots,n_\beta,n_\alpha+1,n_\gamma,\cdots\rangle_B \\
b_\alpha|\cdots,n_\beta,n_\alpha,n_\gamma,\cdots\rangle_B &= \sqrt{n_\alpha}|\cdots,n_\beta,n_\alpha-1,n_\gamma,\cdots\rangle_B
\end{aligned}$$
   上述定义可求得对易关系 $\left[b_\alpha^\dagger, b_\beta^\dagger\right] = [b_\alpha, b_\beta] = 0$, $\left[b_\alpha, b_\beta^\dagger\right] = \delta_{\alpha\beta}$.

1.4.8 费米子的产生湮灭算符

1. 费米产生算符 $c_\alpha^\dagger$, 在单粒子态 $|\alpha\rangle$ 上添加一个费米子, 占据数 $n_\alpha \to n_\alpha + 1$(因此 $n_\alpha = 0$). 因为在 $N+1$ 个位置反对称添加 $|\alpha\rangle$, 所以有
$$c_\alpha^\dagger|\Psi\rangle = \frac{1}{\sqrt{N+1}}|\alpha\rangle\hat{A}_-|\Psi\rangle$$
2. 费米湮灭算符 c_α, 在单粒子态 $|\alpha\rangle$ 上移除一个费米子, 占据数 $n_\alpha \to n_\alpha - 1$(因此 $n_\alpha = 1$). 因为在 N 个位置反对称移除 $|\alpha\rangle$, 所以有
$$c_\alpha|\Psi\rangle = \frac{1}{\sqrt{N}}|\alpha\rangle\hat{D}_-|\Psi\rangle$$

玻色产生湮灭算符对 Fock 态的作用:

1. 单模 Fock 态:
$$\begin{aligned}
&c_\alpha^\dagger|0_\alpha\rangle = |\alpha\rangle\hat{A}_-\mathbb{I} = |\alpha\rangle = |1_\alpha\rangle \\
&c_\alpha^\dagger|1_\alpha\rangle = \frac{1}{\sqrt{2}}|\alpha\rangle\hat{A}_-|\alpha\rangle = \frac{1}{\sqrt{2}}(|\alpha\rangle\otimes|\alpha\rangle - |\alpha\rangle\otimes|\alpha\rangle) = 0 \\
&c_\alpha|0_\alpha\rangle = 0 \\
&c_\alpha|1_\alpha\rangle = |\alpha\rangle\hat{D}_-|\alpha\rangle = |0_\alpha\rangle
\end{aligned}$$
   总结为 $c_\alpha^\dagger|n_\alpha\rangle = \sqrt{1-n_\alpha}|1-n_\alpha\rangle, \quad c_\alpha|n_\alpha\rangle = \sqrt{n_\alpha}|1-n_\alpha\rangle$. 观察到费米子的粒子数算符 $c_\alpha^\dagger c_\alpha|n_\alpha\rangle = n_\alpha|n_\alpha\rangle$.

   单模 Fock 态可以用产生算符 $c_\alpha^\dagger$ 作用于真空态得到: $|n_\alpha\rangle = \left(c_\alpha^\dagger\right)^{n_\alpha}|0_\alpha\rangle$

2. 一般 Fock 态:

$$c_\alpha^\dagger|\cdots,n_\beta,n_\alpha,n_\gamma,\cdots\rangle_F=(-)^{\sum\limits_{\beta<\alpha}n_\beta}\sqrt{1-n_\alpha}|\cdots,n_\beta,1-n_\alpha,n_\gamma,\cdots\rangle_F$$
$$c_\alpha|\cdots,n_\beta,n_\alpha,n_\gamma,\cdots\rangle_F=(-)^{\sum\limits_{\beta<\alpha}n_\beta}\sqrt{n_\alpha}|\cdots,n_\beta,1-n_\alpha,n_\gamma,\cdots\rangle_F$$

上述定义可求得反对易关系 $\left\{c_\alpha^\dagger,c_\beta^\dagger\right\}=\{c_\alpha,c_\beta\}=0,\left\{c_\alpha,c_\beta^\dagger\right\}=\delta_{\alpha\beta}$

可以看出玻色子和费米子的(反)对易关系非常相似, 引入 $[a,b]_{-\zeta}=ab-\zeta ba$ 统一 $[a,b]$ 和 $\{a,b\}$:

$$\left[a_\alpha^\dagger,a_\beta^\dagger\right]_{-\zeta}=[a_\alpha,a_\beta]_{-\zeta}=0,\quad\left[a_\alpha,a_\beta^\dagger\right]_{-\zeta}=\delta_{\alpha\beta},\quad\zeta=\begin{cases}1,&\text{Boson}\\-1,&\text{Fermion}\end{cases}$$

1.4.9 产生湮灭算符的表象变换规律

已知单位算符 $\mathbb{I}=\sum\limits_\alpha|\alpha\rangle\langle\alpha|$, 基矢变换 $|\widetilde{\alpha}\rangle=\sum\limits_\alpha|\alpha\rangle\langle\alpha|\widetilde{\alpha}\rangle$, 真空态涨落 $|\alpha\rangle=a_\alpha^\dagger|0\rangle,\quad|\widetilde{\alpha}\rangle=a_{\widetilde{\alpha}}^\dagger|0\rangle$, 得到产生湮灭算符的基矢变换规律

$$a_{\widetilde{\alpha}}^\dagger=\sum_\alpha\langle\alpha|\widetilde{\alpha}\rangle a_\alpha^\dagger,\quad a_{\widetilde{\alpha}}=\sum_\alpha\langle\widetilde{\alpha}|\alpha\rangle a_\alpha$$

这对玻色子和费米子都成立. 比如计算坐标表象 $|x\rangle$ 下的产生湮灭算符, 此时它被称为场算符:

$$\psi^\dagger(x)=\sum_\alpha\langle\alpha|x\rangle a_\alpha^\dagger=\sum_\alpha\phi_\alpha^*(x)a_\alpha^\dagger$$
$$\psi(x)=\sum_\alpha\langle x|\alpha\rangle a_\alpha=\sum_\alpha\phi_\alpha(x)a_\alpha$$

存在逆变换

$$a_\alpha^\dagger=\int\langle x|\alpha\rangle\psi^\dagger(x)\mathrm{d}x=\int\phi_\alpha(x)\psi^\dagger(x)\mathrm{d}x,$$
$$a_\alpha=\int\langle\alpha|x\rangle\psi(x)\mathrm{d}x=\int\phi_\alpha^*(x)\psi(x)\mathrm{d}x$$

场算符的对易关系为

$$\left[\psi^\dagger(x),\psi^\dagger(y)\right]_{-\zeta}=[\psi(x),\psi(y)]_{-\zeta}=0,\quad\left[\psi(x),\psi^\dagger(y)\right]_{-\zeta}=\delta(x-y)$$

如果考虑 α 为动量表象, 那么一维长 L 空间有

$$a_k=\int_0^L\mathrm{d}x\langle k|x\rangle\psi(x),\quad\psi(x)=\sum_k\langle x|k\rangle a_k,\quad\langle k|x\rangle=\frac{1}{\sqrt{L}}e^{-ikx}$$

1.4.10 单体算符的表示

通过产生湮灭算符可能乘积的线性组合来构造任意算符. 对于 N 粒子体系, 希尔伯特空间 $\mathcal{F}^N$ 中的单体算符 $\hat{U}$ 具有形式 $\hat{U}=\sum\limits_{i=1}^N\hat{U}_i$, 比如动能算符 $-\frac{1}{2}\nabla_i^2$ 和势能算符 $\hat{v}\left(\vec{x}_i\right)$.

考虑 $\hat{U}$ 表象(即选择其本征矢 $|\lambda\rangle$ 为基矢, 此时 $\hat{U}_i$ 将自动对角化为对角矩阵 $\mathrm{Diag}\left\{U_\lambda\right\}$), 即 $\hat{U}=\sum\limits_{i=1}^N\sum\limits_\lambda U_\lambda|\lambda\rangle_i\langle\lambda|_i$, 其中 $U_\lambda=\langle\lambda|U_i|\lambda\rangle$, 在占据数表象下的矩阵元将是

$$
\begin{aligned}
\langle n_1', n_2', \cdots | \hat{U} | n_1, n_2, \cdots \rangle &= \sum_\lambda U_\lambda \langle n_1', n_2', \cdots | \left(\sum_{i=1}^{N} |\lambda\rangle\langle\lambda| \right) |n_1, n_2, \cdots \rangle \\
&= \sum_\lambda U_\lambda \langle n_1', n_2', \cdots | n_\lambda | n_1, n_2, \cdots \rangle \\
&= \langle n_1', n_2', \cdots | \sum_\lambda U_\lambda a_\lambda^\dagger a_\lambda | n_1, n_2, \cdots \rangle
\end{aligned}
$$

因此 $\hat{U} = \sum_\lambda U_\lambda a_\lambda^\dagger a_\lambda = \sum_\lambda \langle\lambda|\hat{U}_i|\lambda\rangle a_\lambda^\dagger a_\lambda$. 使用表象变换 $a_{\widetilde{\alpha}}^\dagger = \sum_\alpha \langle\alpha|\widetilde{\alpha}\rangle a_\alpha^\dagger, \quad a_{\widetilde{\alpha}} = \sum_\alpha \langle\widetilde{\alpha}|\alpha\rangle a_\alpha$:

$$
\begin{aligned}
\hat{U} &= \sum_\lambda U_\lambda \left(\sum_\mu \langle\mu|\lambda\rangle a_\mu^\dagger \right) \left(\sum_\nu \langle\lambda|\nu\rangle a_\nu \right) \\
&= \sum_{\mu\nu} \langle\mu| \left(\sum_\lambda |\lambda\rangle U_\lambda \langle\lambda| \right) |\nu\rangle a_\mu^\dagger a_\nu \\
&= \sum_{\mu\nu} \langle\mu|\hat{U}_i|\nu\rangle a_\mu^\dagger a_\nu
\end{aligned}
$$

几个单体算符的例子:

1. $\vec{x}$ 表象下的粒子数密度: $\hat{n}(\vec{x}) = \psi^\dagger(\vec{x})\psi(\vec{x})$
2. $\vec{x}$ 和 $\vec{k}$ 表象下的总粒子数: $\hat{N} = \int \psi^\dagger(\vec{x})\psi(\vec{x})\mathrm{d}\vec{x} = \sum_{\vec{k}} a_{\vec{k}}^\dagger a_{\vec{k}}$
3. $\vec{x}$ 和 $\vec{k}$ 表象下的动能算符: $\hat{T} = -\frac{1}{2}\int \psi^\dagger(\vec{x}) \left(-\frac{1}{2}\nabla^2\right) \psi(\vec{x})\mathrm{d}\vec{x} = \sum_{\vec{k}} \frac{k^2}{2} a_{\vec{k}}^\dagger a_{\vec{k}}$
4. $\vec{x}$ 和 $\vec{k}$ 表象下的势能算符: $\hat{V} = \int \psi^\dagger(\vec{x}) v(\vec{x}) \psi(\vec{x})\mathrm{d}\vec{x} = \sum_{\vec{k},\vec{q}} v(\vec{q}) a_{\vec{k}+\vec{q}}^\dagger a_{\vec{k}}$, 其中

$$
v(\vec{x}) = \sum_{\vec{q}} v(\vec{q}) e^{i\vec{q}\cdot\vec{x}} v(\vec{q}) = \frac{1}{V}\int v(\vec{x}) e^{-i\vec{q}\cdot\vec{x}} \mathrm{d}\vec{x}
$$

1.4.11 两体及以上多体算符的表示

考虑一般性的两体算符, 在其对角表象下

$$
\hat{O} = \frac{1}{2}\sum_{i\neq j} \hat{O}_{i,j} = \frac{1}{2}\sum_{i\neq j}\sum_{\alpha,\beta} \mathcal{O}_{\alpha\beta} |\alpha\rangle_i |\beta\rangle_j \langle\alpha|_i \langle\beta|_j, \quad \mathcal{O}_{\alpha\beta} = \langle\alpha\beta|\hat{\mathcal{O}}_{i,j}|\alpha\beta\rangle
$$

那么该两体算符在占据数表象下的矩阵元为

$$
\begin{aligned}
\langle n_1', n_2', \cdots | \hat{O} | n_1, n_2, \cdots \rangle &= \frac{1}{2}\sum_{\alpha,\beta} \mathcal{O}_{\alpha\beta} \langle n_1', n_2', \cdots | \sum_{i\neq j} (|\alpha\rangle_i |\beta\rangle_j \langle\alpha|_i \langle\beta|_j) | n_1, n_2, \cdots \rangle \\
&= \frac{1}{2}\sum_{\alpha,\beta} \mathcal{O}_{\alpha\beta} \langle n_1', n_2', \cdots | \hat{N}_{\alpha\beta} | n_1, n_2, \cdots \rangle \\
&= \langle n_1', n_2', \cdots | \frac{1}{2}\sum_{\alpha,\beta} \mathcal{O}_{\alpha\beta} \hat{N}_{\alpha\beta} | n_1, n_2, \cdots \rangle
\end{aligned}
$$

其中 $\sum_{i\neq j}(|\alpha\rangle_i|\beta\rangle_j\langle\alpha|_i\langle\beta|_j)|n_1,n_2,\cdots\rangle=\hat{N}_{\alpha\beta}|n_1,n_2,\cdots\rangle=(\hat{n}_\alpha\hat{n}_\beta-\delta_{\alpha\beta}\hat{n}_\alpha)\,|n_1,n_2,\cdots\rangle$

$$=a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha|n_1,n_2,\cdots\rangle$$

因此

$$\hat{\mathcal{O}}=\frac{1}{2}\sum_{\alpha\beta}\mathcal{O}_{\alpha\beta}\hat{P}_{\alpha\beta}=\frac{1}{2}\sum_{\alpha\beta}\langle\alpha\beta|\mathcal{O}_{ij}|\alpha\beta\rangle a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha$$

使用表象变换, 得到一般表象下的两体算符

$$\hat{\mathcal{O}}=\frac{1}{2}\sum_{\lambda\mu\nu\rho}\langle\lambda\mu|\mathcal{O}_{ij}|\nu\rho\rangle a_\lambda^\dagger a_\mu^\dagger a_\nu a_\rho$$

推广至 N 体算符, 有

$$\hat{R}=\frac{1}{N!}\sum_{\lambda_1\cdots\lambda_N}\sum_{\mu_1\cdots\mu_N}\langle\lambda_1\cdots\lambda_N|R|\mu_1\cdots\mu_N\rangle a_{\lambda_1}^\dagger\cdots a_{\lambda_N}^\dagger a_{\mu_N}\cdots a_{\mu_1}$$

$\vec{x}$ 表象下的库伦势是典型的两体算符:

$$\hat{V}_{ee}=\frac{1}{2}\sum_{\sigma\sigma'}\iint\psi_\sigma^\dagger(\vec{x}_1)\psi_{\sigma'}^\dagger(\vec{x}_2)\frac{1}{r_{12}}\psi_{\sigma'}(\vec{x}_2)\psi_\sigma(\vec{x}_1)\mathrm{d}\vec{x}_1\mathrm{d}\vec{x}_2$$
$$V_{ee}=\frac{1}{2V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}}\sum_{\sigma\sigma'}\frac{4\pi^2}{q^2}c_{\vec{k}_1+\vec{q},\sigma}^\dagger c_{\vec{k}_2-\vec{q},\sigma'}^\dagger c_{\vec{k}_2,\sigma'}c_{\vec{k}_1,\sigma}$$

1.4.12 相互作用电子系统紧束缚模型的一般导出

1.4.12.1 Bloch 表象和 Wannier 表象

1.4.12.2 紧束缚模型

1.4.13 运动方程

1.4.14 理想气体

1.4.15 巨正则系综

1.4.16 理想费米气体

1.4.17 理想玻色气体

1.4.18 平均场近似

1.4.18.1 稀薄玻色气体的 BEC

1.4.18.2 Hartree-Fock 近似

将之前讨论的 Hatree-Fock 近似使用二次量子化体系重新表述:

1. 单体算符: $F=\sum_{\mu\nu}\langle\mu|f|\nu\rangle a_\mu^\dagger a_\nu$
2. 两体算符: $V=\frac{1}{2}\sum_{\lambda\mu\nu\rho}\langle\lambda\mu|v|\nu\rho\rangle a_\lambda^\dagger a_\mu^\dagger a_\rho a_\nu$

3. HF 波函数: $|\psi_{\text{HF}}\rangle = \prod_{\alpha=1}^{N} a_\alpha^\dagger |0\rangle$

那么

$$
\begin{aligned}
\langle \psi_{\text{HF}}|a_\mu^\dagger a_\nu|\psi_{\text{HF}}\rangle &= \delta_{\mu\nu} \\
\langle \psi_{\text{HF}}|a_\lambda^\dagger a_\mu^\dagger a_\rho a_\nu|\psi_{\text{HF}}\rangle &= \delta_{\lambda\nu}\delta_{\mu\rho} - \delta_{\lambda\rho}\delta_{\mu\nu}
\end{aligned}
$$

所以

$$
E_{\text{HF}} = \sum_\mu \langle\mu|f|\mu\rangle + \frac{1}{2}\sum_{\mu\nu}\left(\langle\mu\nu|b|\mu\nu\rangle - \langle\mu\nu|v|\nu\mu\rangle\right)
$$

更一般性地, 考虑包含单体或两体算符, 形式为 $H = A^\dagger B + C^\dagger D^\dagger EF$ 的哈密顿量, 则 Hatree-Fock 的思想是将其平均为

$$
H_{\text{HF}} = A^\dagger B + \langle C^\dagger F\rangle D^\dagger E + \langle D^\dagger E\rangle C^\dagger F - \langle C^\dagger E\rangle D^\dagger F - \langle D^\dagger F\rangle C^\dagger E + \text{Const}
$$

接下来计算的步骤为

1. 对角化 Hatree-Fock 平均场哈密顿量: $H_{\text{HF}} = \sum_\alpha \varepsilon_\alpha a^\dagger a_\alpha$, 构造 Hatree-Fock 基态波函数 $|\psi_{\text{HF}}\rangle = \prod_{\varepsilon_\alpha<0} a_\alpha^\dagger|0\rangle$
2. 计算平均场参数 $\langle C^\dagger F\rangle, \langle D^\dagger E\rangle, \langle C^\dagger E\rangle, \langle D^\dagger F\rangle$, 重复以上计算直至收敛.
3. 或者计算基态能量 $\langle\psi_{\text{HF}}|H|\psi_{\text{HF}}\rangle = \sum_{\varepsilon_\alpha<0}\varepsilon_\alpha - \langle C^\dagger F\rangle\langle D^\dagger E\rangle + \langle C^\dagger E\rangle\langle D^\dagger F\rangle$
4. 在平均场参数空间极小化基态能量

1.4.18.2.1　Hubbard 模型的 Hartree-Fock 近似　Hubbard 模型哈密顿量为

$$
H = -t\sum_{\langle i,j\rangle,\sigma}\left(c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}\right) + U\sum_i \underbrace{c_{i\uparrow}^\dagger c_{i\uparrow}}_{n_{i\uparrow}}\underbrace{c_{i\downarrow}^\dagger c_{i\downarrow}}_{n_{i\downarrow}}
$$

在第二项中由于已经确定自旋表象, 所以可以互换 $c_{i\uparrow}$ 和 $c_{i\downarrow}^\dagger$ 位置从而形成粒子数算符. 那么考虑两格点模型, 且选定矩阵基矢为

$$
c = \begin{pmatrix} c_{1\uparrow} \\ c_{1\downarrow} \\ c_{2\uparrow} \\ c_{2\downarrow} \end{pmatrix}, \quad c^\dagger = \begin{pmatrix} c_{1\uparrow}^\dagger & c_{1\downarrow}^\dagger & c_{2\uparrow}^\dagger & c_{2\downarrow}^\dagger \end{pmatrix}
$$

于是 Hatree-Fock 近似下的哈密顿量可以改写为矩阵形式

$$
H_{\text{MF}} = \begin{pmatrix} c_{1\uparrow}^\dagger & c_{1\downarrow}^\dagger & c_{2\uparrow}^\dagger & c_{2\downarrow}^\dagger \end{pmatrix}\begin{pmatrix} U\langle n_{1\downarrow}\rangle & -U\langle S_1^-\rangle & -t & \\ -U\langle S_1^+\rangle & U\langle n_{1\downarrow}\rangle & & -t \\ -t & & U\langle n_{2\downarrow}\rangle & -U\langle S_2^-\rangle \\ & -t & -U\langle S_2^+\rangle & U\langle n_{2\uparrow}\rangle \end{pmatrix}\begin{pmatrix} c_{1\uparrow} \\ c_{1\downarrow} \\ c_{2\uparrow} \\ c_{2\downarrow} \end{pmatrix} + U\sum_i(\langle S_i^+\rangle\langle S_i^-\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle)
$$

禁用自旋翻转项 $c_{i\uparrow}^\dagger c_{i\downarrow}$ 与 $c_{i\downarrow}^\dagger c_{i\uparrow}$, 矩阵进一步简化为

$$
H_{\text{MF}} = c^\dagger\begin{pmatrix} U\langle n_{1\downarrow}\rangle & & -t & \\ & U\langle n_{1\uparrow}\rangle & & -t \\ -t & & U\langle n_{2\downarrow}\rangle & \\ & -t & & U\langle n_{2\uparrow}\rangle \end{pmatrix} c - U\sum_i\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle
$$

1. $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$ 作为初始值. 则矩阵变为

$$\begin{pmatrix} U/2 & & -t & \\ & U/2 & & -t \\ -t & & U/2 & \\ & -t & & U/2 \end{pmatrix} = VDV^{-1},$$

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} & 1 & & -1 \\ 1 & & -1 & \\ & 1 & & 1 \\ 1 & & 1 & \end{pmatrix}, \quad D = \begin{pmatrix} -t+U/2 & & & \\ & -t+U/2 & & \\ & & t+U/2 & \\ & & & t+U/2 \end{pmatrix}$$

注意对角矩阵 D 的对角线上能量本征值是升序排列的, 这是为了方便观察基态的能量出现在基矢的什么位置. 根据对角分解有 $H = c^\dagger VDV^{-1}c$, 合并 $V^{-1}c$ 为 γ, 即得到矩阵的新基矢为 $\gamma \equiv V^{-1}c$. 同样的, $c = V\gamma$, 或者写作求和约定 $c_\alpha = \sum_i V_{\alpha i}\gamma_i$. 基态被定义为占据最低能量的态, 而根据对角矩阵可以发现最低能量是二重简并的, 是新基矢 γ 的第 $1, 2$ 分量给出的, 因此基态使用产生算符 $\times|0\rangle$ 写出的话将会是 $\prod_{\varepsilon_i<\varepsilon_F}\gamma_i^\dagger|0\rangle = \gamma_1^\dagger\gamma_2^\dagger|0\rangle$. 那么各粒子数平均值为

$$\begin{aligned}\langle n_{1\uparrow}\rangle &= \langle c_{1\uparrow}^\dagger c_{1\uparrow}\rangle = \sum_{i,j} V_{1\uparrow,i}^\dagger V_{1\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle \\ &= \sum_{i,j} V_{1\uparrow,i}^\dagger V_{1\uparrow,j}\delta_{ij} = \sum_i V_{1\uparrow,i}^\dagger V_{1\uparrow,i} = V_{1\uparrow,1}^\dagger V_{1\uparrow,1} + V_{1\uparrow,2}^\dagger V_{1\uparrow,2} \\ &= \frac{1}{2}\end{aligned}$$

同理计算得到 $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \dfrac{1}{2}$. 这是顺磁态, 能量为

$$\begin{aligned}E_{\mathrm{HF}} &= \sum_{\varepsilon_\alpha<0}\varepsilon_\alpha - U\cdot\frac{1}{2}\frac{1}{2}\times 2 = \left(-t+\frac{U}{2}\right)\times 2 - \frac{U}{2} \\ &= -2t + \frac{U}{2}\end{aligned}$$

2. $\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = 1, \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0$ 作为初始值. 那么

$$\begin{pmatrix} & & -t & \\ & U & & -t \\ -t & & & \\ & -t & & U \end{pmatrix} = VDV^{-1},$$

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 & & \\ & & 1 & -1 \\ 1 & 1 & & \\ & & 1 & 1 \end{pmatrix}, \quad D = \begin{pmatrix} -t & & & \\ & t & & \\ & & -t+U & \\ & & & t+U \end{pmatrix}$$

(a) $-t+U<t$, 则能量最低态将由新矩阵基矢 γ 的 $1, 3$ 分量给出, 那么产生算符 $\times|0\rangle$ 将会是 $|\psi_{\mathrm{HF}}\rangle = \gamma_1^\dagger\gamma_3^\dagger|0\rangle$, 粒子数平均值为

$$\begin{aligned}\langle n_{1\uparrow}\rangle &= \sum_{i,j} V_{1\uparrow,i}^\dagger V_{1\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle \\ &= V_{1\uparrow,1}^\dagger V_{1\uparrow,1} + V_{1\uparrow,3}^\dagger V_{1\uparrow,3} \\ &= \frac{1}{2} \\ \langle n_{1\downarrow}\rangle &= \langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}\end{aligned}$$

因此仍处于顺磁态, 即

$$\begin{aligned} E_{\mathrm{MF}} &= \sum_{\varepsilon_\alpha} \epsilon_\alpha - U\sum_i \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle = -t + (-t+U) + U\cdot\frac{1}{2}\times\frac{1}{2}\times 2 \\ &= -2t + \frac{U}{2} \end{aligned}$$

(b) $-t+U>t$, 则能量最低态将由新矩阵基矢的 $1,2$ 分量给出, 那么产生算符 $\times|0\rangle$ 将会是 $|\psi_{\mathrm{HF}}\rangle = \gamma_1^\dagger\gamma_2^\dagger|0\rangle$, 粒子数平均值为

$$\begin{aligned} \langle n_{1\uparrow}\rangle &= \sum_{i,j} V^\dagger_{1\uparrow,i}V_{1\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle \\ &= V^\dagger_{1\uparrow,1}V_{1\uparrow,1} + V^\dagger_{1\uparrow,2}V_{1\uparrow,2} \\ &= 1 \\ \langle n_{1\uparrow}\rangle &= \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0 \end{aligned}$$

和初始的假设值一致(即"收敛"). 此时自旋方向相同, 得到铁磁态解. 平均场能量为

$$E_{\mathrm{MF}} = \sum_{\varepsilon_\alpha}\varepsilon_\alpha - U\sum_i\langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle = -t + t + U(0\cdot 1 + 0\cdot 1) = 0$$

(c)

1.5 微扰论

1.6 量子计算基础

1.7 相对论量子力学

1.8 量子动力学

第二章 Homework

2.1 Homework 1

2.1.1 Hermitian operators

1. **Prove theorem 1: If A is Hermitian operator, then all its eigenvalues are real numbers, and the eigenvectors corresponding to different eigenvalues are orthogonal.**

   (a) Since A is Hermitian, we have $A^\dagger = A$. Let λ be an eigenvalue of A and v the corresponding eigenvector, so

   $$Av = \lambda v.$$

   Consider the inner product

   $$\langle v, Av\rangle = \langle v, \lambda v\rangle = \lambda\langle v, v\rangle = \lambda||v||^2.$$
   $$\langle Av, v\rangle = \langle \lambda v, v\rangle = \lambda^*\langle v, v\rangle = \lambda^*||v||^2.$$

   So we have $\lambda||v||^2 = \lambda^*||v||^2$, which implies $\lambda = \lambda^*$, so λ is real(since $||v||^2$ is not zero, as $v \neq 0$).

   (b) Let λ_1 and λ_2 be two different eigenvalues of A, and v_1 and v_2 the corresponding eigenvectors, so we have

   $$Av_1 = \lambda_1 v_1, \quad Av_2 = \lambda_2 v_2.$$

   Consider the inner product

   $$\langle v_1, Av_2\rangle = \langle v_1, \lambda_2 v_2\rangle = \lambda_2\langle v_1, v_2\rangle,$$
   $$\langle Av_1, v_2\rangle = \langle \lambda_1 v_1, v_2\rangle = \lambda_1\langle v_1, v_2\rangle.$$

   Since A is Hermitian, we have $\langle v_1, Av_2\rangle = \langle Av_1, v_2\rangle$, so we have $(\lambda_1 - \lambda_2)\langle v_1, v_2\rangle = 0$, which implies $\langle v_1, v_2\rangle = 0$(since $\lambda_1 \neq \lambda_2$).□

2. **Prove theorem 2: If A is Hermitian operator, then it can be always diagonalized by unitary transformation.**

   Let $\{\lambda_1, \lambda_2, \cdots, \lambda_n\}$ be the eigenvalues of A, and $\{v_1, v_2, \cdots, v_n\}$ the corresponding eigenvectors.

   By theorem 1, we have $\langle v_1, v_2\rangle = \delta_{ij}$.

   We define the unitary matrix as $U = [v_1, v_2, \cdots, v_n]$, so we have $U^\dagger U = \mathbb{I}$. Now we compute $U^\dagger AU$. Since $Av_i = \lambda_i v_i$, we have

   $$\begin{aligned} U^\dagger AU &= \begin{pmatrix} v_1^\dagger \\ v_2^\dagger \\ \vdots \\ v_n^\dagger \end{pmatrix} A \begin{pmatrix} v_1 & v_2 & \cdots & v_n \end{pmatrix} = \begin{pmatrix} v_1^\dagger Av_1 & v_1^\dagger Av_2 & \cdots & v_1^\dagger Av_n \\ v_2^\dagger Av_1 & v_2^\dagger Av_2 & \cdots & v_2^\dagger Av_n \\ \vdots & \vdots & \ddots & \vdots \\ v_n^\dagger Av_1 & v_n^\dagger Av_2 & \cdots & v_n^\dagger Av_n \end{pmatrix} \\ &= \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix} = \Lambda.\square \end{aligned}$$

3. **Prove theorem 3: Two diagonalizable operators A and B can be simultaneously diagonalized if, and only if, $[A, B] = 0$.**

   (a) Let's say

   $$A|v\rangle = \lambda|v\rangle, \quad B|v\rangle = \mu|v\rangle.$$

   where $|v\rangle$ is the eigenvector of A and B, λ and μ are the corresponding eigenvalues.

   So

   $$[A, B]|v\rangle = (AB - BA)|v\rangle = (AB|v\rangle - BA|v\rangle) = (\lambda\mu - \mu\lambda)|v\rangle = 0.$$

   for all $|v\rangle$, which means $[A, B] = 0$.

   (b) Let's say $[A, B] = 0$. And we have

   $$\begin{aligned} A|v\rangle &= \lambda|v\rangle, \\ AB|v\rangle &= BA|v\rangle = B\lambda|v\rangle = \lambda\left(B|v\rangle\right), \end{aligned}$$

   which means $B|v\rangle$ is also the eigenvector of A with eigenvalue λ. And apply the same method to all $|v\rangle$ of A, we can find a common set of eigenvectors of A and B within the degenerate subspace. $\square$

2.1.2 Matrix diagonalization and unitary transformation

1. **Diagonalizing a matrix L corresponds to finding a unitary transformation V such that $L = V\Lambda V^\dagger$, where Λ is a diagonal matrix whose diagonal elements are eigenvalues, V is an unitary matrix whose column vectors are the corresponding eigenstates. Find a unitary matrix V that can diagonalize the Pauli matrix $\sigma^x_{(z)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and find the eigenvalues of $\sigma^x_{(z)}$.**

   Find the eigenvalues of $\sigma^x_{(z)}$ by solving the characteristic equation

   $$\det(\sigma^x_{(z)} - \lambda I) = \det\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0,$$

   So we have $\boxed{\lambda = \pm 1}$. For $\lambda_+ = 1$, we have

   $$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = v_2.$$

   So the eigenvector corresponding to λ_+ is $|+\rangle^x_{(z)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. For $\lambda_- = -1$, we have

   $$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = -1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = -v_2.$$

   So the eigenvector corresponding to λ_- is $|-\rangle^x_{(z)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. The eigenvectors have been normalized, so the unitary matrix V is $[|+\rangle^x_{(z)}, |-\rangle^x_{(z)}] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. The diagonal matrix Λ contains the eigenvalues on the diagonal, which means

   $$\Lambda = \mathrm{diag}\{\lambda_+, \lambda_-\} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z_{(z)}$$

   Thus we diagonalized the Pauli matrix $\sigma^x_{(z)}$ by the unitary transformation V:

   $$\sigma^x_{(z)} = V^\dagger \Lambda V = V^\dagger \sigma^z_{(z)} V$$

We notice that the diagnosed matrix Λ is just the Pauli matrix $\sigma^z_{(z)}$, which means we can transform the representation of the Pauli matrix σ^z to the σ^x representation by the unitary transformation V:

$$\sigma^x_{(z)} = V^\dagger \sigma^z_{(z)} V = V^\dagger \sigma^x_{(x)} V \Rightarrow \sigma^x_{(x)} = \left(V^\dagger\right)^{-1} \sigma^x_{(z)} (V)^{-1}$$

$\sigma^x_{(z)}$ is the matrix of σ^x in the σ^z representation. Noticed that $V = V^\dagger = V^{-1}$, so

$$\sigma^x_{(x)} = V \sigma^x_{(z)} V$$

2. **The three components of the spin angular momentum operator $\vec{S}$ for spin-$1/2$ are S^x, S^y, and S^z. If we use the S^z representation, their matrix representations are given by $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, where the three components of $\vec{\sigma}$ are the Pauli matrices σ^x, σ^y, and σ^z.**

   Now consider using the S^x representation. Please list the order of basis vectors you have chosen in the S^x representation, and calculate the matrix representations of the three components of the operator $\vec{S}$ in this representation.

   Within S^z representation, we have

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x_{(z)} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

   From the previous question, we have found the eigenvalues and corresponding eigenvectors:

$$|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

   The matrix V that transforms the S^z representation to the S^x representation is

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

   In the S^z representation, we have

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y_{(z)} = \frac{\hbar}{2}\sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z_{(z)} = \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

   So

$$\begin{aligned}
S^x_{(x)} &= V S^x_{(z)} V = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\
S^y_{(x)} &= V S^y_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\
S^z_{(x)} &= V S^z_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}.
\end{aligned}$$

   So the basis vectors in the S^x representation are

$$|+\rangle^x_{(x)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle^x_{(x)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

2.2 Homework 2

2.2.1 Angular momentum for 4-dimensional space

Consider a 4-dimensional space with coordinates (x, y, z, w).

1. **Show that the operators $L_i = \epsilon_{ijk}x_j p_k$ and $K_i = wp_i - x_i p_w$ generate rotations in this space by showing that the transformations generated by these operators leave the four dimensional radius, defined by $R^2 = x^2 + y^2 + z^2 + w^2$, invariant.**

   (a) Since the operator $L_i = \sum_{jk} \epsilon_{ijk}x_j p_k$ is defined in the usual 3-dimension subspace, so we still have

$$
\begin{aligned}
[L_i, x_j] &= \left[\sum_{kl} \epsilon_{ikl}x_k p_l, x_j\right] = \sum_{kl} \epsilon_{ikl}[x_k p_l, x_j] \\
&= \sum_{kl} \epsilon_{ikl}(x_k[p_l, x_j] + \cancel{[x_k, x_j]p_l}) = \sum_{kl} \epsilon_{ikl}x_k(-i\hbar\delta_{lj}) \\
&= \sum_k \epsilon_{ikj}x_k(-i\hbar) = \boxed{i\hbar \sum_k \epsilon_{ijk}x_k}.
\end{aligned}
$$

   So we have

$$
\begin{aligned}
[L_i, R^2] &= [L_i, x^2 + y^2 + z^2 + w^2] = [L_i, x^2] + [L_i, y^2] + [L_i, z^2] + [L_i, w^2], \\
[L_i, x_j^2] &= [L_i, x_j x_j] = x_j[L_i, x_j] + [L_i, x_j]x_j = x_j\left[i\hbar \sum_k \epsilon_{ijk}x_k\right] + \left[i\hbar \sum_k \epsilon_{ijk}x_k\right]x_j \\
&= 2i\hbar \sum_k \epsilon_{ijk}x_j x_k \\
\left[L_i, \sum_j^3 x_j^2\right] &= \sum_j^3 [L_i, x_j^2] = 2i\hbar \sum_{jk} \epsilon_{ijk}x_j x_k = 0, \quad \text{since } j \leftrightarrow k \text{ symmetry} \\
[L_i, w^2] &= [L_i, ww] = w[L_i, w] + [L_i, w]w = 0.
\end{aligned}
$$

   So we have $[L_i, R^2] = 0$, which means the operator L_i leaves the 4-dimension radius invariant.

   (b) $K_i = wp_i - x_i p_w$.

   Now we consider the commutator. Due to the definition of K_i, only the terms with w will be affected. So we have:

$$
\begin{aligned}
[K_i, R^2] &= [K_i, x^2 + y^2 + z^2 + w^2] = \sum_j^3 [K_i, x_j^2] + [K_i, w^2] \\
[K_i, w^2] &= [K_i, w]w + w[K_i, w] \\
[K_i, w] &= [wp_i - x_i p_w, w] = \left[w\left(-i\hbar\frac{\partial}{\partial x_i}\right) - x_i\left(-i\hbar\frac{\partial}{\partial w}\right), w\right]
\end{aligned}
$$

   Assume a sample function $f(x, y, z, w)$, wo we have

$$
\begin{aligned}
&\left[w\left(-i\hbar\frac{\partial}{\partial x_i}\right) - x_i\left(-i\hbar\frac{\partial}{\partial w}\right), w\right] f = (-i\hbar)\left[w\frac{\partial}{\partial x_i} - x_i\frac{\partial}{\partial w}, w\right] f \\
&= (-i\hbar)\left\{\left(w\frac{\partial}{\partial x_i} - x_i\frac{\partial}{\partial w}\right)(wf) - w\left(w\frac{\partial f}{\partial x_i} - x_i\frac{\partial f}{\partial w}\right)\right\} \\
&= (-i\hbar)(-x_i)f \\
&\Rightarrow \boxed{[K_i, w] = i\hbar x_i}
\end{aligned}
$$

   So we have

$$
[K_i, w^2] = [K_i, w]w + w[K_i, w] = i\hbar x_i w + w(i\hbar x_i) = 2i\hbar x_i w
$$

   For the other term, we have

$$
\begin{aligned}
[K_i, x_j] &= w[p_i, x_j] = (-i\hbar)w\delta_{ij} \\
[K_i, x_j^2] &= [K_i, x_j x_j] = x_j[K_i, x_j] + [K_i, x_j]x_j = -2i\hbar x_j w\delta_{ij}
\end{aligned}
$$

Thus we have

$$[K_i, R^2] = [K_i, x^2 + y^2 + z^2 + w^2] = \sum_j^3 [2i\hbar x_j w \delta_{ij}] - 2i\hbar x_i w = 2i\hbar x_i w - 2i\hbar x_i w = 0.$$

□

2. **Compute the commutators $[L_i, K_j]$ and $[K_i, K_j]$.**

(a) $[L_i, K_j]$

$$[L_i, K_j] = [L_i, wp_j - x_j p_w] = [L_i, wp_j] - [L_i, x_j p_w] = w[L_i, p_j] - [L_i, x_j p_w]$$

We have known that $[p_k, p_j] = 0$ and $[x_l, p_j] = i\hbar\delta_{lj}$, so we have

$$[L_i, p_j] = \left[\sum_{lk} \epsilon_{ilk} x_l p_k, p_j\right] = \sum_{lk} \epsilon_{ilk}(\cancel{x_l[p_k, p_j]} + [x_l, p_j]p_k) = \sum_{lk} \epsilon_{ilk} i\hbar\delta_{lj} p_k = i\hbar \sum_k \epsilon_{ijk} p_k$$

$$\Rightarrow \boxed{w[L_i, p_j] = i\hbar \sum_k \epsilon_{ijk} w p_k}$$

For the other term, we have

$$\begin{aligned}
[L_i, x_j p_w] &= x_j[L_i, p_w] + [L_i, x_j]p_w \\
[L_i, x_j] &= \left[\sum_{kl} \epsilon_{ikl} x_k p_l, x_j\right] = \sum_{kl} \epsilon_{ikl}[x_k p_l, x_j] \\
&= \sum_{kl} \epsilon_{ikl}(x_k[p_l, x_j] + \cancel{[x_k, x_j]p_l}) = \sum_{kl} \epsilon_{ikl} x_k(-i\hbar\delta_{lj}) \\
&= \sum_k \epsilon_{ikj} x_k(-i\hbar) = i\hbar \sum_k \epsilon_{ijk} x_k, \\
[L_i, p_w] &= \sum_{jk} \epsilon_{ijk}[x_j p_k, p_w] = \sum_{jk} \epsilon_{ijk}(x_j[p_k, p_w] + [x_j, p_w]p_k) = \epsilon_{ijk}(x_j \cdot 0 + 0 \cdot p_k) = 0 \\
&\Rightarrow [L_i, x_j p_w] = x_j \cdot 0 + i\hbar \sum_k \epsilon_{ijk} x_k \cdot p_w = \boxed{i\hbar \sum_k \epsilon_{ijk} x_k p_w}
\end{aligned}$$

Combining the terms we derived, we have

$$[L_i, K_j] = i\hbar \sum_k \epsilon_{ijk} w p_k - i\hbar \sum_k \epsilon_{ijk} x_k p_w = \boxed{i\hbar \sum_k \epsilon_{ijk} K_k}$$

(b) $[K_i, K_j]$.

$$\begin{aligned}
[K_i, K_j] &= [wp_i - x_i p_w, wp_j - x_j p_w] = [wp_i, wp_j] - [wp_i, x_j p_w] - [x_i p_w, wp_j] + [x_i p_w, x_j p_w] \\
[wp_i, wp_j] &= w^2[p_i, p_j] = 0; \\
[wp_i, x_j p_w] &= x_j(\cancel{w[p_i, p_w]} + [w, p_w]p_i) + (w[p_i, x_j] + \cancel{[w, x_j]p_i})p_w = x_j i\hbar p_i + w(-i\hbar)\delta_{ij} p_w \\
&= i\hbar(x_j p_i - \delta_{ij} w p_w) \\
[x_i p_w, wp_j] &= w(\cancel{x_i[p_w, p_j]} + [x_i, p_j]p_w) + (x_i[p_w, w] + \cancel{[x_i, w]p_w})p_j = wi\hbar\delta_{ij} p_w + x_i(-i\hbar)p_j \\
&= i\hbar(wp_w\delta_{ij} - x_i p_j) \\
[x_i p_w, x_j p_w] &= 0
\end{aligned}$$

So combine the terms we derived, we have

$$[K_i, K_j] = 0 - i\hbar(x_j p_i \cancel{- \delta_{ij} w p_w}) - i\hbar(\cancel{wp_w\delta_{ij}} - x_i p_j) + 0 = i\hbar(x_i p_j - x_j p_i) = \boxed{i\hbar \sum_k \epsilon_{ijk} L_k}$$

2.2.2 Harmonic oscillator

1. **Find the energy eigenvalues E_n and the corresponding wave functions $\psi_n(x)$ for a one-dimensional quantum harmonic oscillator system.**

   We have known that the Hamitonian of a quantum harmonic oscillator is given by
   $$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2$$
   And the energy eigenvalues E_n are given by
   $$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega, \quad n = 0, 1, 2, \cdots}$$
   The corresponding wave functions $\psi_n(x)$ are given by
   $$\boxed{\psi_n(x) = \frac{1}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} H_n\left(\sqrt{\frac{m\omega}{\hbar}}x\right)}$$
   where $H_n(x)$ are the Hermite polynomials.

2. **Calculate $\langle m|x|n\rangle$, $\langle m|p|n\rangle$, $\langle m|x^2|n\rangle$, and $\langle m|p^2|n\rangle$.**

   We have known that the position operator x and the momentum operator p could be expressed by the creation $a^\dagger$ and annihilation a operators:
   $$\begin{aligned}
   \hat{x} &= \sqrt{\frac{\hbar}{2m\omega}}\left(a + a^\dagger\right), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\left(a^\dagger - a\right) \\
   \hat{x}^2 &= \frac{\hbar}{2m\omega}(a + a^\dagger)^2 = \frac{\hbar}{2m\omega}(a^2 + a^{\dagger 2} + a^\dagger a + aa^\dagger) \\
   \hat{p}^2 &= -\frac{\hbar m\omega}{2}(a^\dagger - a)^2 = -\frac{\hbar m\omega}{2}(a^{\dagger 2} - a^\dagger a - aa^\dagger + a^2)
   \end{aligned}$$
   which is governed by
   $$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle$$
   Apply the calculating formula to the matrix elements, and we have
   $$\begin{aligned}
   \langle m|\hat{x}|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}}\left(\langle m|a|n\rangle + \langle m|a^\dagger|n\rangle\right) = \sqrt{\frac{\hbar}{2m\omega}}\left(\langle m|\sqrt{n}|n-1\rangle + \langle m|\sqrt{n+1}|n+1\rangle\right) \\
   &= \boxed{\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})} \\
   \langle m|\hat{p}|n\rangle &= i\sqrt{\frac{\hbar m\omega}{2}}(\langle m|a^\dagger|n\rangle - \langle m|a|n\rangle) = i\sqrt{\frac{\hbar m\omega}{2}}(\langle m|\sqrt{n+1}|n+1\rangle - \langle m|\sqrt{n}|n-1\rangle) \\
   &= \boxed{i\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1})} \\
   \langle m|\hat{x}^2|n\rangle &= \frac{\hbar}{2m\omega}(\langle m|a^2|n\rangle + \langle m|a^{\dagger 2}|n\rangle + \langle m|a^\dagger a|n\rangle + \langle m|aa^\dagger|n\rangle) \\
   &= \frac{\hbar}{2m\omega}(\langle m|\sqrt{n(n-1)}|n-2\rangle + \langle m|\sqrt{(n+1)(n+2)}|n+2\rangle + \langle m|n|n\rangle + \langle m|n+1|n\rangle) \\
   &= \boxed{\frac{\hbar}{2m\omega}(\sqrt{n(n-1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + n\delta_{m,n} + (2n+1)\delta_{m,n})} \\
   \langle m|\hat{p}^2|n\rangle &= -\frac{\hbar m\omega}{2}\left(\langle m|a^{\dagger 2}|n\rangle - \langle m|2a^\dagger a|n\rangle + \langle m|a^2|n\rangle - \langle m|1|n\rangle\right) \\
   &= \boxed{-\frac{\hbar m\omega}{2}(\sqrt{(n+1)(n+2)}\delta_{m,n+2} - (2n+1)2n\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2})}
   \end{aligned}$$

3. **Assume the quantum harmonic oscillator is in a thermal bath at temperature T; find the partition function Z and the average energy $\langle E\rangle$ of the system.**

Note $\frac{1}{k_BT}$ as β for simplicity. Since the energy eigenvalues are given by $E_n = \left(n+\frac{1}{2}\right)\hbar\omega$, the partition function Z is given by

$$Z = \sum_{n=0}^{\infty} e^{-\beta E_n} = \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} = e^{-\frac{1}{2}\beta\hbar\omega}\sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}$$

For the series $\sum_{n=0}^{\infty} x^n$, we have the limit value $\frac{1}{1-x}$ when $|x|<1$. So we have

$$Z = e^{-\frac{1}{2}\beta\hbar\omega}\frac{1}{1-e^{-\beta\hbar\omega}} = \boxed{\frac{e^{-\frac{1}{2}\beta\hbar\omega}}{1-e^{-\beta\hbar\omega}}}$$

The average energy $\langle E\rangle$ is given by

$$\begin{aligned}
\langle E\rangle &= -\frac{\partial \ln Z}{\partial\beta} = -\frac{\partial}{\partial\beta}\left(-\frac{1}{2}\beta\hbar\omega - \ln(1-e^{-\beta\hbar\omega})\right) \\
&= -\left(-\frac{1}{2}\hbar\omega - \frac{1}{1-e^{-\beta\hbar\omega}}(-e^{-\beta\hbar\omega})(-\hbar\omega)\right) \\
&= \boxed{\frac{1}{2}\hbar\omega + \frac{\hbar\omega}{e^{\beta\hbar\omega}-1}}
\end{aligned}$$

4. **Prove that the inner product of coherent states is given by:**

$$\langle\alpha|\beta\rangle = e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha^*\beta}$$

The coherent states are given by

$$|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

$$|\beta\rangle = e^{-\frac{1}{2}|\beta|^2}\sum_{m=0}^{\infty}\frac{\beta^m}{\sqrt{m!}}|m\rangle$$

So the inner product could be derived as

$$\begin{aligned}
\langle\alpha|\beta\rangle &= \left(e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^{*n}}{\sqrt{n!}}\langle n|\right)\left(e^{-\frac{1}{2}|\beta|^2}\sum_{m=0}^{\infty}\frac{\beta^m}{\sqrt{m!}}|m\rangle\right) \\
&= e^{-\frac{1}{2}|\alpha|^2}e^{-\frac{1}{2}|\beta|^2}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty}\frac{(\alpha^*)^n\beta^m}{\sqrt{n!m!}}\langle n|m\rangle
\end{aligned}$$

where $\langle n|m\rangle = \delta_{n,m}$ due to the orthogonality of the energy eigenstates. So we have

$$\langle\alpha|\beta\rangle = e^{-\frac{|\alpha|^2}{2}}e^{-\frac{|\beta|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^{*n}\beta^n}{n!} = e^{-\frac{|\alpha|^2+|\beta|^2}{2}}\sum_{n=0}^{\infty}\frac{(\alpha^*\beta)^n}{n!} = e^{-\frac{|\alpha|^2+|\beta|^2}{2}}e^{\alpha^*\beta}. \quad \square$$

2.3 Homework 3

2.3.1 Schwinger boson representation

A two-dimensional quantum harmonic oscillator contains two decoupled free bosons, whose annihilation operators can be represented as a and b respectively. $a = \frac{1}{\sqrt{2}}(x+ip_x)$, $b = \frac{1}{\sqrt{2}}(y+ip_y)$. They satisfy the commutation relations

$[a, a^\dagger] = [b, b^\dagger] = 1$ **and** $[a, b] = [a, b^\dagger] = 0$**. This system has U(2) symmetry, which includes an SU(2) subgroup. Let's explore how to construct the SU(2) representation using bosonic operators. Define** $S^x = \dfrac{1}{2}(a^\dagger b + b^\dagger a)$**,** $S^z = \dfrac{1}{2}(a^\dagger a - b^\dagger b)$**.**

1. **Express S^y in terms of a and b. [Hint: Make $\vec{S} \times \vec{S} = i\vec{S}$]**

   To satisfy the commutation relation $\vec{S} \times \vec{S} = i\vec{S}$, we have

$$[S^x, S^y] = iS^z, \quad [S^y, S^z] = iS^x, \quad [S^z, S^x] = iS^y$$

   So we have

$$\begin{aligned} S^y &= \frac{1}{i}[S^z, S^x] = \frac{1}{i}\left[\frac{1}{2}\left(a^\dagger a - b^\dagger b\right), \frac{1}{2}\left(a^\dagger b + b^\dagger a\right)\right] \\ &= \frac{1}{4i}[a^\dagger a - b^\dagger b, a^\dagger b + b^\dagger a] \end{aligned}$$

   We have commutation formula that

$$\begin{aligned} [\hat{A}, \hat{B} + \hat{C}] &= [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}] \\ [\hat{A} + \hat{B}, \hat{C}] &= [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}] \\ [\hat{A}, \hat{B}\hat{C}] &= \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C} \\ [\hat{A}\hat{B}, \hat{C}] &= \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B} \\ \Rightarrow [\hat{A}\hat{B}, \hat{C}\hat{D}] &= \hat{A}\hat{C}[\hat{B}, \hat{D}] + \hat{A}[\hat{B}, \hat{C}]\hat{D} + \hat{C}[\hat{A}, \hat{D}]\hat{B} + [\hat{A}, \hat{C}]\hat{D}\hat{B} \end{aligned}$$

   So we have

$$\begin{aligned} S^y &= \frac{1}{4i}\left[a^\dagger a, a^\dagger b\right] + \frac{1}{4i}\left[a^\dagger a, b^\dagger a\right] - \frac{1}{4i}\left[b^\dagger b, a^\dagger b\right] - \frac{1}{4i}\left[b^\dagger b, b^\dagger a\right] \\ \left[a^\dagger a, a^\dagger b\right] &= \cancel{a^\dagger a^\dagger [a, b]} + a^\dagger [a, a^\dagger] b + \cancel{a^\dagger [a^\dagger, b] a} + \cancel{[a^\dagger, a^\dagger] ba} = a^\dagger b \\ \left[a^\dagger a, b^\dagger a\right] &= \cancel{a^\dagger b^\dagger [a, a]} + \cancel{a^\dagger [a, b^\dagger] a} + b^\dagger [a^\dagger, a] a + \cancel{[a^\dagger, b^\dagger] aa} = -b^\dagger a \\ \left[b^\dagger b, a^\dagger b\right] &= \cancel{b^\dagger a^\dagger [b, b]} + \cancel{b^\dagger [b, a^\dagger] b} + a^\dagger [b^\dagger, b] b + \cancel{[b^\dagger, a^\dagger] bb} = -a^\dagger b \\ \left[b^\dagger b, b^\dagger a\right] &= \cancel{b^\dagger b^\dagger [b, a]} + b^\dagger [b, b^\dagger] a + \cancel{b^\dagger [b^\dagger, a] b} + \cancel{[b^\dagger, b^\dagger] ab} = b^\dagger a \\ \Rightarrow S^y &= \frac{1}{4i}\left(a^\dagger b - b^\dagger a + a^\dagger b - b^\dagger a\right) = \boxed{\frac{1}{2i}\left(a^\dagger b - b^\dagger a\right)} \end{aligned}$$

2. **Prove that S^y is actually related to the angular momentum operator of the harmonic oscillator $L = xp_y - yp_x$, namely $S^y = \dfrac{L}{2}$.**

   Define

$$\begin{aligned} x &= \frac{a + a^\dagger}{\sqrt{2}}, \quad p_x = \frac{i(a^\dagger - a)}{\sqrt{2}} \\ y &= \frac{b + b^\dagger}{\sqrt{2}}, \quad p_y = \frac{i(b^\dagger - b)}{\sqrt{2}} \end{aligned}$$

   So the angular momentum operator is

$$\begin{aligned} L &= \left(\frac{a + a^\dagger}{\sqrt{2}}\right)\left(\frac{i(b^\dagger - b)}{\sqrt{2}}\right) - \left(\frac{b + b^\dagger}{\sqrt{2}}\right)\left(\frac{i(a^\dagger - a)}{\sqrt{2}}\right) \\ &= \frac{i}{2}\left[\left(a + a^\dagger\right)\left(b^\dagger - b\right) - \left(b + b^\dagger\right)\left(a^\dagger - a\right)\right] \\ &= \frac{i}{2}\left(ab^\dagger - \cancel{ab} + \cancel{a^\dagger b^\dagger} - a^\dagger b - ba^\dagger + \cancel{ba} - \cancel{b^\dagger a^\dagger} + b^\dagger a\right) \end{aligned}$$

Because $[a,b]=[a,b^\dagger]=0$, we have $ab^\dagger = b^\dagger a$ and $a^\dagger b = ba^\dagger$, so

$$L = \frac{i}{2}\left(ab^\dagger - a^\dagger b - a^\dagger b + ab^\dagger\right) = i(ab^\dagger - a^\dagger b)$$

While $S^y = \frac{1}{2i}(a^\dagger b - ab^\dagger) = \frac{i}{2}(ab^\dagger - a^\dagger b)$, so $S^y = \frac{L}{2}$. □

3. **Define the following set of states, where $s = 0, 1/2, 1, \cdots$, and $m = -s, -s+1, \cdots, s-1, s$ (they are called the Schwinger boson representation),**

$$|s,m\rangle = \frac{(a^\dagger)^{s+m}}{\sqrt{(s+m)!}}\frac{(b^\dagger)^{s-m}}{\sqrt{(s-m)!}}|\Omega\rangle$$

where $|\Omega\rangle$ is the state annihilated by a and b, i.e., $a|\Omega\rangle = b|\Omega\rangle = 0$. Prove that the state $|s,m\rangle$ is indeed a simultaneous eigenstate of $\vec{S}^2 = (S^x)^2 + (S^y)^2 + (S^z)^2$ and S^z , with eigenvalues $s(s+1)$ and m respectively. [Hint: Use the particle number basis.]

We have known that

$$\begin{aligned} S^z &= \frac{1}{2}\left(a^\dagger a - b^\dagger b\right) \\ \vec{S}^2 &= (S^x)^2 + (S^y)^2 + (S^z)^2 \end{aligned}$$

where $a^\dagger a$ counts the number of particles in the a mode, and $b^\dagger b$ counts the number of particles in the b mode. So we have

$$\begin{aligned} a^\dagger a|s,m\rangle = (s+m)|s,m\rangle, \quad b^\dagger b|s,m\rangle = (s-m)|s,m\rangle \\ \Rightarrow S^z|s,m\rangle = \frac{1}{2}\left((s+m)-(s-m)\right)|s,m\rangle = \boxed{m|s,m\rangle} \end{aligned}$$

So $|s,m\rangle$ is an eigenstate of S^z with eigenvalue m.

Define ladder operators $S^\pm = S^x \pm iS^y$:

$$\begin{aligned} S^+ = a^\dagger b, \quad S^- = b^\dagger a \\ \Rightarrow S^2 = S^z S^z + \frac{1}{2}\left(S^+S^- + S^-S^+\right) \end{aligned}$$

So we have

$$\begin{aligned} S^+|s,m\rangle &= a^\dagger b|s,m\rangle = \sqrt{(s+m+1)(s-m)}|s,m+1\rangle \\ S^-|s,m\rangle &= b^\dagger a|s,m\rangle = \sqrt{(s+m)(s-m+1)}|s,m-1\rangle \\ \Rightarrow S^+S^-|s,m\rangle &= S^+\sqrt{(s+m)(s-m+1)}|s,m-1\rangle = (s+m)(s-m+1)|s,m\rangle \\ S^-S^+|s,m\rangle &= S^-\sqrt{(s+m+1)(s-m)}|s,m+1\rangle = (s+m+1)(s-m)|s,m\rangle \\ S^zS^z|s,m\rangle &= m^2|s,m\rangle \end{aligned}$$

Combine the above results, and we have

$$\begin{aligned} S^2|s,m\rangle &= S^zS^z|s,m\rangle + \frac{1}{2}\left(S^+S^- + S^-S^+\right)|s,m\rangle \\ &= m^2|s,m\rangle + \frac{1}{2}\left((s+m)(s-m+1) + (s+m+1)(s-m)\right)|s,m\rangle \\ &= \boxed{s(s+1)|s,m\rangle} \end{aligned}$$

□

2.3.2 1D tight-binding model

The Hamiltonian of a periodic tight-binding chain of length L is given by the following expression:

$$H_{\text{chain}} = -t\sum_{n=1}^{L}\left(\hat{a}_n^\dagger \hat{a}_{n+1} + \hat{a}_{n+1}^\dagger \hat{a}\right)$$

where t is the hopping matrix element between adjacent sites n and $n+1$, $\hat{a}_n^\dagger$ creates a fermion at site n, and the set of operators $\{a_n^\dagger, a_n; n = 1, \cdots, L\}$ satisfies the standard anticommutation relations:

$$\{a_n, a_{n'}^\dagger\} = \delta_{nn'}, \quad \{a_n, a_{n'}\} = 0, \quad \{a_n^\dagger, a_{n'}^\dagger\} = 0$$

We assume periodic boundary conditions, i.e., we consider $a_{L+n}^\dagger = a_n^\dagger$.The purpose of this problem is to prove that this Hamiltonian can be diagonalized by a linear transformation of the discrete Fourier transform form:

$$b_k^\dagger = \frac{1}{\sqrt{L}}\sum_{n=1}^{L} e^{ikn} a_n^\dagger$$

1. **Let's require that $b_k^\dagger$ remains invariant under any shift of the summation index $n \to n + n'$ (''translation invariance''). Prove that this implies that the index k is quantized and determine the set of allowed k values. How many independent $b_k^\dagger$ operators are there?**

   Apply a shift of the summation index $n \to n + n'$, and

   $$b_k^\dagger = \frac{1}{\sqrt{L}}\sum_{n=1}^{L} e^{ik(n+n')} a_n^\dagger = \frac{1}{\sqrt{L}}\sum_{n=1}^{L} e^{ikn} e^{ikn'} a_n^\dagger$$

   Since b_k' remain invariant, so $e^{ikn'} = 1$ for any shift $n' \in \mathbb{Z}$, which means

   $$k = \frac{2\pi}{L}m, \quad m \in \{0, 1, 2, \cdots, L-1\}$$

   So there are $\boxed{L}$ independent $b_k^\dagger$ operators.

2. **Verify that the set of b_k and $b_k^\dagger$ operators also satisfies the above standard anticommutation relations. That is:**

   $$\{b_k, b_{k'}^\dagger\} = \delta_{kk'}, \quad \{b_k, b_{k'}\} = 0, \quad \{b_k^\dagger, b_{k'}^\dagger\} = 0$$

   Hint: Use the identity $\sum_{m=1}^{L} e^{i\frac{2\pi}{L}m} = 0$.

   We have

   $$b_k^\dagger = \frac{1}{\sqrt{L}}\sum_{n=1}^{L} e^{ikn} a_n^\dagger, \quad b_k = \frac{1}{\sqrt{L}}\sum_{n=1}^{L} e^{-ikn} a_n$$

   So

   $$\begin{aligned}\{b_k, b_{k'}^\dagger\} &= \frac{1}{L}\sum_{n,n'} e^{-ikn} e^{ik'n'}\{a_n, a_{n'}^\dagger\} = \frac{1}{L}\sum_{n,n'} e^{-ikn} e^{ik'n'}\delta_{nn'} \\ &= \frac{1}{L}\sum_{n=1}^{L} e^{-ikn} e^{ik'n} = \frac{1}{L}\sum_{n=1}^{L} e^{i(k'-k)n} = \boxed{\delta_{kk'}} \\ \{b_k, b_{k'}\} &= \frac{1}{L}\sum_{n,n'} e^{-ikn} e^{-ik'n'}\{a_n, a_{n'}\} = \boxed{0} \\ \{b_k^\dagger, b_{k'}^\dagger\} &= \frac{1}{L}\sum_{n,n'} e^{ikn} e^{ik'n'}\{a_n^\dagger, a_{n'}^\dagger\} = \boxed{0}\end{aligned}$$

3. **Prove that the inverse transformation of the above has the form:**

$$a_n^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{-ikn} b_k^\dagger$$

where the sum is over the set of allowed k values determined in (a).

We have the definition

$$b_k^\dagger = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger$$

So

$$\begin{aligned}
\frac{1}{\sqrt{L}} \sum_k e^{-ikn} b_k^\dagger &= \frac{1}{\sqrt{L}} \sum_k e^{-ikn} \left(\frac{1}{\sqrt{L}} \sum_{n'} e^{ikn'} a_{n'}^\dagger \right) \\
&= \frac{1}{L} \sum_{n'} \sum_k e^{ik(n'-n)} a_{n'}^\dagger = \sum_{n'} \left(\frac{1}{L} \sum_k e^{ik(n'-n)} \right) a_{n'}^\dagger \\
&= \sum_{n'} (\delta_{nn'}) a_{n'}^\dagger = a_n^\dagger. \quad \square
\end{aligned}$$

4. **Show that $b_k^\dagger$ is indeed a creation operator of a single-particle eigenstate of H_{chain} by proving that its commutator with the Hamiltonian has the form $[H_{\text{chain}}, b_k^\dagger] = \varepsilon_k b_k^\dagger$. Give the explicit expression for the corresponding eigenvalue ε_k.**

We have known that

$$\begin{aligned}
H_{\text{chain}} &= -t \sum_{n=1}^{L} \left(\hat{a}_n^\dagger \hat{a}_{n+1} + \hat{a}_{n+1}^\dagger \hat{a} \right), \quad \hat{a}_{L+1} = \hat{a}_1 \\
b_k^\dagger &= \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger
\end{aligned}$$

So the commutator

$$\begin{aligned}
[H_{\text{chain}}, b_k^\dagger] &= -t \sum_{n=1}^{L} \left(\left[a_n^\dagger a_{n+1}, b_k^\dagger \right] + \left[a_{n+1}^\dagger a_n, b_k^\dagger \right] \right) \\
\left[a_n^\dagger a_{n+1}, b_k^\dagger \right] &= a_n^\dagger \left[a_{n+1}, b_k^\dagger \right] = a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \left[a_{n+1}, a_m^\dagger \right] \\
&= a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \delta_{n+1,m} = a_n^\dagger \frac{1}{\sqrt{L}} e^{ik(n+1)} \\
\left[a_{n+1}^\dagger a_n, b_k^\dagger \right] &= a_{n+1}^\dagger \left[a_n, b_k^\dagger \right] = a_{n+1}^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \left[a_n, a_m^\dagger \right] \\
&= a_{n+1}^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \delta_{n,m} = a_{n+1}^\dagger \frac{1}{\sqrt{L}} e^{ikn} \\
\Rightarrow [H_{\text{chain}}, b_k^\dagger] &= -t \sum_{n=1}^{L} \left(a_n^\dagger \frac{1}{\sqrt{L}} e^{ik(n+1)} + a_{n+1}^\dagger \frac{1}{\sqrt{L}} e^{ikn} \right) \\
&= -t \left(e^{ik} \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger + e^{-ik} \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ik(n+1)} a_{n+1}^\dagger \right) \\
&= -t \left(e^{ik} b_k^\dagger + e^{-ik} b_k^\dagger \right) = \boxed{-2t \cos k} b_k^\dagger
\end{aligned}$$

So the corresponding eigenvalue $\varepsilon_k = -2t \cos k$.

2.4 Homework 4

2.4.1 Mean-field Solutions for Extended Hubbard Model

The Hamiltonian of the extended Hubbard model can be written as:

$$\hat{H} = -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \textbf{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j\rangle} n_i n_j$$

where:

- $c^\dagger_{i\sigma}$ **and** $c_{i\sigma}$ **are the fermionic creation and annihilation operators for an eletron with spin** σ **at site** i**.**
- $n_{i\sigma} = c^\dagger_{i\sigma} c_{i\sigma}$ **is the number operator for electrons with spin** σ **at site** i**.**
- $n_i = \sum_\sigma c^\dagger_{i\sigma} c_{i\sigma}$ **is the number operator for total electrons at site** i**.**
- $U > 0$ **is the strength of the on-site interaction between electrons.**
- $V > 0$ **is the strength of the interaction between electrons at neighboring sites.**
- $t > 0$ **is the hopping strength of the electrons.**

We consider the case of half-filling for two lattice sites ($\langle N\rangle = \langle n_{1\uparrow} + n_{1\downarrow} + n_{2\uparrow} + n_{2\downarrow}\rangle$**). In the mean-field approximation, calculate the ground state energy** E_{MF}**. Please consider initial mean-field values with following four cases.**

In the mean-field approximation, the Hamiltonian can be written as

$$\begin{aligned}
\hat{H} &= -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right) + U \sum_i n_{i\uparrow} n_{i\downarrow} + V \sum_{\langle i,j\rangle} n_i n_j \\
&= -t \sum_{\langle i,j\rangle,\sigma} \left(c^\dagger_{i\sigma} c_{j\sigma} + \text{h.c.}\right) + U \sum_i \left(n_{i\uparrow}\langle n_{i\downarrow}\rangle + ni\downarrow\langle n_{i\uparrow}\langle n_{i\uparrow}\rangle - \langle n_{i\uparrow}\rangle\langle n_{i\downarrow}\rangle\right) \\
&+ V \sum_{\langle i,j\rangle} \left(n_i\langle n_j\rangle + n_j\langle n_i\rangle - \langle n_i\rangle\langle n_j\rangle\right) \\
&= c^\dagger \begin{bmatrix} U\langle n_{1\downarrow}\rangle + V\langle n_2\rangle & & -t & \\ & U\langle n_{1\uparrow}\rangle + V\langle n_2\rangle & & -t \\ -t & & U\langle n_{2\downarrow}\rangle + V\langle n_1\rangle & \\ & -t & & U\langle n_{2\uparrow}\rangle + V\langle n_1\rangle \end{bmatrix} c
\end{aligned}$$

1. **Case 1: Paramagnetic(PM). Initial mean-field value** $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$**.**

   For this case, the interactions are weak, so we expect that the hopping term is dominant. Thus we have

   $$\langle n_{i\uparrow}\rangle = \langle n_{i\downarrow}\rangle = \frac{1}{2}, \quad \text{for all } i.$$

   $$\begin{bmatrix} U\frac{1}{2} + V & & -t & \\ & U\frac{1}{2} + V & & -t \\ -t & & U\frac{1}{2} + V & \\ & -t & & U\frac{1}{2} + V \end{bmatrix} = UDU^{-1}$$

   Except for the different diagnoal elements, this matrix is very similar to the case in the lecture. We can get

   $$U = \frac{1}{\sqrt{2}} \begin{bmatrix} & 1 & & -1 \\ 1 & & -1 & \\ & 1 & & 1 \\ 1 & & 1 & \end{bmatrix}, \quad D = \begin{bmatrix} -t + \frac{U}{2} + V & & & \\ & -t + \frac{U}{2} + V & & \\ & & t + \frac{U}{2} + V & \\ & & & t + \frac{U}{2} + V \end{bmatrix}$$

   $$E_{\text{MF}} = -2t + \frac{U}{2} + V$$

2. **Case 2: Ferromagnetic(FM). Initial mean-field value $\langle n_{i\uparrow}\rangle = 1$ and $\langle n_{i\downarrow}\rangle = 0$.**

When U is large, we expect no double occupancy. For this case, the mean-field values are chosen as

$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0.$$

$$\begin{bmatrix} V & & -t & \\ & U+V & & -t \\ -t & & V & \\ & -t & & U+V \end{bmatrix} = \begin{bmatrix} & & -t & \\ & U & & -t \\ -t & & & \\ & -t & & U \end{bmatrix} + V\mathbb{I} = UDU^{-1}$$

The effect of V is still just shifting the energy, and we get

$$U = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & -1 & & \\ & & 1 & -1 \\ 1 & 1 & & \\ & & 1 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} -t+V & & & \\ & t+V & & \\ & & -t+U+V & \\ & & & t+U+V \end{bmatrix}$$

(a) When $-t+U+V < t+V \iff U < 2t$,

$$\langle n_{1\uparrow}\rangle = \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{13}^* V_{13} = \frac{1}{2}$$
$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}$$

which implies the system is still in PM phase and $E_{\text{MF}} = -2t + \frac{U}{2} + V$.

(b) When $U > 2t$,

$$\langle n_{1\uparrow}\rangle = \sum_{ij} V_{1i}^* V_{1j} \langle \gamma_i^\dagger \gamma_j\rangle = V_{11}^* V_{11} + V_{12}^* V_{12} = 1$$
$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = 1, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = 0$$

Now the system is in FM phase and $E_{\text{FM}} = V$.

3. **Case 3: Anti-ferromagnetic(AFM). Initial mean-field value $\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1-\alpha$ and $\langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \alpha$.**

Another choice when U is large is to give

$$\langle n_{1\uparrow}\rangle = \langle n_{2\downarrow}\rangle = 1-\alpha, \quad \langle n_{1\downarrow}\rangle = \langle n_{2\uparrow}\rangle = \alpha.$$

$$\begin{aligned} &\begin{bmatrix} \alpha U+V & & -t & \\ & (1-\alpha)U+V & & -t \\ -t & & (1-\alpha)U+V & \\ & -t & & \alpha U+V \end{bmatrix} \\ =& \begin{bmatrix} & & -t & \\ & (1-2\alpha)U & & -t \\ -t & & (1-2\alpha)U & \\ & -t & & \end{bmatrix} + (\alpha U+V)\mathbb{I} = UDU^{-1} \end{aligned}$$

The effect of $\bar{V} = \alpha U + V$ is still just shifting the energy. Similar to the contents in the lecture note, mark $\bar{U} = (1-2\alpha)U$ and shift each eigenenergy with $\bar{V}$, we get

$$\begin{aligned} E_{\text{MF}} &= \bar{U} - \sqrt{4t^2 + \bar{U}^2} + 2\alpha U + 2V + 2\alpha(1-\alpha)U - V \\ &= (1+2\alpha-2\alpha^2)U - \sqrt{4t^2+\bar{U}^2} + V \end{aligned}$$

and the self-consistent equation is

$$\alpha = \frac{4t^2}{4t^2 + [\sqrt{4t^2 + (1-2\alpha)U^2} + (1-2\alpha)U]^2}$$

(a) When $U \gg t$, we get $\alpha \approx 0$ and $E_{\text{MF}} \approx -\dfrac{4t^2}{U} + V$. This corresponds to an AFM solution, which is lower than FM.

(b) When $U \ll t$, we get $\alpha \approx \frac{1}{2}$ and back to the PM solution.

4. **Case 4: Charge density wave(CDW). Initial mean-field value $\langle n_{1\uparrow}\rangle = \langle n_{1\downarrow}\rangle = 1-\alpha$ and $\langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \alpha$.**

When V is much stronger, we expect a double occupancy will occur. Thus the mean-field values are chosen as

$$\langle n_{1\uparrow}\rangle = \langle n_{1\downarrow}\rangle = 1-\alpha, \quad \langle n_{2\uparrow}\rangle = \langle n_{2\downarrow}\rangle = \alpha.$$

$$\begin{bmatrix} (1-\alpha)U + 2\alpha V & & -t & \\ & (1-\alpha)U + 2\alpha V & & -t \\ -t & & \alpha U + 2(1-\alpha)V & \\ & -t & & \alpha U + 2(1-\alpha)V \end{bmatrix} = UDU^{-1}$$

The result is a little complicated and one can solve the matrix by Mathematica easily. Note $\beta = (1-2\alpha)(U-2V)$ and $\gamma = 2t$, we have

$$D = \frac{1}{2}\left((U+2V)\mathbb{I} + \sqrt{\beta^2+\gamma^2}\begin{bmatrix} -1 & & & \\ & -1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix}\right)$$

The self-consistent equation is

$$1-\alpha = \frac{2\beta^2 + \gamma^2 - 2\beta\sqrt{\beta^2+\gamma^2}}{2\beta^2 + 2\gamma^2 - 2\beta\sqrt{\beta^2+\gamma^2}}$$

(a) When $\beta^2 \gg \gamma^2 \iff V \gg \frac{U}{2}$ and $V \gg t$, we have

$$\begin{aligned} \alpha \approx 0, \quad \langle n_{1\sigma}\rangle = 1, \quad \langle n_{2\sigma}\rangle = 0; \\ H_{\text{MF}} \approx U. \end{aligned}$$

(b) When $\beta^2 \ll \gamma^2 \iff V \ll t$ and $U \ll t$, we have $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$ which corresponds to the PM solution.

2.5 Homework 5

2.5.1 Quantum Rotor Model

The angular coordinate of a quatum rotor is $\theta \in [0, 2\pi)$, note that $\theta \pm 2\pi$ and θ are equivalent. The eigenstate of the operator $\hat{\theta}$ is represented by $|\theta\rangle$, and $\theta \pm 2\pi\rangle$ represents the same state as $|\theta\rangle$. Define the rotation operator for the quantum rotator as $\hat{R}(\alpha)$,

$$\hat{R}(\alpha) = \int_0^{2\pi} \mathrm{d}\theta |\theta - \alpha\rangle\langle\theta|$$

Thus $\hat{R}(\alpha)|\theta\rangle = |\theta - \alpha\rangle$, and $\hat{R}(2\pi)$ is the identity operator.

The rotation operator $\hat{R}(\alpha)$ is a unitary operator, its generator is the Hermitian operator $\hat{N}$, which is related to the angular momentum operator of the quantum rotator $\hat{L}$ by $\hat{L} = \hbar\hat{N}$, so $\hat{R}(\alpha) = e^{i\hat{N}\alpha}$, and in the $\hat{\theta}$ representation, we have $\hat{N} = -i\frac{\partial}{\partial\theta}$.

Consider a specific quantum rotor model, its Hamiltonian is

$$\hat{H} = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2 - g\cos 2\hat{\theta}$$

where $g\cos 2\hat{\theta}$ is a small external potential, which can be treated as a perturbation. Assuming $|N\rangle$ is the eigenstate of the operator $\hat{N}$ with eigenvalue N, i.e., $\hat{N}|N\rangle = N|N\rangle$. It can be calculated that $|N\rangle$ is expanded in terms of $|\theta\rangle$ as

$$|N\rangle = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle$$

1. **Use the fact that $\hat{R}(2\pi)$ is the identity operator to prove that N must be an integer.**

   Since $\hat{R}(2\pi) = \mathbb{I}$, so we have $|\theta - 2\pi\rangle = |\theta\rangle$. For eigenstate $|N\rangle$ of operator $\hat{N}$, we have

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta-2\pi\rangle &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle \\
\iff \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta\rangle &= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta\rangle \\
\iff e^{iN\theta} &= e^{iN(\theta-2\pi)} = e^{iN\theta}e^{-i2\pi N}
\end{aligned}$$

   So N should be an integer to keep the invariance of the shift of θ by 2π.

2. **Consider the unperturbed Hamiltonian $\hat{H}_0 = \frac{1}{2}\left(\frac{1}{2}\hat{N} - \frac{1}{2}\right)^2$, prove that $|N\rangle$ is also an eigenstate of $\hat{H}_0$, and find its eigenenergy, demonstrating that each energy level is doubly degenerate.**

$$\begin{aligned}
\hat{H}_0|N\rangle = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2|N\rangle = \frac{1}{2}\left(N - \frac{1}{2}\right)^2|N\rangle &\Rightarrow E_N^{(0)} = \frac{1}{2}\left(N - \frac{1}{2}\right)^2 \\
\Rightarrow N_\pm - \frac{1}{2} = \pm\sqrt{2E_N^{(0)}} &\Rightarrow N_\pm = \frac{1}{2} \pm \sqrt{2E_N^{(0)}}
\end{aligned}$$

   which means for any N, there exists $N' = 1 - N$ to make the energy level degenerate.

3. **Using the basis set $\{|N\rangle\}$, write down the representation matrix for the perturbation term $\hat{V} = -g\cos 2\hat{\theta}$, and prove that the perturbation does not connect degenerate levels (i.e., if $|N\rangle$ and $|N'\rangle$ are degenerate, then $\langle N|\hat{V}|N'\rangle = 0$). Therefore, although the energy levels of $\hat{H}_0$ are degenerate, we can still use non-degenerate perturbation theory.**

$$\begin{aligned}
\cos 2\hat{\theta} &= \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right) \\
e^{i2\hat{\theta}}|N\rangle &= e^{i2\hat{\theta}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle\right) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}e^{i2\hat{\theta}}|\theta\rangle \\
&= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{i(N+2)\theta}|\theta\rangle = |N+2\rangle \\
\Rightarrow \cos 2\hat{\theta}|N\rangle &= \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)|N\rangle = \frac{1}{2}\left(|N+2\rangle + |N-2\rangle\right) \\
\Rightarrow \langle N|\hat{V}|N'\rangle &= -g\langle N|\cos 2\hat{\theta}|N'\rangle = -\frac{g}{2}\left(\langle N|N'+2\rangle + \langle N|N'-2\rangle\right) \\
&= -\frac{g}{2}(\delta_{N,N'+2} + \delta_{N,N'-2})
\end{aligned}$$

   As the discussion before, if $|N\rangle$ and $|N'\rangle$ are degenerate, then $N + N' = 1$, which means the delta note equals to 0 when $N \in \mathbb{Z}$, so the perturbation does not connect degenerate levels.

4. **Calculate the perturbation correction to each energy level E_N up to second order in g, and prove that all degeneracies of the energy levels remain unlifted.**

$$
\begin{aligned}
E_N^{(1)} &= \langle N|\hat{V}|N\rangle = -\frac{g}{2}\left(\langle N|N+2\rangle + \langle N|N-2\rangle\right) = 0 \\
E_N^{(2)} &= \sum_{N'\neq N} \frac{|\langle N|\hat{V}|N'\rangle|^2}{E_N^{(0)} - E_{N'}^{(0)}} = \sum_{N'\neq N} \frac{\left(-\frac{g}{2}(\delta_{N,N'+2} + \delta_{N,N'-2})\right)^2}{\frac{1}{2}\left(N-\frac{1}{2}\right)^2 - \frac{1}{2}\left(N'-\frac{1}{2}\right)^2} \\
&= \boxed{\frac{g^2}{(2N-3)(2N+1)}}
\end{aligned}
$$

So the corrected energy level is

$$
E_N \approx \frac{1}{2}\left(N-\frac{1}{2}\right)^2 + \frac{g^2}{(2N-3)(2N+1)}
$$

Apply $N' = 1 - N$ to check if the degeneracy is lifted, we have

$$
\begin{aligned}
E_{N'} &= \frac{1}{2}\left(1-N-\frac{1}{2}\right)^2 + \frac{g^2}{[2(1-N)-3][2(1-N)+1]} \\
&= \frac{1}{2}\left(N-\frac{1}{2}\right)^2 + \frac{g^2}{(2N+1)(2N-3)} = E_N
\end{aligned}
$$

so the degeneracy of the energy levels remains unlifted.

第三章　2022秋高等量子力学期末考核

3.1　单项选择

1. 让大量热化的自旋通过 **Stern-Gerlach** 装置**SG** $\hat{z}$,测得 S_+^z 的概率是?

   大量热化自旋表示充分随机, 所以 $P(S_+^z) = ||\chi_+^{z\dagger}\frac{1}{\sqrt{2}}(\chi_+^z + \chi_-^z)||^2 = \boxed{\frac{1}{2}}$

2. **Pauli** 矩阵 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, $\sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$, $\sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, 那么 $\sigma^x\sigma^z$ 等于?

   $\sigma^x\sigma^z = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}$

3. 混态可以用混态的密度矩阵来描述. 假设系统处于态 $|\phi_i\rangle$ 的概率为 p_i, 注意 $\sum_i p_i = 1$, 那么该系统的密度矩阵为 $\rho = \sum_i |\phi_i\rangle p_i \langle\phi_i|$, 那么 **Tr**$[\rho]$ 应满足?

   因为密度矩阵的迹表示系统的总概率, 而概率必须归一化, 即 $\mathrm{Tr}[\rho] = \sum_i p_i = \boxed{1}$

4. 如果 ρ 是混态的密度矩阵, 那么 **Tr**$[\rho^2]$ 应满足?

   对任意密度矩阵总有$\hat{\rho} = \sum_\alpha p_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|$. 那么$\hat{\rho}^2 = \sum_\alpha p_\alpha|\psi_\alpha\rangle\langle\psi_\alpha|\sum_\beta p_\beta|\psi_\beta\rangle\langle\psi_\beta| = \sum_\alpha p_\alpha^2|\psi_\alpha\rangle\langle\psi_\alpha|$. 对于纯态($p_n^2 = p_n$) $\mathrm{Tr}[\rho^2] = \mathrm{Tr}[\rho] = 1$, 而混态($p_n^2 \neq p_n$)则是 $\mathrm{Tr}[\rho^2]\boxed{< 1}$.

5. 考虑系统哈密顿量 H 不显含时间, 时间演化算符为 $U(t,0) = e^{-iHt/\hbar}$. 在海森堡绘景中, 我们让算符承载时间演化, 海森堡绘景中的算符定义为 $A_H(t) = U^\dagger(t,0)AU(t,0)$, 其中 A 是薛定谔绘景中的算符, 如果 A 不显含时间, 那么 $\mathrm{d}A_H(t)/\mathrm{d}t$ 等于?

$$\begin{aligned}
\frac{\mathrm{d}A_H(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}Ae^{-iHt/\hbar}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}\right)Ae^{-iHt/\hbar} + e^{iHt/\hbar}\frac{\mathrm{d}}{\mathrm{d}t}\left(Ae^{-iHt/\hbar}\right) \\
&= \frac{iH}{\hbar}e^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}A\frac{iH}{\hbar}e^{-iHt/\hbar} = \frac{i}{\hbar}\left(He^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}Ae^{-iHt/\hbar}H\right) \\
&= \frac{i}{\hbar}[H, A_H(t)] = \boxed{\frac{1}{i\hbar}[A_H(t), H]}
\end{aligned}$$

6. 电磁场中电荷为 q 的单粒子哈密顿量为 $H = \frac{(\vec{p} - q\vec{A})^2}{2m} + q\phi$, 那么薛定谔方程 $i\hbar\frac{\partial\psi}{\partial t} = H\psi$ 满足规范不变性: $\vec{A} \to \vec{A} - \nabla\Lambda$, $\phi \to \phi + \frac{\partial\Lambda}{\partial t}$, $\psi \to$?

   推导极其麻烦, 建议直接背结论, 不要试图考场现推. 假设 $\psi' = \psi e^{if(\vec{r},t)}$ 是满足规范变换的, 其中 $f(\vec{r},t)$ 是待定函数. 连同其它的规范变换, 代入薛定谔方程得到 $f(\vec{r},t)$ 的微分方程:

$$
\begin{aligned}
i\hbar\frac{\partial}{\partial t}\left[\psi e^{if(\vec{r},t)}\right] &= \left[\frac{(-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda))^2}{2m}+q\left(\phi+\frac{\partial\Lambda}{\partial t}\right)\right]\left[\psi e^{if(\vec{r},t)}\right] \\
i\hbar\frac{\partial}{\partial t}\left[\psi e^{if(\vec{r},t)}\right] &= \left[i\hbar\frac{\partial\psi}{\partial t}-\hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)} \\
\vec{\nabla}\left(\psi e^{if(\vec{r},t)}\right) &= \left(\vec{\nabla}\psi+\psi i\vec{\nabla}f\right)e^{if(\vec{r},t)} \\
\left[-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda)\right]\left[\psi e^{if(\vec{r},t)}\right] &= \left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}
\end{aligned}
$$

$$
\begin{aligned}
&\left[-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda)\right]^2\left[\psi e^{if(\vec{r},t)}\right] = \left[-i\hbar\vec{\nabla}-q(\vec{A}-\vec{\nabla}\Lambda)\right]\left\{\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}\right\} \\
&= (-i\hbar)\left\{\left[-i\hbar\nabla^2\psi+\hbar(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\hbar\psi\nabla^2 f-q(\vec{\nabla}\cdot\vec{A}-\nabla^2\Lambda)\psi-q(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right]e^{if(\vec{r},t)}\right. \\
&\left.+\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]\cdot i(\vec{\nabla}f)e^{if(\vec{r},t)}\right\} \\
&-q(\vec{A}-\vec{\nabla}\Lambda)\cdot\left[-i\hbar\vec{\nabla}\psi+\hbar\psi\vec{\nabla}f-q(\vec{A}-\vec{\nabla}\Lambda)\psi\right]e^{if(\vec{r},t)}
\end{aligned}
$$

展开变换前的薛定谔方程:

$$
i\hbar\frac{\partial\psi}{\partial t} = \left[\frac{(-i\hbar\vec{\nabla}-q\vec{A})^2}{2m}+q\phi\right]\psi = -\frac{\hbar^2}{2m}\nabla^2\psi+\frac{i\hbar q}{2m}(\vec{\nabla}\cdot\vec{A})\psi+\frac{i\hbar q}{m}\vec{A}\cdot(\vec{\nabla}\psi)+\frac{q^2A^2}{2m}\psi+q\phi\psi \tag{①}
$$

展开变换后的薛定谔方程:

$$
\begin{aligned}
&\left[i\hbar\frac{\partial\psi}{\partial t}-\hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)} \\
&= e^{if(\vec{r},t)}\left[-\frac{\hbar^2}{2m}\nabla^2\psi-\frac{i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)-\frac{i\hbar^2}{2m}\psi\nabla^2 f+\frac{i\hbar q}{2m}(\vec{\nabla}\cdot\vec{A}-\nabla^2\Lambda)\psi+\frac{i\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right. \\
&+\frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi-\frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi \\
&+\frac{i\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi)-\frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi+\frac{q^2}{2m}(\vec{A}-\vec{\nabla}\Lambda)^2\psi \\
&\left.+q\left(\phi+\frac{\partial\Lambda}{\partial t}\right)\psi\right]
\end{aligned} \tag{②}
$$

$(②)-(①)\cdot e^{if(\vec{r},t)}$, 得到

$$
\begin{aligned}
&\left[\cancel{i\hbar\frac{\partial\psi}{\partial t}}-\hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)} \\
&= e^{if(\vec{r},t)}\left[\cancel{-\frac{\hbar^2}{2m}\nabla^2}\psi-\frac{i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)-\frac{i\hbar^2}{2m}\psi\nabla^2 f+\frac{i\hbar q}{2m}(\cancel{\vec{\nabla}\cdot\vec{A}}-\nabla^2\Lambda)\psi+\frac{i\hbar q}{2m}(\cancel{\vec{A}}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi)\right. \\
&+\frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f)+\frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi-\frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi \\
&+\frac{i\hbar q}{2m}(\cancel{\vec{A}}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi)-\frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi+\frac{q^2}{2m}\left(\cancel{A^2}+(\vec{\nabla}\Lambda)^2-2\vec{A}\cdot(\vec{\nabla}\Lambda)\right)\psi \\
&\left.+q\left(\cancel{\phi}+\frac{\partial\Lambda}{\partial t}\right)\psi\right]
\end{aligned}
$$

$$
\begin{aligned}
-\hbar\psi\frac{\partial f}{\partial t} = & -\frac{i\hbar^2}{m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f) - \frac{i\hbar^2}{2m}\psi\nabla^2 f - \frac{i\hbar q}{2m}\psi\nabla^2\Lambda - \frac{i\hbar q}{m}(\vec{\nabla}\Lambda)\cdot(\vec{\nabla}\psi) \\
& + \frac{\hbar^2}{2m}\psi(\nabla f)^2 - \frac{\hbar q}{m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi \\
& + \frac{q^2}{2m}\left[(\vec{\nabla}\Lambda)^2 - 2\vec{A}\cdot(\vec{\nabla}\Lambda)\right]\psi \\
& + q\frac{\partial\Lambda}{\partial t}\psi
\end{aligned}
$$

重点观察含 $\vec{A}$ 的项, 由于需要对任意 $\vec{A}$ 都成立, 所以 $\vec{A}$ 的系数必须为 0, 即

$$
\vec{A}\cdot\left(-\frac{\hbar q}{m}\vec{\nabla}f - \frac{q^2}{2m}2\vec{\nabla}\Lambda\right) = 0
$$

最简单的解法即 $f = \frac{-q\Lambda}{\hbar}$, 所以规范变换后的波函数为 $\psi' = \boxed{\psi e^{-iq\Lambda/\hbar}}$. 需要关注一开始给出的 Λ 的符号, 从而影响整体变换的正负.

7. **角动量的对易关系为 $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$, 升降算符定义为 $J_\pm = J_x \pm iJ_y$, 那么 $[J_+, J_-] =$?**

$$
\begin{aligned}
[J_+, J_-] &= [J_x + iJ_y, J_x - iJ_y] \\
&= [J_x, J_x] - i[J_x, J_y] + i[J_y, J_x] + [J_y, J_y] = -2i[J_x, J_y] = -2i(i\hbar J_z) \\
&= \boxed{2\hbar J_z}
\end{aligned}
$$

8. **二维谐振子的哈密顿量为 $H = \hbar\omega\left(a_1^\dagger a_1 + a_2^\dagger a_2 + 1\right)$ 其第一激发态的简并度为?**

二维谐振子的哈密顿量用粒子数算符写作 $\hat{H} = \hbar\omega\left(\hat{n}_1 + \hat{n}_2 + \frac{1}{2}\right)$, 所以第一激发态即 $n_1 + n_2 = 1$, 这代表了 $|01\rangle$ 和 $|10\rangle$ 两个正交态, 所以简并度为 $\boxed{2}$.

9. **量子比特 A 和 B 构成双量子比特体系, 双量子比特态 $|\psi\rangle$ 中量子比特 A 的纠缠熵定义为 $S(A) = -\mathbf{Tr}[\rho_A \ln\rho_A]$, 其中 ρ_A 是约化密度矩阵, 由密度矩阵求迹掉量子比特 B 的自由度得到. 考虑自旋单态 $|\psi\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, 计算可得量子比特 A 的纠缠熵为?**

密度矩阵为

$$
\begin{aligned}
\rho = |\psi\rangle\langle\psi| &= \frac{1}{\sqrt{2}}\left(|\uparrow\rangle_A\otimes|\downarrow\rangle_B - |\downarrow\rangle_A\otimes|\uparrow\rangle_B\right)\frac{1}{\sqrt{2}}\left(\langle\uparrow|_A\langle\downarrow|_B - \langle\downarrow|_A\langle\uparrow|_B\right) \\
&= \frac{1}{2}\left(|\uparrow\rangle_A\langle\uparrow|_A\otimes|\downarrow\rangle_B\langle\downarrow|_B - |\uparrow\rangle_A\langle\downarrow|_A\otimes|\downarrow\rangle_B\langle\uparrow|_B - |\downarrow\rangle_A\langle\uparrow|_A\otimes|\uparrow\rangle_B\langle\downarrow|_B + |\downarrow\rangle_A\langle\downarrow|_A\otimes|\uparrow\rangle_B\langle\uparrow|_B\right)
\end{aligned}
$$

接下来进行部分求迹, 从而得到所需的约化密度矩阵 ρ_A. 迹被定义为对角线元素之和, 所以我们通过矢量 $\mathbb{I}_A\otimes|\uparrow\rangle_B$ 和$\mathbb{I}_A\otimes|\downarrow\rangle_B$ 来提取对角元素. 具体方法是

$$
\begin{aligned}
&(\mathbb{I}_A\otimes\langle\uparrow|_B)\rho(\mathbb{I}_A\otimes|\uparrow\rangle_B) = \frac{1}{2}|\downarrow\rangle_A\langle\downarrow|_A, \\
&(\mathbb{I}_A\otimes\langle\downarrow|_B)\rho(\mathbb{I}_A\otimes|\downarrow\rangle_B) = \frac{1}{2}|\uparrow\rangle_A\langle\uparrow|_A, \\
&\qquad\Rightarrow \rho_A = \sum_i^{\uparrow,\downarrow}(\mathbb{I}_A\otimes\langle i|_B)\rho(\mathbb{I}_A\otimes|i\rangle_B) = \frac{1}{2}\left(|\downarrow\rangle_A\langle\downarrow|_A + |\uparrow\rangle_A\langle\uparrow|_A\right) = \frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}
\end{aligned}
$$

计算 ρ_A 的纠缠熵:

$$S(A) = -\mathrm{Tr}[\rho_A \ln \rho_A] = -\sum_i^{\uparrow,\downarrow}(\langle i|_A)\rho_A(|i\rangle_A)\ln\left[(\langle i|_A)\rho_A(|i\rangle_A)\right]$$
$$= -\left(\frac{1}{2}\ln\frac{1}{2}+\frac{1}{2}\ln\frac{1}{2}\right) = \boxed{\ln 2 = 1\ \mathrm{bit}}$$

10. **假设哈密顿量 H 是厄密的, 其基态能量为 E_0, 给定某个态 Ψ, 测得能量期望值为 $E[\Psi]=\dfrac{\langle\Psi|H|\Psi\rangle}{\langle\Psi|\Psi\rangle}$, $E(\Psi)$ 和 E_0 的关系为?**

任意态均可通过基矢展开, 形式为 $|\Psi\rangle = \sum_n |n\rangle\langle n|\Psi\rangle$, 则

$$E[\Psi] = \left(\sum_m \langle\Psi|m\rangle\langle m|\right)\hat{H}\left(\sum_n |n\rangle\langle n|\Psi\rangle\right) = \sum_{m,n}\langle\Psi|m\rangle\langle m|\hat{H}|n\rangle\langle n|\Psi\rangle$$
$$= \sum_{m,n} c_m^* E_n \delta_{mn} c_n = \sum_n |c_n|^2 E_n \geq \sum_n |c_n|^2 E_0 = E_0$$

3.2　多项选择

1. **与总角动量算符的平方 $\vec{J}^2$ 对易的算符在 $(J_x, J_y, J_z, J_+, J_-)$ 中有?**

已知角动量的基本对易关系 $[J_i, J_j] = i\hbar\epsilon_{ijk}J_k$, 那么

$$[J^2, J_l] = [\sum_i^3 J_i^2, J_l] = \sum_i^3 [J_i^2, J_l] = \sum_i^3 \left(J_i[J_i,J_l] + [J_i,J_l]J_i\right)$$
$$= \sum_i^3 \left(J_i i\hbar\epsilon_{ilk}J_k + i\hbar\epsilon_{ilk}J_kJ_i\right)$$
$$= i\hbar\sum_i^3(\epsilon_{ilk}J_iJ_k - \epsilon_{kli}J_kJ_i) = 0.$$

其中利用了 ϵ_{ijk} 的反对称性质以及 $k \iff i$ 的地位等价. 而 $J_\pm = J_x \pm iJ_y$ 是 $\{J_l\}$ 的线性组合, 根据对易关系的线性性质可知 $[J^2, J_\pm] = 0$, 所以待选项均为正确答案.

2. **在原子单位制下 $\hbar = c = 1$, 和能量同单位的量在 (距离, 动量, 时间, 质量, 角动量) 中有?**

能量单位为 J=kg·m^2/s^2, 距离单位为 m, 动量单位为 kg·m/s, 时间单位为 s, 质量单位为 kg, 角动量单位为 kg·m^2/s. 现在要求 kg·m^2/s=m/s=1, 即寻找如何通过除以 $\hbar(\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s})$, $c(\mathrm{m/s})$ 来进行量纲变换

(a) 距离. $\dfrac{E}{\hbar c} = \dfrac{\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}^2}{\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}\cdot\mathrm{m/s}} = \dfrac{1}{\mathrm{m}}$, 说明距离和能量在单位上互为倒数.

(b) $\boxed{\text{动量}}$. $E = pc$

(c) 时间. $E = \hbar\omega = \hbar\dfrac{1}{\tau}$, 所以时间和能量单位互为倒数.

(d) $\boxed{\text{质量}}$. $E = mc^2$.

(e) 角动量. 角动量的量纲正好是 kg·m^2/s, 即无量纲数, 而能量无法通过除以 $\hbar$ 或 c 来变成角动量的量纲, 所以角动量和能量不同单位.

3. **宇称算符 $\mathbb{P}$ 连续作用两次为恒等变换, 这说明宇称算符 $\mathbb{P}$ 的本征值在 $(0, 1, -1, i, -i)$ 中有?**

不妨设 $\mathbb{P}\psi = \lambda\psi$, 那么 $\mathbb{P}^2\psi = \lambda^2\psi = \psi$, 所以 $\lambda^2 = 1$, 即 $\lambda = \pm 1$. 所以宇称算符的本征值为 $\boxed{1, -1}$.

4. **如果算符 A 满足 $A^2 = A$, 那么算符 A 的本征值有 $(0, 1, -1, i, -i)$ 中有?**

不妨设 $A\psi = \lambda\psi$, 那么 $A^2\psi = A(\lambda\psi) = \lambda^2\psi$, $\lambda^2 = \lambda$, 即 $\lambda = 0, 1$. 所以算符 A 的本征值为 $\boxed{0, 1}$.

5. **玻色子产生和湮灭算符满足对易关系 $\left[b_\alpha^\dagger, b_\beta^\dagger\right] = [b_\alpha, b_\beta] = 0$, $\left[b_\alpha, b_\beta^\dagger\right] = \delta_{\alpha\beta}$, 那么和总粒子数算符 $N = \sum\limits_\alpha b_\alpha^\dagger b_\alpha$ 对易的算符在 $(b_\alpha, b_\alpha^\dagger b_\alpha, b_\alpha^\dagger b_\beta, b_\alpha^\dagger b_\beta b_\mu, b_\alpha^\dagger b_\beta b_\mu^\dagger b_\nu)$ 中有?**

已知 $[N, A] = \sum\limits_i \left[b_i^\dagger b_i, A\right] = \sum\limits_i \left\{b_i^\dagger [b_i, A] + \left[b_i^\dagger, A\right] b_i\right\}$, 代入以上各算符 A 判断是否对易.

(a) $[N, b_\alpha] = \sum\limits_i \left\{b_i^\dagger [b_i, b_\alpha] + \left[b_i^\dagger, b_\alpha\right] b_i\right\} = \sum\limits_i \{0 + (-\delta_{i\alpha}) b_\alpha\} = -b_\alpha$

(b)

$$\begin{aligned}
\boxed{[N, b_\alpha^\dagger b_\alpha]} &= \sum_i \left[b_i^\dagger b_i, b_\alpha^\dagger b_\alpha\right] = \sum_i \left\{b_i^\dagger [b_i, b_\alpha^\dagger b_\alpha] + \left[b_i^\dagger, b_\alpha^\dagger b_\alpha\right] b_i\right\} \\
&= \sum_i \left\{b_i^\dagger \left(b_\alpha^\dagger [b_i, b_\alpha] + \left[b_i, b_\alpha^\dagger\right] b_\alpha\right) + \left(b_\alpha^\dagger [b_i^\dagger, b_\alpha] + [b_i^\dagger, b_\alpha^\dagger] b_\alpha\right) b_i\right\} \\
&= \sum_i \left\{b_i^\dagger (b_\alpha^\dagger \cdot 0 + \delta_{i\alpha} b_\alpha) + (b_\alpha^\dagger (-\delta_{i\alpha}) + 0 \cdot b_\alpha) b_i\right\} \\
&= \sum_i \delta_{i\alpha} (b_i^\dagger b_\alpha - b_\alpha^\dagger b_i) = 0
\end{aligned}$$

(c)

$$\begin{aligned}
\boxed{[N, b_\alpha^\dagger b_\beta]} &= \sum_i \left[b_i^\dagger b_i, b_\alpha^\dagger b_\beta\right] = \sum_i \left\{b_i^\dagger [b_i, b_\alpha^\dagger b_\beta] + \left[b_i^\dagger, b_\alpha^\dagger b_\beta\right] b_i\right\} \\
&= \sum_i \left\{b_i^\dagger (b_\alpha^\dagger [b_i, b_\beta] + [b_i, b_\alpha^\dagger] b_\beta) + (b_\alpha^\dagger [b_i^\dagger, b_\beta] + [b_i^\dagger, b_\alpha^\dagger] b_\beta) b_i\right\} \\
&= \sum_i \left\{b_i^\dagger (b_\alpha^\dagger \cdot 0 + \delta_{i\alpha} b_\beta) + (b_\alpha^\dagger (-\delta_{i\beta}) + 0 \cdot b_\beta) b_i\right\} \\
&= \sum_i \left(b_i^\dagger b_\beta \delta_{i\alpha} - b_\alpha^\dagger b_i \delta_{i\beta}\right) = 0.
\end{aligned}$$

(d)

$$[N, b_\alpha^\dagger b_\beta b_\mu] = b_\alpha^\dagger b_\beta [N, b_\mu] + [N, b_\alpha^\dagger b_\beta] b_\mu = -b_\alpha^\dagger b_\beta b_\mu$$

(e)

$$\boxed{[N, b_\alpha^\dagger b_\beta b_\mu^\dagger b_\nu]} = b_\alpha^\dagger b_\beta [N, b_\mu^\dagger b_\nu] + [N, b_\alpha^\dagger b_\beta] b_\mu^\dagger b_\nu = 0 + 0 = 0$$

可以不严谨地总结出一条规律: 粒子数算符 $\hat{N}$ 只会与另一个粒子数算符对易, 而与单独的产生湮灭算符均不对易.

3.3 简答题

1. **中心势场中的单粒子哈密顿量为 $H = \dfrac{\vec{p}^2}{2M} + V(r)$. 轨道角动量 $\vec{L} = \vec{r} \times \vec{p}$, 那么 $[\vec{L}, H] =$?**

由于是中心势场, 不妨设 $V(r)=r^n$, 则

$$
\begin{aligned}
[\vec{L},H] &= \left[\sum_{ijk}\epsilon_{ijk}\hat{x}_i x_j p_k, \sum_{\alpha}^{3}\frac{p_\alpha^2}{2m}+r^n\right] = \frac{1}{2m}\sum_{ijk\alpha}\epsilon_{ijk}\hat{x}_i[x_jp_k,p_\alpha^2]+\sum_{ijk}\epsilon_{ijk}\hat{x}_i[x_jp_k,r^n] \\
&= \frac{1}{2m}\sum_{ijk\alpha}\hat{x}_i\epsilon_{ijk}\left\{\cancel{x_jp_\alpha[p_k,p_\alpha]}+\cancel{x_j[p_k,p_\alpha]p_\alpha}+p_\alpha[x_j,p_\alpha]p_k+[x_j,p_\alpha]p_\alpha p_k\right\}+\sum_{ijk}\epsilon_{ijk}\hat{x}_ix_j[-i\hbar\frac{\partial}{\partial x_k},r^n] \\
&= \frac{1}{2m}\sum_{ijk\alpha}2i\hbar\delta_{j\alpha}p_\alpha p_k+\sum_{ijk}\epsilon_{ijk}\hat{x}_ix_j\left(-i\hbar n r^{n-1}r^{-\frac{1}{2}}x_k\right) \\
&= \sum_{ijk}\epsilon_{ijk}\hat{x}_i\left\{\frac{i\hbar}{m}p_jp_k+(-i\hbar n r^{n-\frac{3}{2}})x_jx_k\right\}
\end{aligned}
$$

注意到 $j \iff k$ 和 ϵ_{ijk} 的反对称性质, 可以得到 $[\vec{L},H]=\boxed{0}$.

2. **考虑一阶近似, 当 $i\neq f$ 时, 跃迁概率为**

$$
P_{i\to f}(t)=\frac{1}{\hbar^2}\left|\int_0^t \mathrm{d}t'\langle f|V(t')|i\rangle e^{\mathrm{i}\omega_{fi}t'}\right|^2
$$

其中 $\hbar\omega_{fi}=E_f-E_i$. 当微扰为

$$
V(t)=\begin{cases} Ve^{-\mathrm{i}\omega t} & t>0 \\ 0 & t<0 \end{cases}
$$

跃迁概率为?

$$
\begin{aligned}
P_{i\to f}(t) &= \frac{1}{\hbar^2}\left\|\int_0^t \mathrm{d}t'\langle f|Ve^{-\mathrm{i}\omega t'}|i\rangle e^{\mathrm{i}\omega_{fi}t'}\right\|^2 = \frac{1}{\hbar^2}\left\|\int_0^t \mathrm{d}t'\langle f|V|i\rangle e^{-\mathrm{i}\omega t'}e^{\mathrm{i}\omega_{fi}t'}\right\|^2 \\
&= \frac{1}{\hbar^2}\left\|\int_0^t \mathrm{d}t'\langle f|V|i\rangle e^{\mathrm{i}(\omega_{fi}-\omega)t'}\right\|^2 = \frac{1}{\hbar^2}\left\|\int_0^t \mathrm{d}t'\langle f|V|i\rangle e^{\mathrm{i}\Delta\omega t'}\right\|^2 \\
\left\|\int_0^t \mathrm{d}t' e^{\mathrm{i}\Delta\omega t'}\right\|^2 &= \left\|\frac{e^{\mathrm{i}\Delta\omega t}-1}{\mathrm{i}\omega}\right\|^2 = \frac{(e^{\mathrm{i}\Delta\omega t}-1)(e^{-\mathrm{i}\Delta\omega t}-1)}{(\Delta\omega)^2} = \frac{2-2\cos\Delta t}{(\Delta\omega)^2} = \frac{4}{(\Delta\omega)^2}\sin^2\left(\frac{\Delta\omega t}{2}\right) \\
P_{i\to f}(t) &= \boxed{\frac{4\left|\langle f|V|i\rangle\right|^2}{\hbar^2(\Delta\omega)^2}\sin^2\left(\frac{\Delta\omega t}{2}\right)}
\end{aligned}
$$

3. *算符 $\Omega(t)\equiv U^{-1}(t)U_0(t)$, 算符 $\Omega_\pm\equiv\lim_{t\to\mp\infty}\Omega(t)$, 其中
   - $U_0(t)=e^{-\mathrm{i}H_0t/\hbar}$ 是自由系统 H_0 的时间演化算符;
   - $U(t)=e^{-\mathrm{i}Ht/\hbar}$ 是短程势散射系统的时间演化算符.

   $H=H_0+V$. 散射算符定义为 $S\equiv\Omega_-^\dagger\Omega_+$, 那么 $[S,H_0]=?$

4. **动量空间中自由粒子的 Dirac 方程可以写为**

$$
(E-\vec{\sigma}\cdot\vec{p})\,\chi_+(\vec{p})=m\chi_-(\vec{p}),\quad (E+\vec{\sigma}\cdot\vec{p})\,\chi_-(\vec{p})=m\chi_+(\vec{p})
$$

当质量 $m=0$时, 两个 Weyl 旋量之间没有耦合, 得到动量空间中的 Weyl 方程

$$
(E-\vec{\sigma}\cdot\vec{p})\,\chi_+=0,\quad (E+\vec{\sigma}\cdot\vec{p})\,\chi_-=0
$$

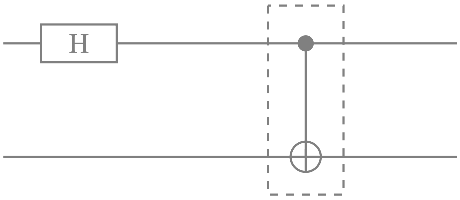
定义螺旋度算符为 $\frac{1}{2}\hat{\vec{p}}\cdot\vec{\sigma}$, 其中 $\hat{\vec{p}}=\frac{\vec{p}}{|\vec{p}|}$, 那么可知 Weyl 旋量 $\chi_\pm$ 恰好是螺旋度算符的本征态, 本征值分别为?

当 $m=0$ 且 $|\vec{p}|=E$ 时, 原 Dirac 方程即为

$$
\begin{aligned}
&(1-\hat{\vec{p}}\cdot\vec{\sigma})\chi_+(\vec{p})=0, \quad (1+\hat{\vec{p}}\cdot\vec{\sigma})\chi_-(\vec{p})=0\\
\Rightarrow\ &(1-2\hat{h})\chi_+(\vec{p})=0, \quad (1+2\hat{h})\chi_-(\vec{p})=0
\end{aligned}
$$

其中 $\hat{h}$ 即为螺旋度算符. 显然 χ_+ 和 χ_- 分别是 $\hat{h}$ 的本征态, 本征值则为 $\boxed{\pm\frac{1}{2}}$

5. *一个可以制备 Bell 态的简单量子线路为



它包含两个张量: 一个 Hadamard gate (H) 和一个 controlled NOT gate (CNOT)(虚线框里), 在 S^z 表象下它们的矩阵表示为,

$$
\begin{aligned}
H&=\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix},\\
\text{CNOT}&=\exp\left\{\mathrm{i}\pi\frac{1}{4}(\mathbb{I}-\sigma_1^z)\otimes(\mathbb{I}-\sigma_2^x)\right\}
\end{aligned}
$$

将以上量子线路作用到 $|\uparrow\uparrow\rangle$ 上得到的态为?

注意到

$$
\begin{aligned}
A&=\frac{1}{4}(\mathbb{I}-\sigma_1^z)\otimes(\mathbb{I}-\sigma_2^x)=\frac{1}{4}\begin{pmatrix} & \\ & 2\end{pmatrix}\otimes\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}=\begin{pmatrix} & & & \\ & & & \\ & & \frac{1}{2} & -\frac{1}{2}\\ & & -\frac{1}{2} & \frac{1}{2}\end{pmatrix}\\
A^2&=A\\
e^{i\alpha A}&=\sum_{n=0}^{\infty}\frac{1}{n!}(i\alpha A)^n=\mathbb{I}+\sum_{n=1}^{\infty}\frac{1}{n!}(i\alpha)^n(A)^n=\mathbb{I}+A\left(\sum_{n=0}^{\infty}\frac{1}{n!}(i\alpha)^n-1\right)\\
&=\mathbb{I}+A(e^{i\alpha}-1)\\
\Rightarrow \text{CNOT}&=\mathbb{I}-2A=\begin{pmatrix}1 & & & \\ & 1 & & \\ & & & 1\\ & & 1 & \end{pmatrix}.
\end{aligned}
$$

因此, CNOT 的作用是调换第三, 第四元素的位置, 这个作用当且仅当第一个量子比特为 $|\downarrow\rangle=\begin{pmatrix}0\\1\end{pmatrix}$ 时才会发生.

$$
\begin{aligned}
&\left(\hat{H}_{(1)}\otimes\mathbb{I}_{(2)}\right)|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}=\hat{H}_{(1)}|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}=\left[\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}\right]\otimes\begin{pmatrix}1\\0\end{pmatrix}\\
&=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)}+|\downarrow\rangle_{(1)})\otimes|\uparrow\rangle_{(2)}=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}+|\downarrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}).\\
&\text{CNOT}\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}+|\downarrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)})=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}+\text{CNOT}|\downarrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)})\\
&=\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)}\otimes|\uparrow\rangle_{(2)}+|\downarrow\rangle_{(1)}\otimes|\downarrow\rangle_{(2)})=\boxed{\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle+|\downarrow\downarrow\rangle)}, \quad \text{for simplicity.}
\end{aligned}
$$

3.4 应用题

1. 矩阵对角化和表象变换

   (a) **对角化矩阵 L 就是去找到幺正变换 V, 使得 $L = V\Lambda V^{\dagger}$, 其中 Λ 是一个对角矩阵, 它的对角元是本征值. V 是一个幺正矩阵, 它的列矢量是本征矢, 和 Λ 中的本征值一一对应. 找到一个能对角化 Pauli 矩阵 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ 的幺正矩阵 V, 并找到 σ^x 的本征值.**

   通过求解其特征方程以得到 $\sigma^x_{(z)}$ 的本征值:

$$\det(\sigma^x_{(z)} - \lambda I) = \det\begin{pmatrix} -\lambda & 1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 - 1 = 0,$$

   解得 $\boxed{\lambda = \pm 1}$. 对于 $\lambda_+ = 1$ 有:

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = v_2.$$

   所以对应于 λ_+ 的本征矢是 $|+\rangle^x_{(z)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$. 对于 $\lambda_- = -1$ 有

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = -1 \cdot \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \Rightarrow v_1 = -v_2.$$

   所以对应于 λ_- 的本征矢是 $|-\rangle^x_{(z)} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. 在求解过程中已经对这些本征矢进行了归一化, 所以可以得到幺正矩阵 $V = [|+\rangle^x_{(z)}, |-\rangle^x_{(z)}] = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. 对角矩阵 Λ 对角线上依次是本征值, 即

$$\Lambda = \mathrm{diag}\{\lambda_+, \lambda_-\} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \sigma^z_{(z)}$$

   于是我们可以通过幺正矩阵 V 来对 $\sigma^x_{(z)}$ 进行对角化:

$$\sigma^x_{(z)} = V^{\dagger}\Lambda V = V^{\dagger}\sigma^z_{(z)} V$$

   我们注意到, 对角矩阵 Λ 和 $\sigma^z_{(z)}$ 形式完全一致, 这意味着不同表象 i 下, $\sigma^i_{(i)}$ 的形式都是 $\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$, 这就是我们通过 V 来改变表象的依据:

$$\sigma^x_{(z)} = V^{\dagger}\sigma^z_{(z)} V = V^{\dagger}\sigma^x_{(x)} V \Rightarrow \sigma^x_{(x)} = \left(V^{\dagger}\right)^{-1}\sigma^x_{(z)}(V)^{-1}$$

   我们标记 $\sigma^x_{(z)}$ 为 σ^x 在 σ^z 表象下的矩阵. 注意 $V = V^{\dagger} = V^{-1}$, 所以

$$\sigma^x_{(x)} = V\sigma^x_{(z)} V$$

   (b) **自旋 $1/2$ 的自旋角动量算符 $\vec{S}$ 的三个分量为S^x, S^y, S^z. 如果采用 S^z 表象, 它们的矩阵表示为 $\vec{S} = \frac{\hbar}{2}\vec{\sigma}$, 其中 $\vec{\sigma}$ 的三个分量为 Pauli 矩阵 σ^x, σ^y, σ^z. 现在考采用 S^x 表象, 请列出 S^x 表象中你约定的基矢顺序, 并求出在该表象下算符 $\vec{S}$ 的三个分量的矩阵表示.**

   在 S^z 表象下有

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x_{(z)} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

   从前文中可知, $\sigma^x_{(z)}$ 的本征矢为:

$$|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

用以将 S^z 表象转换为 S^x 表象的幺正矩阵为

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

在 S^z 表象中有

$$S^x_{(z)} = \frac{\hbar}{2}\sigma^x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S^y_{(z)} = \frac{\hbar}{2}\sigma^y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad S^z_{(z)} = \frac{\hbar}{2}\sigma^z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

因此

$$\begin{aligned} S^x_{(x)} &= V S^x_{(z)} V = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ S^y_{(x)} &= V S^y_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \\ S^z_{(x)} &= V S^z_{(z)} V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \end{aligned}$$

在 S^x 表象中的基矢为

$$|+\rangle^x_{(x)} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |-\rangle^x_{(x)} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

2. 谐振子问题

一维谐振子的哈密顿量为

$$H = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

坐标算符 x 和动量算符 p 满足对易式 $[x,p] = i\hbar$. 对动量算符和坐标算符进行重新标度

$$p = P\sqrt{\hbar m\omega}, \quad x = Q\sqrt{\frac{\hbar}{m\omega}}$$

注意新的坐标算符 Q 和动量算符 P 是无量纲的, 哈密顿量重新写为

$$H = \frac{1}{2}\hbar\omega(P^2 + Q^2)$$

引入玻色子产生和湮灭算符, $a^\dagger$ 和 a.

$$a = \frac{1}{\sqrt{2}}(Q + iP), \quad a^\dagger = \frac{1}{\sqrt{2}}(Q - iP)$$

(a) 计算 $[Q,P]$, $[a,a^\dagger]$, $[a,a^\dagger a]$, $[a^\dagger,a^\dagger a]$;

$$
\begin{aligned}
[Q,P] &= [\sqrt{\frac{m\omega}{\hbar}}x, \sqrt{\frac{1}{\hbar m\omega}}p] = \frac{1}{\hbar}[x,p] = \frac{1}{\hbar}i\hbar = \boxed{i}, \\
[a,a^\dagger] &= \left[\frac{1}{\sqrt{2}}(Q+iP), \frac{1}{\sqrt{2}}(Q-iP)\right] \\
&= \frac{1}{2}[Q+iP, Q-iP] = \frac{1}{2}\left([Q,Q] - i[Q,P] + i[P,Q] + [P,P]\right) \\
&= \frac{1}{2}[0 - i\cdot i + i\cdot(-i) + 0] = \boxed{1}, \\
[a,a] &= \left[\frac{1}{\sqrt{2}}(Q+iP), \frac{1}{\sqrt{2}}(Q+iP)\right] \\
&= \frac{1}{2}[Q+iP, Q+iP] = \frac{1}{2}\left([Q,Q] + i[Q,P] + i[P,Q] + [P,P]\right) \\
&= \frac{1}{2}[0 + i\cdot i + i\cdot(-i) + 0] = 0, \\
[a^\dagger,a^\dagger] &= \left[\frac{1}{\sqrt{2}}(Q-iP), \frac{1}{\sqrt{2}}(Q-iP)\right] \\
&= \frac{1}{2}[Q-iP, Q-iP] = \frac{1}{2}([Q,Q] - i[Q,P] - i[P,Q] + [P,P]) \\
&= \frac{1}{2}(0 - i\cdot i - i\cdot(-i) + 0) = 0, \\
[a,a^\dagger a] &= a^\dagger[a,a] + [a,a^\dagger]a = a^\dagger\cdot 0 + 1\cdot a = \boxed{a}, \\
[a^\dagger,a^\dagger a] &= a^\dagger[a^\dagger,a] + [a^\dagger,a^\dagger]a = a^\dagger\cdot(-1) + 0\cdot a = \boxed{-a^\dagger}.
\end{aligned}
$$

(b) 将哈密顿量 H 用 a 和 $a^\dagger$ 表示. 并求出全部能级;

$$
\begin{aligned}
& a = \frac{1}{\sqrt{2}}(Q+iP), \quad a^\dagger = \frac{1}{\sqrt{2}}(Q-iP) \\
\Rightarrow\ & Q = \frac{1}{\sqrt{2}}(a+a^\dagger), \quad P = \frac{1}{\sqrt{2}i}(a-a^\dagger) \\
\Rightarrow\ & H = \frac{1}{2}\hbar\omega(P^2+Q^2) = \frac{1}{2}\hbar\omega\left\{\left[\frac{1}{\sqrt{2}i}(a-a^\dagger)\right]^2 + \left[\frac{1}{\sqrt{2}}(a+a^\dagger)\right]^2\right\} \\
&= \frac{1}{2}\hbar\omega\left\{-\frac{1}{2}\left(aa - aa^\dagger - a^\dagger a + a^\dagger a^\dagger\right) + \frac{1}{2}\left(aa + aa^\dagger + a^\dagger a + a^\dagger a^\dagger\right)\right\} \\
&= \frac{1}{2}\hbar\omega\left(a^\dagger a + aa^\dagger\right)
\end{aligned}
$$

当然, 也可以利用 $[a,a^\dagger] = 1 \iff aa^\dagger = a^\dagger a + 1$ 将 H 变换为熟知的粒子数表象形式:

$$\boxed{H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)}$$

所以 $\boxed{E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n = 0, 1, 2, \cdots}$

(c) 在能量表象中, 计算 a 和 $a^\dagger$ 的矩阵元.

能量表象的本征矢满足 $H|n\rangle = E_n|n\rangle$, 则矩阵元为

$$
\begin{aligned}
& a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle \\
\Rightarrow\ & \langle m|a|n\rangle = \boxed{\sqrt{n}\delta_{m,n-1}}, \quad \langle m|a^\dagger|n\rangle = \boxed{\sqrt{n+1}\delta_{m,n+1}}
\end{aligned}
$$

3. **角动量耦合**

两个大小相等, 属于不同自由度的角动量 $\vec{J}_1$ 和 $\vec{J}_2$ 耦合成总角动量 $\vec{J}=\vec{J}_1+\vec{J}_2$, 设 $\vec{J}_1^2=\vec{J}_2^2=j(j+1)\hbar^2$, $J^2=J(J+1)\hbar^2$, $J=2j,2j-1,\cdots,1,0$. 在总角动量量子数 $J=0$ 的状态下, 求 $J_{1,z}$ 和 $J_{2,z}$ 的可能取值及相应概率.

4. **自旋-1 模型**

考虑自旋-1 体系, 自旋算符为 $\vec{S}$, 考虑 $(\vec{S}^2,S^z)$ 表象, 基矢顺序为 $|1,1\rangle$, $|1,0\rangle$, $|1,-1\rangle$, 简记为 $|+1\rangle$, $|0\rangle$, $|-1\rangle$. 设 $\hbar=1$.

(a) **写出 S^x 和 S^z 的矩阵表示.**

由于是在 $(\vec{S}^2,S^z)$ 表象, 所以 S^z 的矩阵一定是对角矩阵. 选定基矢为 $\{|s,m\rangle\}$, 即$|1,1\rangle=\begin{pmatrix}1\\0\\0\end{pmatrix}$, $|1,0\rangle=\begin{pmatrix}0\\1\\0\end{pmatrix}$, $|1,-1\rangle=\begin{pmatrix}0\\0\\1\end{pmatrix}$. 根据本征方程 $S^z|s,m\rangle=m|s,m\rangle$, 得到

$$S^z=\boxed{\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}}$$

而对于 S^x (包括题解不要求的 S^y), 我们实际上是使用的升降算符 $S^\pm$ 来定义的.

$$\begin{aligned}
S^+|s,m\rangle&=\sqrt{s(s+1)-m(m+1)}|s,m+1\rangle,\\
S^-|s,m\rangle&=\sqrt{s(s+1)-m(m-1)}|s,m-1\rangle.\\
\Rightarrow S^+|1,1\rangle=0,\quad &S^+|1,0\rangle=\sqrt{2}|1,1\rangle,\quad S^+|1,-1\rangle=\sqrt{2}|1,0\rangle,\\
S^-|1,1\rangle=\sqrt{2}|1,0\rangle,\quad &S^-|1,0\rangle=\sqrt{2}|1,-1\rangle,\quad S^-|1,-1\rangle=0.\\
\Rightarrow S^+&=\begin{pmatrix}0&\sqrt{2}&0\\0&0&\sqrt{2}\\0&0&0\end{pmatrix},\quad S^-=\begin{pmatrix}0&0&0\\\sqrt{2}&0&0\\0&\sqrt{2}&0\end{pmatrix}.\\
\Rightarrow S^x&=\frac{1}{2}\left(S^++S^-\right)=\boxed{\frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}}
\end{aligned}$$

(b) **考虑哈密顿量 $H(\lambda)=H_0+\lambda V$, 其中 $H_0=(S^z)^2$, $V=S^x+S^z$. 考虑为 λV 微扰, 利用微扰论计算微扰后的各能级和各能态, 其中能级微扰准确到二阶, 能态微扰准确到一阶.**

$$\begin{aligned}
H_0|s,m\rangle&=\left(S^z\right)^2|s,m\rangle=m^2|s,m\rangle\\
\Rightarrow E_{-1}^{(0)}&=1,\quad E_0=0,\quad E_1=1
\end{aligned}$$

注意到 m^2 会带来 $m=\pm1$ 的简并, 所以后续计算时会涉及简并态的微扰处理. 首先观察简并态, 简并态矢张

成独立子空间, 于是求解这个子空间中 V 的矩阵:

$$
\begin{aligned}
V_{\text{sub}} &= \begin{pmatrix} \langle 1,1|V|1,1\rangle & \langle 1,1|V|1,-1\rangle \\ \langle 1,-1|V|1,1\rangle & \langle 1,-1|V|1,-1\rangle \end{pmatrix} \\
\langle 1,1|V|1,1\rangle &= \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 1, \\
\langle 1,1|V|1,-1\rangle &= \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0, \\
\langle 1,-1|V|1,1\rangle &= 0, \\
\langle 1,-1|V|1,-1\rangle &= \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = -1. \\
\Rightarrow V_{\text{sub}} &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}
\end{aligned}
$$

注意到计算得到的子空间中 V_{sub} 完成了对角化, 这说明沿用的 $|s,m\rangle$ 基矢已经是 "好量子态". 所以回归到非简并微扰论的方法. 一阶能量修正各为

$$
\begin{aligned}
E_1^{(1)} &= \langle 1,1|V|1,1\rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \boxed{1}, \\
E_0^{(1)} &= \langle 1,0|V|1,0\rangle = \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \boxed{0}, \\
E_{-1}^{(1)} &= \langle 1,-1|V|1,-1\rangle = \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \boxed{-1},
\end{aligned}
$$

二阶能量修正由公式 $E_m^{(n)} = \sum\limits_{n\neq m} \dfrac{|\langle n|V|m\rangle|^2}{E_m^{(0)} - E_n^{(0)}}$ 给出:

$$
\begin{aligned}
E_1^{(2)} &= \frac{|\langle 1,0|V|1,1\rangle|^2}{E_1^{(0)} - E_0^{0}} + \frac{|\langle 1,-1|V|1,1\rangle|^2}{E_1^{(0)} - E_{-1}^{(0)}} = \frac{\left(\frac{1}{\sqrt{2}}\right)^2}{1-0} + \frac{0^2}{1-1} = \boxed{\frac{1}{2}}, \\
E_0^{(2)} &= \frac{|\langle 1,1|V|1,0\rangle|^2}{E_0^{(0)} - E_1^{(0)}} + \frac{|\langle 1,-1|V|1,0\rangle|^2}{E_0^{(0)} - E_{-1}^{(0)}} = \frac{\left(\frac{1}{\sqrt{2}}\right)^2}{0-1} + \frac{0^2}{0-(-1)} = \boxed{-\frac{1}{2}}, \\
E_{-1}^{(2)} &= \frac{|\langle 1,0|V|1,-1\rangle|^2}{E_{-1}^{(0)} - E_0^{(0)}} + \frac{|\langle 1,1|V|1,-1\rangle|^2}{E_{-1}^{(0)} - E_1^{(0)}} = \frac{\left(\frac{1}{\sqrt{2}}\right)^2}{-1-0} + \frac{0^2}{1-1} = \boxed{-\frac{1}{2}}
\end{aligned}
$$

可见, 只要在 $E_i^{(1)} - E_j^{(1)} = 0$ 时分子也为 0, 我们就可以无视分母为 0 的问题. 接下来是对态函数的微扰修正.

一阶修正由 $|m\rangle^{(1)} = \sum_{n\neq m} |n\rangle \frac{\langle n|V|m\rangle}{E_m^{(0)} - E_n^{(0)}}$ 给出:

$$\begin{aligned}
|1,1\rangle^{(1)} &= |1,0\rangle \frac{\langle 1,0|V|1,1\rangle}{E_1^{(0)} - E_0^{(0)}} + |1,-1\rangle \frac{\langle 1,-1|V|1,1\rangle}{E_1^{(0)} - E_{-1}^{(0)}} = |1,0\rangle \frac{1}{\sqrt{2}} \frac{1}{1-0} + |1,-1\rangle \cdot 0 \\
&= \boxed{\frac{1}{\sqrt{2}}|1,0\rangle} \\
|1,0\rangle^{(1)} &= |1,1\rangle \frac{\langle 1,1|V|1,0\rangle}{E_0^{(0)} - E_1^{(0)}} + |1,-1\rangle \frac{\langle 1,-1|V|1,0\rangle}{E_0^{(0)} - E_{-1}^{(0)}} = |1,1\rangle \frac{1}{\sqrt{2}} \frac{1}{0-1} + |1,-1\rangle \frac{1}{\sqrt{2}} \cdot \frac{1}{0-(-1)} \\
&= \boxed{\frac{1}{\sqrt{2}}(-|1,1\rangle + |1,-1\rangle)} \\
|1,-1\rangle^{(1)} &= |1,1\rangle \frac{\langle 1,1|V|1,-1\rangle}{E_{-1}^{(0)} - E_1^{(0)}} + |1,0\rangle \frac{\langle 1,0|V|1,-1\rangle}{E_{-1}^{(0)} - E_0^{(0)}} = |1,1\rangle \cdot 0 + |1,0\rangle \frac{1}{\sqrt{2}} \cdot \frac{1}{-1-0} \\
&= \boxed{-\frac{1}{\sqrt{2}}|1,0\rangle}
\end{aligned}$$

总结:

$$\begin{aligned}
E_1 &= 1 + 1\lambda + \frac{1}{2}\lambda^2 + o(\lambda^2) \\
E_0 &= 0 + 0\lambda - \frac{1}{2}\lambda^2 + o(\lambda^2) \\
E_{-1} &= 1 - 1\lambda - \frac{1}{2}\lambda^2 + o(\lambda^2) \\
|1,1\rangle &= |1,1\rangle + \frac{\lambda}{\sqrt{2}}|1,0\rangle + o(\lambda) \\
|1,0\rangle &= |1,0\rangle + \frac{\lambda}{\sqrt{2}}(-|1,1\rangle + |1,-1\rangle) + o(\lambda) \\
|1,-1\rangle &= |1,-1\rangle - \frac{\lambda}{\sqrt{2}}|1,0\rangle + o(\lambda)
\end{aligned}$$

对于这类可以使用矩阵形式讨论的问题, 还有一种笨办法, 就是直接严格对角化含 λ 微扰的哈密顿量, 然后进行 Taylor 展开得到各级数. 但是在三阶矩阵下的计算已经非常复杂, 所以还是建议使用一般微扰论方法, 毕竟考试时是会给出公式的.

5. **均匀电子气**

考虑三维相互作用均匀电子气, 哈密顿量为 $H = H_0 + H_I$. 考虑系统体积为 $V = L^3$, 每个方向的系统尺寸为 L. 采用箱归一化, 所以 $\vec{k}$ 是离散的, $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$, n_x, n_y, n_z 为整数. 采用二次量子化的语言, 可给出哈密顿量在动量空间的形式. H_0 为单体部分:

$$H_0 = \sum_{\vec{k}\sigma} \varepsilon_{\vec{k}} c_{\vec{k}\sigma}^\dagger c_{\vec{k}\sigma}$$

其中 $\varepsilon_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m}$ 是自由电子的色散关系. 用 ε_F 表示费米能, k_F 表示费米波矢的大小.

H_I 为两体相互作用部分,

$$H_I = \frac{1}{2V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \sum_{\sigma\sigma'} v(q) c_{\vec{k}_1+\vec{q},\sigma}^\dagger c_{\vec{k}_2-\vec{q},\sigma'}^\dagger c_{\vec{k}_2\sigma'} c_{\vec{k}_1\sigma}$$

$v(q)$ 是相互作用 $v(x)$ 的傅里叶变换形式, $q = |\vec{q}|$, $x = |\vec{x}|$,

$$v(q) = \frac{1}{V} \int v(x) e^{-i\vec{q}\cdot\vec{x}} \mathrm{d}^3\vec{x}$$

这里我们考虑短程势, 也就是说 $v(q=0)$ 不发散.

自由电子气零温下处于电子填充到费米能 ε_F 的费米海态(Fermi sea state), 简记为 FS, 利用费米子产生算符作用到真空态上可以表示 FS 态为

$$|\mathbf{FS}\rangle = \prod_{k<k_F,\sigma} c^\dagger_{\vec{k}\sigma}|0\rangle$$

(a) **考虑零温下的自由电子气, 计算总粒子数 N 和粒子数密度 n, 计算总能量 $E^{(0)}$ 并把总能量密度 $E^{(0)}/V$ 表示成粒子数密度 n 的函数.**

使用分离变量法, 求解自由电子气的薛定谔方程 $\frac{\hbar^2\hat{k}^2}{2m}\psi = E\psi$. 于是能量本征值为 $\frac{\hbar^2k^2}{2m} = \sum_i \frac{\hbar^2k_i^2}{2m}$. 其中 $k_i = \frac{\sqrt{2mE_i}}{\hbar}$. 由于使用了箱归一化, 即有边界条件 $k_il_i = n_i\pi(n_i\in\mathbb{N}^*)$, 代入即得

$$E = \frac{\hbar^2}{2m}\left[\sum_i^3\left(\frac{\pi}{l_i}\right)^2 n_i^2\right] = \frac{\hbar^2\pi^2}{2m}\left(\sum_i^3\frac{n_i^2}{l_i^2}\right)$$

每个波矢 $\vec{k} = \left(\frac{\pi}{l_x}n_x, \frac{\pi}{l_y}n_y, \frac{\pi}{l_z}n_z\right)$ 都是在 $\vec{k}$ 空间中的一个格点, 这种格点所占据的 $\vec{k}$ 空间体积为 $\prod_i^3\frac{\pi}{l_i} = \frac{\pi^3}{l_xl_yl_z} = \frac{\pi^3}{V}$, 其中 V 代表了物质在 $\vec{x}$ 空间的体积(实体积). 电子是全同费米子, 每个格点上(每个状态)能且只能容纳两个电子. 而费米-狄拉克分布为$f(\epsilon) = \frac{1}{1+e^{\beta(\epsilon-\mu)}}$. 绝对零度($\beta\to\infty$)下, 电子可占据的最高能级即为费米能级 $\lim_{\beta\to\infty}\mu = \varepsilon_F$, 对应波矢 $|k|\leq k_F$. 由于前面讨论 $k_i\in\mathbb{N}^*$, 因此 $k\leq k_F$ 在 $\vec{k}$ 空间中会形成 $\frac{1}{8}$ 球体. 由于题解要求, 我们略去讨论各原子贡献的自由电子数目, 而是直接使用总粒子(电子)数 N:

$$\frac{1}{8}\left(\frac{4}{3}\pi k_F^3\right) = \frac{N}{2}\left(\frac{\pi^3}{V}\right)$$

其中 N 除以 2 是因为泡利不相容原理. 具体到题目中, 有 $l_i = L, \forall i$, 于是进一步化简得到

$$\boxed{N = \frac{k_F^3V}{3\pi^2}}, \quad \frac{N}{V} = \boxed{n = \frac{k_F^3}{3\pi^2}}$$

接下来计算总能量. 由于 N 充分大, 使得电子的态能遍布整个 $\frac{1}{8}$ 费米球, 于是求和化为积分形式, 即有 $E_{\text{tot}} = \sum_i^{k\leq k_F}\frac{\hbar^2}{2m}$

其中 $f(k)$ 是态密度, 表示在同一能量 $\frac{\hbar^2k^2}{2m}$ 上的电子数目, 所以这就要求我们对电子态密度进行计算. 对于半径为 k, 厚度为 $\mathrm{d}k$ 的 $\frac{1}{8}$ 球壳, 在这个球壳上电子的能量都是相同的. 而这个球壳的体积为 $\frac{1}{8}(4\pi k^2\mathrm{d}k)$, 又已知每个格点体积为 $\frac{\pi^3}{V}$, 因此球壳中电子数目为

$$\text{格点数}\times 2 = \frac{\frac{1}{8}(4\pi k^2\mathrm{d}k)}{\frac{\pi^3}{V}}\times 2 = \frac{k^2V}{\pi^2}\mathrm{d}k = f(k)\mathrm{d}k$$

因此总能量为

$$E^{(0)} = \int_0^{k_F}\frac{\hbar^2k^2}{2m}\frac{k^2V}{\pi^2}\mathrm{d}k = \frac{\hbar^2V}{2m\pi^2}\int_0^{k_F}k^4\mathrm{d}k = \frac{\hbar^2V}{2m\pi^2}\frac{k_F^5}{5} = \boxed{\frac{\hbar^2Vk_F^5}{10m\pi^2}}$$

反解粒子数密度表达式得到 $k_F(n)$, 代入 $E^{(0)}$ 计算总能量密度:

$$k_F = (3\pi^2n)^{\frac{1}{3}}$$

$$\frac{E^{(0)}}{V} = \frac{\hbar^2k_F^5}{10m\pi^2} = \frac{\hbar^2}{10m\pi^2}\cdot(3\pi^2n)^{\frac{5}{3}} = \boxed{\frac{(3n)^{\frac{5}{3}}\hbar^2\pi^{\frac{4}{3}}}{10m}}$$

(b) 计算能量的一阶修正 $E^{(1)} = \langle \mathbf{FS}|H_I|\mathbf{FS}\rangle$.

(c) 利用 **Hatree Fock** 平均场近似, 并假设平均场参数是自旋对角的, 并且保持了自旋对称性, 以及平移对称性, 因此我们期待 $\left\langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}'\sigma'} \right\rangle = \left\langle c^\dagger_{\vec{k}\sigma} c_{\vec{k}\sigma} \right\rangle \delta_{\vec{k},\vec{k}'} \delta_{\sigma,\sigma'}$, 以及 $\left\langle c^\dagger_{\vec{k}\uparrow} c_{\vec{k}\uparrow} \right\rangle = \left\langle c^\dagger_{\vec{k}\downarrow} c_{\vec{k}\downarrow} \right\rangle$. 计算系统总能量, 并与 $E^{(0)} + E^{(1)}$ 比较大小.

6. 量子转子模型

量子转子的角度坐标 $\theta \in [0, 2\pi)$, 注意 $\theta \pm 2\pi$ 和 θ 是等价的. 用 $|\theta\rangle$ 表现 $\hat{\theta}$ 算符的本征态, $|\theta \pm 2\pi\rangle$ 和 $|\theta\rangle$ 是相同的态. 定义量子转子的转动算符为 $\hat{R}(\alpha)$,

$$\hat{R}(\alpha) = \int_0^{2\pi} \mathrm{d}\theta |\theta - \alpha\rangle\langle\theta|$$

所以 $\hat{R}(\alpha)|\theta\rangle = |\theta - \alpha\rangle$, 并且 $\hat{R}(2\pi)$ 是单位算符.

转动算符 $\hat{R}S(\alpha)$ 是一个幺正算符, 它的产生子为厄米算符 $\hat{N}$, 与量子转子的角动量算符 $\hat{L}$ 的关系为 $\hat{L} = \hbar\hat{N}$, 所以 $\hat{R}(\alpha) = e^{i\hat{N}\alpha}$, 在 $\hat{\theta}$ 表象下可求得 $\hat{N} = -i\frac{\partial}{\partial\theta}$.

考虑一个特定的量子转子模型, 它的哈密顿量为

$$H = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2 - g\cos\left(2\hat{\theta}\right)$$

其中 $g\cos\left(2\hat{\theta}\right)$ 是一个小的外势, 可以当成微扰处理. 假设 $|N\rangle$ 是算符 $\hat{N}$ 的本征态, 本征值为 N, 即 $\hat{N}|N\rangle = N|N\rangle$. 可计算出 $|N\rangle$ 用 $|\theta\rangle$ 展开为

$$|N\rangle = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} e^{iN\theta}|\theta\rangle$$

(a) 利用 $\hat{R}(2\pi)$ 是单位算符证明 N 必须是整数.

因为 $\hat{R}(2\pi) = \mathbb{I}$, 所以有 $|\theta - 2\pi\rangle = |\theta\rangle$. 对于算符 $\hat{N}$ 的本征态 $|N\rangle$ 有

$$\begin{aligned}
\frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta - 2\pi\rangle &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle \\
\Longleftrightarrow \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta\rangle &= \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta-2\pi)}|\theta\rangle \\
\Longleftrightarrow e^{iN\theta} &= e^{iN(\theta-2\pi)} = e^{iN\theta}e^{-i2\pi N}
\end{aligned}$$

因此为了保持 θ 转动 2π 后的不变性, N 应当是整数.

(b) 考虑无微扰时的哈密顿量 $H_0 = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2$, 证明 $|N\rangle$ 也是 H_0 的本征态, 并求出本征能量, 证明每个能级都是两重简并的.

$$\begin{aligned}
\hat{H}_0|N\rangle = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2|N\rangle = \frac{1}{2}\left(N - \frac{1}{2}\right)^2|N\rangle &\Rightarrow E_N^{(0)} = \frac{1}{2}\left(N - \frac{1}{2}\right)^2 \\
&\Rightarrow N_\pm - \frac{1}{2} = \pm\sqrt{2E_N^{(0)}} \Rightarrow N_\pm = \frac{1}{2} \pm \sqrt{2E_N^{(0)}}
\end{aligned}$$

这意味着对于任意整数 N, 都对应存在着 $N' = 1 - N$ 使得能级简并.

(c) 采用 $\{|N\rangle\}$ 作为基组, 写出微扰项 $V = -g\cos\left(2\hat{\theta}\right)$ 的表示矩阵, 并证明微扰不会连接简并的能级(即如果 $|N\rangle$ 和 $|N'\rangle$ 简并, 那么 $\langle N|V|N'\rangle$). 因此尽管 H_0 的能级是简并的, 我们仍然可以使用非简并微扰论.

$$
\begin{aligned}
\cos 2\hat{\theta} &= \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right) \\
e^{i2\hat{\theta}}|N\rangle &= e^{i2\hat{\theta}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}|\theta\rangle\right) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN\theta}e^{i2\hat{\theta}}|\theta\rangle \\
&= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{i(N+2)\theta}|\theta\rangle = |N+2\rangle \\
\Rightarrow \cos 2\hat{\theta}|N\rangle &= \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)|N\rangle = \frac{1}{2}\left(|N+2\rangle + |N-2\rangle\right) \\
\Rightarrow \langle N|\hat{V}|N'\rangle &= -g\langle N|\cos 2\hat{\theta}|N'\rangle = -\frac{g}{2}\left(\langle N|N'+2\rangle + \langle N|N'-2\rangle\right) \\
&= -\frac{g}{2}(\delta_{N,N'+2} + \delta_{N,N'-2})
\end{aligned}
$$

和前文一致, 如果 $|N\rangle$ 和 $|N'\rangle$ 简并, 那么 $N+N'=1$ 使得只要 $N\in\mathbb{Z}$, 那么$\delta\neq 0$. 所以仍然可以使用非简并微扰论.

(d) **计算每个能级 E_N 的微扰修正到 g 的二阶, 并证明此时所有的能级简并仍然没有被解除.**

$$
\begin{aligned}
E_N^{(1)} &= \langle N|\hat{V}|N\rangle = -\frac{g}{2}\left(\langle N|N+2\rangle + \langle N|N-2\rangle\right) = 0 \\
E_N^{(2)} &= \sum_{N'\neq N}\frac{|\langle N|\hat{V}|N'\rangle|^2}{E_N^{(0)} - E_{N'}^{(0)}} = \sum_{N'\neq N}\frac{\left(-\frac{g}{2}(\delta_{N,N'+2}+\delta_{N,N'-2})\right)^2}{\frac{1}{2}\left(N-\frac{1}{2}\right)^2 - \frac{1}{2}\left(N'-\frac{1}{2}\right)^2} \\
&= \boxed{\frac{g^2}{(2N-3)(2N+1)}}
\end{aligned}
$$

微扰修正后的能级为

$$
E_N \approx \frac{1}{2}\left(N-\frac{1}{2}\right)^2 + \frac{g^2}{(2N-3)(2N+1)}
$$

代入 $N'=1-N$ 以检查能级简并性:

$$
\begin{aligned}
E_{N'} &= \frac{1}{2}\left(1-N-\frac{1}{2}\right)^2 + \frac{g^2}{[2(1-N)-3][2(1-N)+1]} \\
&= \frac{1}{2}\left(N-\frac{1}{2}\right)^2 + \frac{g^2}{(2N+1)(2N-3)} = E_N
\end{aligned}
$$

所以简并度未变化.