ADVANCED QUANTUM MECHANICS

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第一章　课堂讲义

1.1　导论

1.2　对称性

1.2.1　群的定义

集合 $\mathcal{G}$ 包含元素 g_i, 使用乘法 $\cdot$, 满足

1. $\forall g_1, g_2 \in \mathcal{G}, \quad g_1 \cdot g_2 \in \mathcal{G}$;
2. $(g_1 \cdot g_2) \cdot g_3 = g_1 \cdot (g_2 \cdot g_3)$;
3. $1 \in \mathcal{G}, \quad \text{s.t.} \quad 1 \cdot g = g \cdot 1 = g$;
4. $\forall g \in \mathcal{G}, \quad \exists g^{-1} \in \mathcal{G} \quad \text{s.t.} \quad g \cdot g^{-1} = g^{-1} \cdot g = 1$

1.2.2　群的表示举例

1.2.3　连续对称性和守恒律

一个对称变换对应一个幺正算符 U. 若 $[U, H] = 0$, 则 $H = U^\dagger H U$, U 是 H 的一个对称性. 若 $H|\psi_n\rangle = E_n|\psi_n\rangle$, 那么 $HU|\psi_n\rangle = E_n U|\psi_n\rangle$. 如果 E_n 是 m 重简并的, 那么会存在其简并子空间, 通过基矢 $\{|\psi_{n,m}\rangle\}$ 张成. 而 U 相当于使 $|\psi_n\rangle$ 在这个子空间内转动, 如

$$
\begin{aligned}
U|\psi_{n,i}\rangle &= \left(\sum_{k=1}^{m} |\psi_{n,k}\rangle\langle\psi_{n,k}|\right) U|\psi_{n,i}\rangle \\
&= \sum_{k=1}^{m} |\psi_{n,k}\rangle \Big(\langle\psi_{n,k}|U|\psi_{n,i}\rangle\Big)
\end{aligned}
$$

也就是说, 对于幺正变换 U, 在 E_n 的简并子空间中, 可以使用矩阵来进行描述, 矩阵元是 $\langle\psi_{n,k}|U|\psi_{n,i}\rangle$, 观察发现共有 n, k, i 三个指标, 所以矩阵可以用 $D^{(n)}(U)_{ki}$ 来表示. 存在关系 $D^{(n)}(U_2)D^{(n)}(U_1) = D^{(n)}(U_2U_1)$.

可以通过一系列无穷小对称变换累积构造出的对称变换是连续对称性, 反之是离散对称性.

若物理量 $G = G^\dagger$ 守恒, 则 $\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{1}{i\hbar}[G, H] = 0$, 即 $[G, H] = 0$. 那么定义幺正算符 $U = e^{i\theta G/\hbar}$, 它将满足

$$
\begin{aligned}
U^\dagger H U &= \left(1 + \frac{i\theta}{\hbar} G\right) H \left(1 - \frac{i\theta}{\hbar} G\right) \\
&= H + \frac{i\theta}{\hbar}[G, H] = H
\end{aligned}
$$

G 被称作该对称性的生成元.

1.2.3.1 空间平移

对于 $x \to x + a$, 有平移算符 $T(a) = e^{-ipa/\hbar}$. 这是一个幺正算符, 具有性质

1. $[T(a)]^{-1} = T(-a)$.
2. $T(a_1)T(a_2) = T(a_1 + a_2)$.
3. $T^\dagger(a)xT(a) = x + a$, 用到公式 $e^B A e^{-B} = A + [B, A] + \frac{1}{2!}[B, [B, A]] + \cdots$

推广至 d 维($x_i \to x_i + a_i$), 平移算符为

$$
T(\{a_i\}) = \prod_i T_i(a_i) = \prod_i e^{-ip_i a_i/\hbar}
$$
$$
[T_i(a_i), T_j(a_j)] = 0 \iff [p_i, p_j] = 0
$$

1.2.3.2 时间平移

时间平移表示能量守恒 $\dfrac{\mathrm{d}H}{\mathrm{d}t} = 0$, 对应幺正算符为 $U(t) = e^{-iHt/\hbar}$

1.2.3.3 转动

1.2.3.3.1 角动量是转动的生成元 对于 d 维空间, 转动使得 $\vec{x}_i \to \vec{x}'_i = \sum_{j=1}^{d} R_{ij}\vec{x}_j$. 转动操作具有保内积性质 $\vec{x} \cdot \vec{y} = \vec{x}' \cdot \vec{y}'$,

$$
\begin{aligned}
\sum_i x_i y_i = \sum_i x'_i y'_i &= \sum_i \left(\sum_j R_{ij} x_j\right)\left(\sum_k R_{ik} y_k\right) = \sum_i \sum_j \sum_k R_{ij} R_{ik} x_j y_k \\
&= \sum_j \sum_k \left(\sum_i R_{ij} R_{ik}\right) x_j y_k \stackrel{?}{=} \sum_j \sum_k \delta_{kj} x_j y_k = \sum_j x_j y_j \\
\Rightarrow \sum_i R_{ij} R_{ik} = \sum_i R^T_{ji} R_{ik} &= \delta_{kj} \to R^T R = \mathbb{I}
\end{aligned}
$$

而 R 和 R^{-1} 的行列式值相同, 所以 $\det R = \pm 1$. 其中 $\det R = 1$ 表示的是正常转动, 组成 SO(d) (特殊正交)群.

R 对应一个幺正算符 $\mathcal{D}(R)$, 即 $|\alpha_R\rangle = \mathcal{D}(R)|\alpha\rangle$. 设矢量算符 $\vec{V}$, 那么

$$
\begin{aligned}
\langle \beta_R | V_i | \alpha_R \rangle = \langle \beta | \mathcal{D}^\dagger(R) V_i \mathcal{D}(R) | \alpha \rangle &= R_{ij} \langle \beta | V_j | \alpha \rangle \\
\Rightarrow \mathcal{D}^\dagger(R) V_i \mathcal{D}(R) &= R_{ij} V_j
\end{aligned}
$$

使用无穷小转动 $R \approx \mathbb{I} - \omega + \mathcal{O}(\omega^2)$, 而 $R^T R \approx (\mathbb{I} - \omega^T)(\mathbb{I} - \omega) = \mathbb{I}$, 因此 $\omega^T = -\omega$, 这代表 ω 是一个反对称阵. 对应于 $\mathcal{D}(R)$, 进行展开

$$
\mathcal{D}(R) = 1 - \frac{i}{2\hbar} \sum_{i,j} \omega_{ij} J_{ij} + \mathcal{O}(\omega^2)
$$

1.2.3.3.2 角动量代数 角动量对易关系 $[J_i, J_j] = i\hbar\epsilon_{ijk} J_k, \quad [\vec{J}^2, J_i] = 0$. 由于 $\vec{J}^2$ 和 J_z 有共同本征态, 各取一个参数 j, m 标记, 即 $|j, m\rangle$.

$$
\vec{J}^2 |j, m\rangle = a |j, m\rangle, \quad J_z |j, m\rangle = b |j, m\rangle
$$

引入升降算符 $J_\pm = J_x \pm iJ_y$, 有对易关系 $[J_+, J_-] = 2\hbar J_z, \quad [J_z, J_\pm] = \pm\hbar J_\pm, \quad [J^2, J_\pm] = 0$

注意到, 升降算符会使 J_z 的本征值升降 $\hbar$:

$$
J_z J_\pm |j, m\rangle = (J_\pm J_z \pm \hbar J_\pm)|j, m\rangle = (b \pm \hbar) J_\pm |j, m\rangle
$$

$$\vec{J}^2 = J_x^2 + J_y^2 + J_z^2 = J_z^2 + \frac{1}{2}(J_+J_- + J_-J_+) = J_z^2 + \frac{1}{2}\left(J_+J_+^\dagger + J_-J_-^\dagger\right)$$

这说明 $\langle j,m|\vec{J}^2 - \vec{J}_z^2|j,m\rangle = a - b^2 \geq 0, \quad \forall |j,m\rangle$, 因此存在一个最大值 $b_{\max}$ 使得 $-b_{\max} \leq b \leq b_{\max}$. 那么升降算符不能无限地升降 J_z 的本征值. 所以添加限制 $J_\pm|b\rangle = J_\pm|b_{\max}\rangle = J_\pm|{}^{\max}_{\min}\rangle = 0$.

$$\begin{aligned}
J_-J_+|\max\rangle &= (J_x - iJ_y)(J_x + iJ_y)|\max\rangle = (\vec{J}^2 - J_z^2 - \hbar J_z)|\max\rangle = 0\\
a - b_{\max}^2 - \hbar b_{\max} = 0 &\to a = b_{\max}(b_{\max} + \hbar)\\
J_+J_-|\min\rangle &= (J_x + iJ_y)(J_x - iJ_y)|\min\rangle = (\vec{J}^2 - J_z^2 + \hbar J_z)|\min\rangle = 0\\
a - b_{\min}^2 + \hbar b_{\min} = 0 &\to a = b_{\min}(b_{\min} - \hbar), \quad b_{\min} = -b_{\max}
\end{aligned}$$

假定从 $|\min\rangle$ 到 $|\max\rangle$ 需要 n 次 J_+, 即有 $b_{\max} = -b_{\max} + n\hbar \iff b_{\max} = \frac{n}{2}\hbar \equiv j\hbar$, 这就将前面选定的 j,m 联系起来了:

$$\begin{aligned}
&a = j(j+1)\hbar^2, \quad j \in \frac{1}{2}\mathbb{Z}\\
&b = m\hbar, \quad m = -j, -j+1, \cdots, j-1, j
\end{aligned}$$

既然已选定基矢, 那么就可以计算矩阵元.

$$\begin{aligned}
\langle j',m'|\vec{J}^2|j,m\rangle &= j(j+1)\hbar^2\delta_{jj'}\delta_{mm'}\\
\langle j',m'|J_z|j,m\rangle &= m\hbar\delta_{jj'}\delta_{mm'}\\
\langle j,m|J_-J_+|j,m\rangle &= \langle j,m|\vec{J}^2 - J_z^2 - \hbar J_z|j,m\rangle = [j(j+1) - m^2 - m]\hbar^2\\
&= (J_+|j,m\rangle)^\dagger(J_+|j,m\rangle) = (c_{j,m}|j,m\rangle)^\dagger c_{j,m}|j,m\rangle = |c_{j,m}|^2\\
\Rightarrow c_{j,m} &= \sqrt{j(j+1) - m(m+1)}\hbar\\
\langle j,m|J_+J_-|j,m\rangle &= \langle j,m|\vec{J}^2 - J_z^2 + \hbar J_z|j,m\rangle = [j(j+1) - m^2 + m]\hbar^2\\
&= (J_-|j,m\rangle)^\dagger(J_-|j,m\rangle) = (c'_{j,m}|j,m\rangle)^\dagger c'_{j,m}|j,m\rangle = |c'_{j,m}|^2\\
\Rightarrow c'_{j,m} &= \sqrt{j(j+1) - m(m-1)}\hbar\\
\langle j',m'|J_\pm|j,m\rangle &= \hbar\sqrt{j(j+1) - m(m\pm 1)}\delta_{j,j'}\delta_{m,m'\pm 1}
\end{aligned}$$

既然升降算符已定, 那么就可反解出 J_x, J_y. 一般需要先确定角动量量子数 j, 从而确定矩阵的大小. 比如 $j = \dfrac{1}{2}$ 时, 所得的各矩阵就是泡利矩阵; $j = 1$ 时, 则有

$$J_z = \hbar\begin{pmatrix}1 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & -1\end{pmatrix}, \quad J_x = \frac{J_+ + J_-}{2} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & 1 & 0\\ 1 & 0 & 1\\ 0 & 1 & 0\end{pmatrix}, \quad J_y = \frac{J_+ - J_-}{2i} = \frac{\hbar}{\sqrt{2}}\begin{pmatrix}0 & -i & 0\\ i & 0 & -i\\ 0 & i & 0\end{pmatrix}$$

1.2.3.3.3 SO(3), SU(2)

1.2.3.3.4 中心势场中的单粒子问题

1.2.3.3.5 角动量相加 若两个系统 1 和 2 分别有角动量 j_1 和 j_2, 这个复合系统的 Hilbert 空间为 $\mathcal{H}_1 \otimes \mathcal{H}_2$. 要确定复合系统的角动量, 就需要选定一个基矢, 常用方法是子系统基矢的直积; 对应地, 复合系统的算符也是子系统算符的直积, 即

$$\begin{aligned}
|j_1, m_2; j_2, m_2\rangle &= |j_1, m_1\rangle \otimes |j_2, m_2\rangle\\
\vec{J} = \vec{J}_1 + \vec{J}_2 &\equiv \vec{J}_1 \otimes \mathbb{I}_2 + \mathbb{I}_1 \otimes \vec{J}_2
\end{aligned}$$

为了简便, 常常去除直积符号和单位算符, 而只是简单的相加. 不同子系统的角动量互不干涉, 所以 $[J_{1\alpha}, J_{2\beta}] = 0$. 但是总角动量 $\vec{J}^2$ 并不单独与子系统角动量 $J_{\alpha,z}$对易, 所以基矢 $|j_1, m_1; j_2, m_2\rangle$ 不是 $\vec{J}^2$ 的本征矢.

由于 $\vec{J}_2, J_z, \vec{J}_1^2, J_2^2$ 相互对易, 所以基矢为 $|j,m;j_1,j_2\rangle$.比如熟悉的两电子系统 $\frac{1}{2}\otimes\frac{1}{2}$,

$$\left|\frac{1}{2},\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle = |++\rangle; \quad \left|\frac{1}{2},\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle = |+-\rangle;$$
$$\left|\frac{1}{2},-\frac{1}{2};\frac{1}{2},\frac{1}{2}\right\rangle = |-+\rangle; \quad \left|\frac{1}{2},-\frac{1}{2};\frac{1}{2},-\frac{1}{2}\right\rangle = |--\rangle$$
$$\text{单态:}\quad |0,0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$
$$\text{三重态:}\quad |1,1\rangle = |++\rangle, \quad |1,0\rangle = \frac{1}{\sqrt{2}}\left(|+-\rangle + |-+\rangle\right), \quad |1,-1\rangle = |--\rangle$$

这就涉及到基矢变换 $|j_1,m_1;j_2,m_2\rangle \to |j,m;j_1,j_2\rangle$:

$$\begin{aligned}|j,m;j_1,j_2\rangle &= \sum_{m_1,m_2}|j_1,m_1;j_2,m_2\rangle \overbrace{\langle j_1,m_1;j_2,m_2|j,m;j_1,j_2\rangle}^{\text{CG 系数}} \\ &= \sum_{m_1,m_2} C^{j,m}_{j_1,j_2,m_1,m_2}|j_1,m_1;j_2,m_2\rangle\end{aligned}$$

1. 磁量子数守恒. $J_z = J_{1,z} + J_{2,z}$.
2. $|j_1 - j_2| \le j \le j_1 + j_2$.
3. 若 $j_1, j_2 \in \mathbb{Z}$ 或 $j_1, j_2 \in \frac{1}{2}\mathbb{Z}$, 则 $j \in \mathbb{Z}$. 不失一般性地, 若 $j_1 \in \mathbb{Z}$, $j_2 \in \frac{1}{2}\mathbb{Z}$, 则 $j \in \frac{1}{2}\mathbb{Z}$.
4. 递推公式. 为了后续方便 $\langle i|j\rangle = \delta_{ij}$ 的计算, 在原求和公式的 m_1, m_2 添加上标 $'$ 以示区别.

$$\langle j_1,m_1;j_2,m_2|J_\pm|j,m;j_1,j_2\rangle = \langle j_1,m_1;j_2,m_2|(J_{1\pm}+J_{2\pm})\sum_{m_1',m_2'} C^{j,m}_{j_1,j_2,m_1',m_2'}|j_1,m_1';j_2,m_2'\rangle$$

$$\begin{aligned}&\sqrt{j(j+1)-m(m\pm1)}\langle j_1,m_1;j_2,m_2|j,m\pm1;j_1,j_2\rangle \\ &= \langle j_1,m_1;j_2,m_2|\sum_{m_1',m_2'}\sqrt{j_1(j_1+1)-m_1'(m_1'\pm1)}|j_1,m_1'\pm1;j_2,m_2'\rangle C^{j,m}_{j_1,j_2,m_1',m_2'} \\ &+ \langle j_1,m_1;j_2,m_2|\sum_{m_1,m_2}\sqrt{j_2(j_2+1)-m_2'(m_2'\pm1)}|j_1,m_1';j_2,m_2'\pm1\rangle C^{j,m}_{j_1,j_2,m_1',m_2'}\end{aligned}$$

$$\begin{aligned}&\sqrt{j(j+1)-m(m\pm1)}C^{j,m\pm1}_{j_1,j_2,m_1,m_2} \\ &= \sum_{m_1',m_2'}\sqrt{j_1(j_1+1)-m_1'(m_1'\pm1)}\delta_{m_1,m_1'\pm1}\delta_{m_2,m_2'}C^{j,m}_{j_1,j_2,m_1',m_2'} \\ &+ \sum_{m_1',m_2'}\sqrt{j_2(j_2+1)-m_2(m_2\pm1)}\delta_{m_1,m_1'}\delta_{m_2,m_2'\pm1}C^{j,m}_{j_1,j_2,m_1',m_2'}\end{aligned}$$

通过求和消去 δ 函数, 第一项即 $m_1' = m_1 \mp 1$ 且 $m_2 = m_2'$, 第二项即 $m_1 = m_1'$ 且 $m_2' = m_2 \mp 1$. 化简得到

$$\begin{aligned}&\sqrt{j(j+1)-m(m\pm1)}C^{j,m\pm1}_{j_1,j_2,m_1,m_2} \\ &= \sqrt{j_1(j_1+1)-(m_1\mp1)m_1}C^{j,m}_{j_1,j_2,m_1\mp1,m_2} + \sqrt{j_2(j_2+1)-(m_2\mp1)m_2}C^{j,m}_{j_1,j_2,m_1,m_2\mp1}\end{aligned}$$

通过约定 $\langle j_1,j_1;j_2,j_2|j_1+j_2,j_1+j_2;j_1,j_2\rangle = C^{j_1+j_2,j_1+j_2}_{j_1,j_2,j_1,j_2} = 1$, 就能递推出各系数.

1.2.4 离散对称性

1.2.4.1 宇称

1.2.4.1.1 波函数的宇称

1.2.4.1.2 动量本征态和角动量本征态的宇称

1.2.4.1.3 宇称选择定则

1.2.4.2 时间反演

1.2.4.2.1 时间反演和自旋

1.2.4.2.2 无自旋粒子

1.2.4.2.3 时间反演对称不对应守恒律

1.2.4.2.4 半整数自旋体系的 Kramer 定理

1.2.4.3 晶格平移

1.3 单体问题的代数解法

1.3.1 类氢原子

1.3.1.1 量级分析

$$H=\frac{\vec{p}^2}{2\mu}-\frac{Ze^2}{4\pi\epsilon_0 r},\quad \mu=\frac{m_e M}{m_e+M}$$

使用不确定性原理临界 $\Delta x\Delta p\sim\hbar$ 可知

$$\begin{aligned}H(\Delta r)&\sim\frac{\hbar^2}{2\mu(\Delta r)^2}-\frac{Ze^2}{4\pi\epsilon_0\Delta r}\\ \Rightarrow r&\sim\frac{4\pi\epsilon_0\hbar^2}{Ze^2\mu}\equiv\frac{1}{Z}\frac{m_e}{\mu}a_0\\ E_0&\sim-\frac{1}{2}\frac{\mu}{\hbar^2}\left(\frac{Ze^2}{4\pi\epsilon_0}\right)^2\equiv-Z^2\frac{\mu}{m_e}\mathrm{Ry},\quad \mathrm{Ry}=\frac{1}{2}\frac{e^2}{4\pi\epsilon_0 a_0}\end{aligned}$$

1.3.1.2 径向波函数

$$\begin{aligned}&\nabla^2=\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right),\quad \psi(r,\theta,\phi)=R(r)Y(\theta,\phi)\\ &\Rightarrow\begin{cases}\dfrac{1}{R}\dfrac{\mathrm{d}}{\mathrm{d}r}\left(r^2\dfrac{\mathrm{d}R}{\mathrm{d}r}\right)-\dfrac{2mr^2}{\hbar^2}\left[\dfrac{1}{4\pi\epsilon_0}\dfrac{1}{r}-E\right]=l(l+1)\\ \dfrac{1}{Y}\left\{\dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial Y}{\partial\theta}\right)+\dfrac{1}{\sin^2\theta}\dfrac{\partial^2 Y}{\partial\phi^2}\right\}=-l(l+1)\end{cases}\end{aligned}$$

令 $\kappa\equiv\dfrac{\sqrt{-2m_eE}}{\hbar}$, $\rho\equiv\kappa r$, 径向波函数化为

$$\begin{aligned}&\frac{\mathrm{d}^2u}{\mathrm{d}\rho^2}=\left[1-\frac{\rho_0}{\rho}+\frac{l(l+1)}{\rho^2}\right]u.\quad \rho_0\equiv\frac{m_e e^2}{2m_e\varepsilon_0\hbar^2\kappa}\\ &\lim_{\rho\to\infty}u\sim Ae^{-\rho},\quad \lim_{\rho\to 0}u\sim C\rho^{l+1}\Rightarrow u(\rho)=\rho^{l+1}e^{-\rho}v(\rho)\\ &\Rightarrow\rho\frac{\mathrm{d}^2v}{\mathrm{d}\rho^2}+2(l+1-\rho)\frac{\mathrm{d}v}{\mathrm{d}\rho}+\Big[\rho_0-2(l+1)\Big]v=0\end{aligned}$$

设 $v(\rho)=\sum_{j=0}^{\infty}c_j\rho_j$, 代入得到递推关系

$$c_{j+1}=\frac{2(j+l+1)-\rho_0}{(j+1)\Big[j+2(l+1)\Big]}c_j$$

1.3.2 简谐振子

1.3.2.1 一维谐振子

1.3.2.1.1 哈密顿量

$$H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2,\quad \omega=\sqrt{\frac{k}{m}}$$
$$\text{无量纲化:}\quad p=P\sqrt{\hbar m\omega},\quad x=Q\sqrt{\frac{\hbar}{m\omega}}$$
$$\Rightarrow H=\frac{1}{2}\hbar\omega(P^2+Q^2),\quad [P,Q]=i$$

1.3.2.1.2 玻色子概念 $E_n=\hbar\omega\left(n+\frac{1}{2}\right),\quad n=0,1,2,\cdots$. 每个单位能量 $\hbar\omega$ 对应的是玻色子的激发. 产生: $a^\dagger:|0\rangle\to|1\rangle\to|2\rangle\to\cdots$, 湮灭: $a:\cdots\to|2\rangle\to|1\rangle\to|0\rangle$.

1.3.2.1.3 产生湮灭算符

$$a=\frac{1}{\sqrt{2}}(Q+iP)$$
$$a^\dagger=\frac{1}{\sqrt{2}}(Q-iP)$$
$$[a,a^\dagger]=1\Leftrightarrow aa^\dagger=a^\dagger a+1$$

1.3.2.1.4 玻色子占据数表象

$$a|n\rangle=\sqrt{n}|n-1\rangle$$
$$a^\dagger|n\rangle=\sqrt{n+1}|n+1\rangle$$
$$a^\dagger a|n\rangle=n|n\rangle,\quad aa^\dagger|n\rangle=(n+1)|n\rangle$$

1.3.2.1.5 Fock 空间的构造 定义粒子数算符 $\hat{n}=a^\dagger a$, 本征态为 $|n\rangle$, 本征值 $\lambda_n=n$.

1.3.2.1.6 矩阵表示 选定矩阵基矢为 $|0\rangle = \begin{pmatrix}1\\0\\0\\\vdots\end{pmatrix}, \quad |1\rangle = \begin{pmatrix}0\\1\\0\\\vdots\end{pmatrix}, \quad |2\rangle = \begin{pmatrix}0\\0\\1\\\vdots\end{pmatrix}, \quad \cdots$, 即可计算产生湮灭算符的矩阵表示:

$$
\begin{aligned}
&a_{mn} = \langle m|a|n\rangle = \sqrt{n}\langle m|n-1\rangle = \sqrt{n}\delta_{m,n-1}\\
&a^\dagger_{mn} = \langle m|a^\dagger|n\rangle = \sqrt{n+1}\langle m|n+1\rangle = \sqrt{n+1}\delta_{m,n+1}\\
&a = \begin{pmatrix}0 & \sqrt{1} & & & \cdots\\ & 0 & \sqrt{2} & & \cdots\\ & & 0 & \sqrt{3} & \cdots\\ & & & 0 & \ddots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}, \quad a^\dagger = \begin{pmatrix}0 & & & & \cdots\\ \sqrt{1} & 0 & & & \cdots\\ & \sqrt{2} & 0 & & \cdots\\ & & \sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}\\
&Q = \frac{a+a^\dagger}{\sqrt{2}} = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & \sqrt{1} & & & \cdots\\ \sqrt{1} & 0 & \sqrt{2} & & \cdots\\ & \sqrt{2} & 0 & \sqrt{3} & \cdots\\ & & \sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}, \quad P = \frac{a-a^\dagger}{\sqrt{2}i} = \frac{1}{\sqrt{2}i}\begin{pmatrix}0 & +\sqrt{1} & & & \cdots\\ -\sqrt{1} & 0 & +\sqrt{2} & & \cdots\\ & -\sqrt{2} & 0 & +\sqrt{3} & \cdots\\ & & -\sqrt{3} & 0 & \cdots\\ \vdots & \vdots & \vdots & \vdots & \ddots\end{pmatrix}
\end{aligned}
$$

1.3.2.1.7 能谱

$$
\begin{aligned}
H = \hbar\left(a^\dagger a + \frac{1}{2}\right) &\to E_n = \hbar\omega\left(n+\frac{1}{2}\right)\\
|n\rangle = \frac{1}{\sqrt{n!}}\left[a^\dagger\right]^n|0\rangle, &\quad \hat{n}|n\rangle = a^\dagger a|n\rangle = \frac{1}{\sqrt{n!}}a^\dagger a\left[a^\dagger\right]^n|0\rangle\\
a\left[a^\dagger\right]^n = aa^\dagger\left[a^\dagger\right]^{n-1} &= (a^\dagger a+1)\left[a^\dagger\right]^{n-1} = a^\dagger a\left[a^\dagger\right]^{n-1} + [a^\dagger]^{n-1}\\
a^\dagger a\left[a^\dagger\right]^{n-1} = a^\dagger aa^\dagger\left[a^\dagger\right]^{n-2} &= a^\dagger\left(a^\dagger a+1\right)\left[a^\dagger\right]^{n-2} = \left[a^\dagger\right]^2 a\left[a^\dagger\right]^{n-2} + \left[a^\dagger\right]^{n-1}\\
\Rightarrow \hat{n}|n\rangle = \frac{1}{\sqrt{n!}}a^\dagger\left\{\cancel{\left[a^\dagger\right]^n a} + n\left[a^\dagger\right]^{n-1}\right\}|0\rangle &= \frac{n}{\sqrt{n!}}\left[a^\dagger\right]^n|0\rangle = n|n\rangle
\end{aligned}
$$

1.3.2.1.8 波函数 根据 $a|0\rangle = 0$, 且应用 $P = -i\dfrac{\partial}{\partial Q}$, 基态 $|0\rangle$ 满足 $\left(Q + \dfrac{\partial}{\partial Q}\right)\psi_0(Q) = 0$. 所以 $\psi_0(Q) = \dfrac{1}{\pi^{\frac{1}{4}}}e^{-\frac{1}{2}Q^2}$. 通过 $a^\dagger$ 产生激发态, 如第一激发态 $|1\rangle = a^\dagger|0\rangle$:

$$
\begin{aligned}
\psi_1(Q) &= \frac{1}{\sqrt{2}}\left(Q - \frac{\partial}{\partial Q}\right)\psi_0(Q) = \frac{1}{\pi^{\frac{1}{4}}}\sqrt{2}Qe^{-\frac{1}{2}Q^2}\\
\psi_n(Q) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}}H_n(Q)e^{-\frac{1}{2}Q^2}\\
\bar{\psi}_n(P) &= \frac{1}{\pi^{\frac{1}{4}}\sqrt{2^n n!}}H_n(P)e^{-\frac{1}{2}P^2}
\end{aligned}
$$

1.3.2.1.9 不确定性关系

$$
\Delta Q\delta P \geq \frac{1}{2}\left|[Q,P]\right|^2 = \frac{1}{2}
$$

使用 Fock 态 $|n\rangle$ 检验. ΔQ 和 ΔP 即标准差, 有

$$Q = \frac{a + a^\dagger}{\sqrt{2}}, \quad P = \frac{a - a^\dagger}{\sqrt{2}i}$$
$$\langle n|Q|n\rangle = 0, \quad \langle n|Q^2|n\rangle = \frac{1}{2}\langle n|(a + a^\dagger)^2|n\rangle = n + \frac{1}{2}$$
$$\to \Delta Q = \sqrt{\langle n|q^2|n\rangle - (\langle n|Q|n\rangle)^2} = \sqrt{n + \frac{1}{2}}$$
$$\langle n|P|n\rangle = 0, \quad \langle n|P^2|n\rangle = -\frac{1}{2}\langle n|(a - a^\dagger)^2|n\rangle = -n - \frac{1}{2}$$
$$\to \Delta P = \sqrt{\langle n|P^2|n\rangle - (\langle n|P|n\rangle)^2} = \sqrt{n + \frac{1}{2}}$$
$$\Rightarrow \Delta Q\Delta P = \sqrt{n + \frac{1}{2}}\sqrt{n + \frac{1}{2}} = n + \frac{1}{2} \geq \frac{1}{2}$$

1.3.2.2 相干态

1.3.2.2.1 定义 相干态是湮灭算符 a 的本征态, 也是使得不确定性最小的态.

$$a|\alpha\rangle = \alpha|\alpha\rangle, \quad \alpha \in \mathbb{C}, \quad \langle\alpha_1|\alpha_2\rangle \neq \delta(\alpha_1 - \alpha_2)$$
$$\langle\alpha|Q|\alpha\rangle = \langle\alpha|\frac{a + a^\dagger}{\sqrt{2}}|\alpha\rangle = \frac{\alpha^* + \alpha}{\sqrt{2}} = \sqrt{2}\mathrm{Re}(\alpha)$$
$$\langle\alpha|Q^2|\alpha\rangle = \langle\alpha|\frac{[a^\dagger]^2 + aa^\dagger + a^\dagger a + a^2}{2}|\alpha\rangle = \frac{\alpha^2 + 2\alpha^*\alpha + [\alpha^*]^2 + 1}{2} = \frac{(\alpha^* + \alpha)}{2} + \frac{1}{2} = 2[\mathrm{Re}\alpha]^2 + \frac{1}{2}$$
$$\Rightarrow \Delta Q = \sqrt{\langle\alpha|x^2|\alpha\rangle - (\langle\alpha|x|\alpha\rangle)^2} = \frac{1}{\sqrt{2}}$$
$$\langle\alpha|P|\alpha\rangle = \langle\alpha|\frac{a - a^\dagger}{\sqrt{2}i}|\alpha\rangle = \frac{\alpha^* - \alpha}{\sqrt{2}i} = \sqrt{2}\mathrm{Im}(\alpha)$$
$$\langle\alpha|P^2|\alpha\rangle = \langle\alpha|\frac{[a^\dagger]^2 - aa^\dagger - a^\dagger a + a^2}{2}|\alpha\rangle = \frac{\alpha^2 - 2\alpha^*\alpha + [\alpha^*]^2 + 1}{2} = \frac{(\alpha^* - \alpha)}{2} + \frac{1}{2} = 2[\mathrm{Im}\alpha]^2 + \frac{1}{2}$$
$$\Rightarrow \Delta P = \sqrt{\langle\alpha|P^2|\alpha\rangle - (\langle\alpha|P|\alpha\rangle)^2} = \frac{1}{\sqrt{2}}$$
$$\Delta Q\Delta P = \frac{1}{2}$$

1.3.2.2.2 Fock 态表象 以 Fock 态为基矢展开相干态 $|\alpha\rangle = e^{-\frac{1}{2}|\alpha|^2}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$. 它的含义是, 遍历所有可能的 $|n\rangle$, 并使用对应的 n 个湮灭算符将其降阶至基态 $|0\rangle$.

1. $|0\rangle$ 也是相干态, 相当于 $\alpha = 0$.
2. 相干态 $|\alpha = n\rangle$ 和粒子数表象的 $|n\rangle$ 不同.
3. 在相干态 $|\alpha\rangle$ 中测得 n 个玻色子的概率为 $p_\alpha(n) = |\langle n|\alpha\rangle|^2 = \frac{|\alpha|^{2n}}{n!}e^{-|\alpha|^2} \equiv \frac{\lambda^2}{n!}e^{-\lambda}$, 也就是说这是一个 Poisson 分布. 这也是 $\langle n\rangle_\alpha = \langle\alpha|\hat{n}|\alpha\rangle = |\alpha|^2$ 的例证.

1.3.2.2.3 时间演化

$$
\begin{aligned}
U(t) &= e^{-iHt/\hbar} = e^{-i\omega\left(\hat{n}+\frac{1}{2}\right)t} = e^{-\frac{i\omega t}{2}} e^{-i\omega t\hat{n}} \\
U(t)|\alpha\rangle &= e^{-\frac{i\omega t}{2}} e^{-i\omega t\hat{n}} e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}}|n\rangle = e^{-\frac{i\omega t}{2}} e^{-\frac{1}{2}|\alpha|^2} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} e^{-i\omega t n}|n\rangle \\
&= e^{-\frac{i\omega t}{2}} e^{-\frac{1}{2}|\alpha e^{-i\omega t}|^2} \sum_{n=0}^{\infty} \frac{(\alpha e^{-i\omega t})^n}{\sqrt{n!}}|n\rangle = |\alpha e^{-i\omega t}\rangle \\
\Rightarrow \alpha(t) &= \alpha(0)e^{-i\omega t}
\end{aligned}
$$

1.3.2.2.4 U(1)对称性

1.3.2.2.5 坐标表象

1.3.2.2.6 BCH 公式

1.3.2.2.7 位移公式

1.3.2.2.8 超完备性

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

1. 非正交性: $\langle\beta|\alpha\rangle \neq \delta_{\alpha\beta}$.
2. 完备性关系:

$$
\begin{aligned}
\frac{1}{\pi}\int_{\mathbb{C}} \mathrm{d}\alpha|\alpha\rangle\langle\alpha| &= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}\int_{\mathbb{C}}\mathrm{d}\alpha e^{-|\alpha|^2}\alpha^m[\alpha^*]^n|m\rangle\langle n| \\
\alpha = re^{i\varphi}: \quad &= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}\int_0^{\infty} r\mathrm{d}re^{-r^2}r^{m+n}\int_0^{2\pi}\mathrm{d}\varphi e^{i(m-n)\varphi}|m\rangle\langle n| \\
&= \frac{1}{\pi}\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{1}{\sqrt{m!n!}}2\pi\delta_{mn}\int_0^{\infty} r\mathrm{d}re^{-r^2}r^{m+n}|m\rangle\langle n| \\
s = r^2: \quad &= \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{1}{n!}\pi\int_0^{\infty}\mathrm{d}se^{-s}s^n|n\rangle\langle n| \\
&= \frac{1}{\pi}\sum_{n=0}^{\infty}\frac{1}{\cancel{n!}}\pi\cancel{\Gamma(n+1)}|n\rangle\langle n| \\
&= \sum_{n=0}^{\infty}|n\rangle\langle n| = \mathbb{I}
\end{aligned}
$$

3. 超完备性(任何相干态都可以用其它相干态展开):

$$
|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}\beta|\beta\rangle\langle\beta|\alpha\rangle = \frac{1}{\pi}\int_{\mathbb{C}}\mathrm{d}\beta|\beta\rangle e^{-\frac{1}{2}(|\alpha|^2+|\beta|^2)+\alpha\beta^*}
$$

1.3.2.3 三维谐振子

1.3.2.3.1 哈密顿量

$$
\begin{aligned}
H &= \frac{\hbar\omega}{2}\left(\vec{P}^2+\vec{Q}^2\right), \quad [Q_i,P_j]=i\delta_{ij}, \quad [Q_i,Q_j]=[P_i,P_j]=0 \\
\vec{a} &= \frac{1}{\sqrt{2}}(\vec{Q}+i\vec{P}), \quad \vec{a}^\dagger=\frac{1}{\sqrt{2}}(\vec{Q}-i\vec{P}), \quad [a_i,a_j^\dagger]=\delta_{ij}, \quad [a_i,a_j]=[a_i^\dagger,a_j^\dagger]=0 \\
H &= \hbar\omega\left(\vec{a}^\dagger\cdot\vec{a}+\frac{3}{2}\right)=\hbar\omega\left(a_1^\dagger a_1+a_2^\dagger a_2+a_3^\dagger a_3+\frac{3}{2}\right)
\end{aligned}
$$

1.3.2.3.2 能级和简并

$$
\begin{aligned}
E &= \hbar\omega\left(n_1+n_2+n_3+\frac{3}{2}\right)=\hbar\omega\left(N+\frac{3}{2}\right) \\
D &= \sum_{n_1,n_2,n_3}\delta_{N,n_1+n_2,n_3}=\frac{1}{2}(N+1)(N+2)
\end{aligned}
$$

1.3.2.3.3 角动量算符

$$
\vec{L}=\vec{x}\times\vec{p} \iff L_i=\epsilon_{ijk}x_jp_k \iff L_i=-i\epsilon_{ijk}a_j^\dagger a_k
$$

1.3.2.3.4 Fock 态表象

1.4 全同粒子

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

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

通过构造 $P_{12}HP_{12}=H$ 证明 $[P_{12},H]=0$. 则 P_{12} 的本征态为 $|k'k''\rangle_\pm=\frac{1}{\sqrt{2}}(|k'\rangle|k''\rangle\pm|k''\rangle|k'\rangle)$, 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

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

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

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

1.4.3.2 变分原理

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

1.4.3.3 Hatree-Fock 近似

设系统波函数可由 Slater 行列式近似, 即 $\Psi = \dfrac{1}{\sqrt{N!}}\det[\psi_{q(1)}\psi_{q(2)}\cdots\psi_{q(N)}]$, $\psi_q(\vec{x})$ 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.

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

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 $\displaystyle\int \psi_i^*(\vec{x})\psi_j(\vec{x})\mathrm{d}\vec{x} = \delta_{ij}$ 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

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

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: $\int \frac{1}{r} e^{-i\vec{q}\cdot\vec{r}} \mathrm{d}\vec{r} = \frac{4\pi}{q^2}$, 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 $\int \mathrm{d}^3\vec{x} e^{i\vec{k}\cdot\vec{x}} = (2\pi)^3 \delta^{(3)}(\vec{k}, \vec{0})$:

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

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

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

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

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

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.

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

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:

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

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:

$$b_\alpha^\dagger|n_\alpha\rangle = \frac{1}{\sqrt{n_\alpha+1}}|\alpha\rangle\hat{A}_+|\alpha\rangle\otimes^{n_\alpha} = \frac{n_\alpha+1}{\sqrt{n_\alpha+1}}|\alpha\rangle\otimes^{(n_\alpha+1)} = \sqrt{n_\alpha+1}|n_\alpha+1\rangle$$
$$b_\alpha|n_\alpha\rangle = \frac{1}{\sqrt{n_\alpha}}|\alpha\rangle\hat{D}_+|\alpha\rangle\otimes^{n_\alpha} = \frac{n_\alpha}{\sqrt{n_\alpha}}|\alpha\rangle\otimes^{(n_\alpha-1)} = \sqrt{n_\alpha}|n_\alpha-1\rangle$$

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:

$$b_\alpha^\dagger|\cdots, n_\beta, n_\alpha, n_\gamma, \cdots\rangle_B = \sqrt{n_\alpha+1}|\cdots, n_\beta, n_\alpha+1, n_\gamma, \cdots\rangle_B$$
$$b_\alpha|\cdots, n_\beta, n_\alpha, n_\gamma, \cdots\rangle_B = \sqrt{n_\alpha}|\cdots, n_\beta, n_\alpha-1, n_\gamma, \cdots\rangle_B$$

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:

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

   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:

$$\begin{aligned}
\psi^\dagger(x) &= \sum_\alpha \langle\alpha|x\rangle a_\alpha^\dagger = \sum_\alpha \phi_\alpha^*(x) a_\alpha^\dagger \\
\psi(x) &= \sum_\alpha \langle x|\alpha\rangle a_\alpha = \sum_\alpha \phi_\alpha(x) a_\alpha
\end{aligned}$$

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 $\hat{U} = \sum_{i=1}^N \hat{U}_i$, 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 $\hat{U} = \sum_{i=1}^N \sum_\lambda U_\lambda |\lambda\rangle_i\langle\lambda|_i$, 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

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

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 $\begin{aligned}\sum_{i\neq j}(|\alpha\rangle_i|\beta\rangle_j\langle\alpha|_i\langle\beta|_j)|n_1, n_2, \cdots\rangle &= \hat{N}_{\alpha\beta}|n_1, n_2, \cdots\rangle = (\hat{n}_\alpha\hat{n}_\beta - \delta_{\alpha\beta}\hat{n}_\alpha)\,|n_1, n_2, \cdots\rangle \\ &= a_\alpha^\dagger a_\beta^\dagger a_\beta a_\alpha|n_1, n_2, \cdots\rangle\end{aligned}$

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:

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

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

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

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. 如果追加半满条件, 即两个格点共有两个电子, 后续通过产生算符作用于真空态得到基态波函数时就会使用两个产生算符, 具体是什么产生算符需要看能量最低的两个本征值的位置.

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

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

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

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

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

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

$$\begin{pmatrix} & \frac{U+\sqrt{4t^2+U^2}}{\sqrt{4t^2+(\sqrt{4t^2+U^2}+U)^2}} & & \frac{U-\sqrt{4t^2+U^2}}{\sqrt{4t^2+(\sqrt{4t^2+U^2}-U)^2}} \\ \frac{-U+\sqrt{4t^2+U^2}}{\sqrt{4t^2+(\sqrt{4t^2+U^2}-U)^2}} & & \frac{-U-\sqrt{4t^2+U^2}}{\sqrt{4t^2+(\sqrt{4t^2+U^2}+U)^2}} & \\ & \frac{2t}{\sqrt{4t^2+(\sqrt{4t^2+U^2}+U)^2}} & & \frac{2t}{\sqrt{4t^2+(\sqrt{4t^2+U^2}-U)^2}} \\ \frac{2t}{\sqrt{4t^2+(\sqrt{4t^2+U^2}-U)^2}} & & \frac{2t}{\sqrt{4t^2+(\sqrt{4t^2+U^2}+U)^2}} & \end{pmatrix}$$

$$D=\frac{1}{2}\begin{pmatrix} U-\sqrt{4t^2+U^2} & & & \\ & U-\sqrt{4t^2+U^2} & & \\ & & U+\sqrt{4t^2+U^2} & \\ & & & U+\sqrt{4t^2+U^2} \end{pmatrix}$$

能量最低态由新基矢的 $1,2$ 分量给出, 产生算符 $\times|0\rangle$ 将会是 $|\psi_{\text{HF}}\rangle=\gamma_1^\dagger\gamma_2^\dagger|0\rangle$, 粒子数平均值为

$$\begin{aligned}\langle n_{1\uparrow}\rangle=\langle c_{1\uparrow}^\dagger c_{1\uparrow}\rangle&=\sum_{i,j}(V_{1\uparrow,i})^\dagger V_{1\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle=(V_{1\uparrow,1})^\dagger V_{1\uparrow,1}+(V_{1\uparrow,2})^\dagger V_{1\uparrow,2}\\&=\frac{(U+\sqrt{4t^2+U^2})^2}{4t^2+(\sqrt{4t^2+U^2}+U)^2}\end{aligned}$$

发现粒子数平均值并未收敛, 需要将粒子数平均值作为变量进行迭代计算.

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

$$\begin{pmatrix} \alpha U & & -t & \\ & (1-\alpha)U & & -t \\ -t & & (1-\alpha)U & \\ & -t & & \alpha U \end{pmatrix}=\begin{pmatrix} & & -t & \\ & (1-2\alpha)U & & -t \\ -t & & (1-2\alpha)U & \\ & -t & & \end{pmatrix}+\alpha U\mathbb{I}=VDV^{-1}$$

观察可知, 这种情况相当于将 U 替换为 $\bar{U}=(1-2\alpha)U$, 能量本征值再统一加 αU 值. 能量最低态由新基矢的 $1,2$ 分量给出, 所以平均场能量为

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

收敛即代入 $\langle n_{i\sigma}\rangle$ 的值等于最后根据 V 计算得到的 $\langle n_{i\sigma}\rangle$, 这被称作 self-consistent 方程. 比如取 $\langle n_{1\downarrow}\rangle$, 能量最低态由新基矢的 $1,2$ 分量给出, 那么

$$\begin{aligned}\langle n_{2\uparrow}\rangle=\langle c_{2\uparrow}^\dagger c_{2\uparrow}\rangle&=\sum_{i,j}(V_{2\uparrow,i})^\dagger V_{2\uparrow,j}\langle\gamma_i^\dagger\gamma_j\rangle=(V_{2\uparrow,1})^\dagger V_{2\uparrow,1}+(V_{2\uparrow,2})^\dagger V_{2\uparrow,2}\\&=0\cdot 0+\left(\frac{2t}{\sqrt{4t^2+(\bar{U}+\sqrt{4t^2+\bar{U}^2})^2}}\right)^2\\&=\frac{4t^2}{4t^2+(\sqrt{4t^2+[(1-2\alpha)U]^2}+(1-2\alpha)U)^2}=\alpha\end{aligned}$$

取 $U\gg t$ 极限, 即有 $\alpha\to 0$,

1.4.18.2.2　Hubbard 模型在动量空间的平均场　考虑傅里叶变换 $c_{i,\sigma} = \frac{1}{\sqrt{N}}\sum_{k} c_{k,\sigma} e^{i\vec{k}\cdot\vec{r}_i}$, 那么单体算符部分有

$$
\begin{aligned}
H_0 &= -t\sum_{i,\delta} c^\dagger_{i,\sigma} c_{i+\delta,\sigma} - \mu \sum_{i,\sigma} n_{i,\sigma} \\
&= \sum_{\vec{k}} (\varepsilon_{\vec{k}} - \mu) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma}
\end{aligned}
$$

对于两体算符 $n_{i,\uparrow}n_{i,\downarrow} = c^\dagger_{i,\uparrow}c_{i,\uparrow}c^\dagger_{i,\downarrow}c_{i,\downarrow}$ 部分,

$$
\begin{aligned}
H_U &= U \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} c^\dagger_{\vec{k}_1,\uparrow} c_{\vec{k}_2,\uparrow} c^\dagger_{\vec{k}_3,\downarrow} c_{\vec{k}_4,\downarrow} \frac{1}{N^2} \sum_i e^{-i[(\vec{k}_1-\vec{k}_2)-(\vec{k}_4-\vec{k}_3)]\cdot\vec{r}_i} \\
&= U \sum_{\vec{k}_1,\vec{k}_2,\vec{k}_3,\vec{k}_4} c^\dagger_{\vec{k}_1,\uparrow} c_{\vec{k}_2,\uparrow} c^\dagger_{\vec{k}_3,\downarrow} c_{\vec{k}_4,\downarrow} \frac{1}{N} \delta_{\vec{k}_1-\vec{k}_2,\vec{k}_4-\vec{k}_3} \\
&= U \sum_{\vec{k}_2,\vec{q}_1,\vec{k}_4,\vec{q}_2} c^\dagger_{\vec{k}_2+\vec{q}_1,\uparrow} c_{\vec{k}_2,\uparrow} c^\dagger_{\vec{k}_4+\vec{q}_2,\downarrow} c_{\vec{k}_4,\downarrow} \frac{1}{N} \delta_{\vec{q}_1,-\vec{q}_2} \\
&= U \sum_{\vec{k}_2,\vec{q}_1,\vec{k}_4} c^\dagger_{\vec{k}_2+\vec{q}_1,\uparrow} c_{\vec{k}_2,\uparrow} c^\dagger_{\vec{k}_4-\vec{q}_1,\downarrow} c_{\vec{k}_4,\downarrow} \frac{1}{N}
\end{aligned}
$$

式子中的 $\delta_{\vec{q}_1,-\vec{q}_2}$ 代表的是动量交换守恒. 引入属于动量空间中的 ”粒子数算符” $\rho_{\vec{q},\sigma} = \frac{1}{\sqrt{N}}\sum_{\vec{k}} c^\dagger_{\vec{k}+\vec{q},\sigma} c_{\vec{k},\sigma}$, 即有

$$
\begin{aligned}
H_U &= U \sum_{\vec{q}_1} \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}_2} c^\dagger_{\vec{k}_2+\vec{q}_1,\uparrow} c_{\vec{k}_2,\uparrow} \right) \left(\frac{1}{\sqrt{N}} \sum_{\vec{k}_4} c^\dagger_{\vec{k}_2-\vec{q}_1,\downarrow} c_{\vec{k}_2,\downarrow} \right) \\
&= U \sum_{\vec{q}} \rho_{\vec{q},\uparrow} \rho_{-\vec{q},\downarrow} \\
&\approx U \sum_{\vec{q}} \langle \rho_{\vec{q},\uparrow} \rangle \rho_{-\vec{q},\downarrow} + \rho_{\vec{q},\uparrow} \langle \rho_{-\vec{q},\downarrow} \rangle - \langle \rho_{\vec{q},\uparrow} \rangle \langle \rho_{-\vec{q},\downarrow} \rangle
\end{aligned}
$$

最后一行应用了平均场近似. 综合以上讨论, 得到平均场哈密顿量

$$
H_{\mathrm{MF}} = \sum_{\vec{k}} (\varepsilon_{\vec{k}} - \mu) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} + U \sum_{\vec{q}} \langle \rho_{\vec{q},\uparrow} \rangle \rho_{-\vec{q},\downarrow} + \rho_{\vec{q},\uparrow} \langle \rho_{-\vec{q},\downarrow} \rangle - \langle \rho_{\vec{q},\uparrow} \rangle \langle \rho_{-\vec{q},\downarrow} \rangle
$$

1.5　微扰论

1.6　量子计算基础

1.6.1　量子纠缠

1.6.1.1　双量子比特态

量子比特有两种状态 $|\uparrow\rangle = \begin{pmatrix}1\\0\end{pmatrix}$ 和 $|\downarrow\rangle = \begin{pmatrix}0\\1\end{pmatrix}$. 通过张量积规则 $\begin{pmatrix}a_1\\a_2\end{pmatrix} \otimes \begin{pmatrix}b_1\\b_2\end{pmatrix} = \begin{pmatrix} a_1\begin{pmatrix}b_1\\b_2\end{pmatrix} \\ a_2\begin{pmatrix}b_1\\b_2\end{pmatrix}\end{pmatrix} = \begin{pmatrix}a_1b_1\\a_1b_2\\a_2b_1\\a_2b_2\end{pmatrix}$ 计算复合系统的基矢 $|\uparrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\downarrow\downarrow\rangle$. 所以双量子比特 Hilbert 空间中的态可以展开为基矢的线性组合:

$$
|\psi\rangle = \psi_1|\uparrow\uparrow\rangle + \psi_2|\uparrow\downarrow\rangle + \psi_3|\downarrow\uparrow\rangle + \psi_4|\downarrow\downarrow\rangle = \begin{pmatrix}\psi_1\\\psi_2\\\psi_3\\\psi_4\end{pmatrix}
$$

1.6.1.2 双量子比特算符

通过 Pauli 矩阵约定 $\sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\sigma^{1,2,3} = \sigma^{x,y,z}$, 且其张量积积简写为 $\sigma_A^i \otimes \sigma_B^j \equiv \sigma^{ij}$, 矩阵张量积规则为

$$\sigma^{32} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \otimes \sigma^2 = \begin{pmatrix} 1\sigma^2 & 0\sigma^2 \\ 0\sigma^2 & -1\sigma^2 \end{pmatrix} = \begin{pmatrix} & -i & & \\ i & & & \\ & & & i \\ & & -i & \end{pmatrix}$$

这相当于是在给定算符的 ”基”. 即观测量矩阵都可以展开为这些矩阵张量积的线性组合. 谈论单量子比特的观测量时, 相当于默认另一个量子比特算符为 $\mathbb{I} = \sigma^0$, 使得算符基为 $(\sigma^{10}, \sigma^{20}, \sigma^{30})$ 和 $(\sigma^{01}, \sigma^{02}, \sigma^{03})$.

1.6.1.3 双量子比特模型

双量子比特 Heisenberg 模型哈密顿量为 $H = \dfrac{J}{4}\vec{\sigma}_A \cdot \vec{\sigma}_B$, 将其写作矩阵形式:

$$H = \frac{J}{4}(\sigma^{11} + \sigma^{22} + \sigma^{33}) = \frac{J}{4}\begin{pmatrix} 1 & & & \\ & -1 & 2 & \\ & 2 & -1 & \\ & & & 1 \end{pmatrix}$$

将其对角化以计算本征值, 并找到本征值对应的本征态, 结果为

$$E_s = -\frac{3}{4}J, \quad |s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle), \quad \text{自旋单态}$$

$$E_t = \frac{J}{4}, \quad \begin{cases} |t_1\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle) \\ |t_2\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \\ |t_3\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle) \end{cases}, \quad \text{自旋三重态}$$

1.6.1.4 自旋单态

$$|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \vec{\sigma}_A = (\sigma^{10}, \sigma^{20}, \sigma^{30}) = \left(\begin{pmatrix} & & 1 & \\ & & & 1 \\ 1 & & & \\ & 1 & & \end{pmatrix}, \begin{pmatrix} & & -i & \\ & & & -i \\ i & & & \\ & i & & \end{pmatrix}, \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix}\right)$$

1.6.1.5 纠缠熵

双量子比特态 $|\psi\rangle$ 中量子比特 A 的纠缠熵: $S(A) = -\mathrm{Tr}[\rho_A \ln \rho_A]$. 其中约化密度矩阵 $\rho_A = \mathrm{Tr}_B|\psi\rangle\langle\psi|$

更广义的 Renyi 纠缠熵 $S^{(n)}(A) = \dfrac{1}{1-n}\ln \mathrm{Tr}\rho_A^n$.

接下来介绍如何部分求迹.

1. 自旋单态 $|\psi\rangle = |s\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$. 其总密度矩阵为

$$\rho = |s\rangle\langle s| = \frac{1}{2}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}\begin{pmatrix}0 & 1 & -1 & 0\end{pmatrix} = \frac{1}{2}\begin{pmatrix} & & & \\ & 1 & -1 & \\ & -1 & 1 & \\ & & & \end{pmatrix}$$

$$\rho_A = \mathrm{Tr}_B\rho = \frac{1}{2}\begin{pmatrix}\mathrm{Tr}\begin{pmatrix} & \\ & 1\end{pmatrix} & \mathrm{Tr}\begin{pmatrix} & \\ -1 & \end{pmatrix}\\ \mathrm{Tr}\begin{pmatrix} & -1\\ & \end{pmatrix} & \mathrm{Tr}\begin{pmatrix}1 & \\ & \end{pmatrix}\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 0\\0 & 1\end{pmatrix}, \quad \lambda_A^1 = \frac{1}{2}, \quad \lambda_A^2 = \frac{1}{2}$$

$$S(A) = -\mathrm{Tr}\rho_A \ln\rho_A = -\sum_i \lambda_A^i \ln\lambda_A^i = -\left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = \ln 2$$

2. 乘积态 $|\psi\rangle = \dfrac{1}{2}(|\uparrow\uparrow\rangle + |\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle + |\downarrow\downarrow\rangle)$. 总密度矩阵为

$$\rho = |\psi\rangle\langle\psi| = \frac{1}{4}\begin{pmatrix}1\\1\\1\\1\end{pmatrix}\begin{pmatrix}1 & 1 & 1 & 1\end{pmatrix} = \frac{1}{4}\begin{pmatrix}1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\\1 & 1 & 1 & 1\end{pmatrix}$$

$$\rho_A = \mathrm{Tr}_B\rho = \frac{1}{4}\begin{pmatrix}\mathrm{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} & \mathrm{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\\ \mathrm{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} & \mathrm{Tr}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}\end{pmatrix} = \frac{1}{4}\begin{pmatrix}2 & 2\\2 & 2\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix}, \quad \lambda_A^1 = 0, \quad \lambda_A^2 = 1$$

$$S(A) = -\mathrm{Tr}\rho_A \ln\rho_A = -\sum_i \lambda_A^i \ln\lambda_A^i = -(0\ln 0 + 1\ln 1) = 0.$$

1.6.1.6　互信息

双量子比特体系, A 和 B 之间的互信息为

$$I(A:B) = S(A) + S(B) - S(A\cup B)$$

1.6.1.7　EPR 佯谬和 Bell 不等式

1.7　相对论量子力学

1.7.1　洛伦兹协变性

1.7.1.1　单位制约定

原子单位制: $\hbar(\mathrm{kg}\cdot\mathrm{m}^2/\mathrm{s}^2) = c(\mathrm{m/s}) = 1$.

1. $c = 1$: 速度 v 无量纲; 时间 t 和距离 x 同量纲; 质量 m, 动量 p, 能量 E 同量纲.
2. $\hbar = 1$: 时间 t 和距离 x 乘积后与能量 E 同量纲.

1.7.1.2　协变逆变记号

来源于相对论. $\begin{cases}\text{逆变:}a^\mu & = (a^0, +\vec{a})\\ \text{协变:}a_\mu & = (a^0, -\vec{a})\end{cases}$. 其中 $a_\mu = \eta_{\mu\nu}a^\nu$. $\eta_{\mu\nu} = \begin{pmatrix}+1 & 0 & 0 & 0\\0 & -1 & 0 & 0\\0 & 0 & -1 & 0\\0 & 0 & 0 & -1\end{pmatrix}$

4-矢量的内积: $a^\mu b_\mu = a^0b^0 - \vec{a}\cdot\vec{b}$.

时空 4-矢量 $x^\mu = (t, \vec{x})$, 逆变 4-梯度: $\dfrac{\partial}{\partial x_\mu} \equiv \partial^\mu = \left(\dfrac{\partial}{\partial t}, -\nabla\right)$, 协变 4-梯度: $\dfrac{\partial}{\partial x^\mu} \equiv \partial_\mu = \left(\dfrac{\partial}{\partial t}, \nabla\right)$

1.7.1.3 洛伦兹群

若 Λ_ν^μ 令 $x^\mu = \Lambda_\nu^\mu x_\nu$, 使得 $x^\mu x_\mu = x^\nu x_{nu}$, 则该变换属于 Lorentz 变换.

1.7.2 Klein-Gordon 方程

1.7.2.1 Klein-Gordon 方程的推导

相对论的能动关系: $E^2 = p^2 + m^2$. 对其使用一次量子化 $p \to \hat{p} = -i\nabla, \quad E \to \hat{H} = i\dfrac{\partial}{\partial t}$, 得到 Klein-Gordon 方程:

$$\begin{aligned}
&\left(\frac{\partial^2}{\partial t^2} - \nabla^2 + m^2\right)\psi = 0 \\
&\Rightarrow \left(\partial_\mu \partial^\mu + m^2\right)\psi = 0
\end{aligned}$$

平面波解 $\psi(\vec{x},t) = Ae^{i\vec{p}\cdot\vec{x}}e^{-iEt} = Ae^{-i(Et-\vec{p}\cdot\vec{x})} \overset{p^\mu=(E,\vec{p}),x_\mu=(t,-\vec{x})}{\Longrightarrow} Ae^{-ip^\mu x_\mu}$, 它意味着 $E = \pm\sqrt{\vec{p}^2 + m^2}$.

常规理解 K-G 方程会带来负能量, 负概率等难以解释的问题. 解决方法是引入自然存在正负的电荷 q. K-G 方程用于描述自旋为 0 的粒子.

K-G 具有 Lorentz 协变性, 因此完美适用电磁作用. 那么推广至 $\begin{cases} E & \to E - q\phi \\ \vec{p} & \to \vec{p} - q\vec{A} \end{cases}$, $p_\mu \to A_\mu = (\phi, -\vec{A})$, K-G 方程形式维持:

$$\begin{aligned}
&\left[D_\mu D^\mu + m^2\right]\psi = 0, \quad \text{协变微分: } D_\mu = \partial_\mu + iqA_\mu \\
&D_\mu D^\mu = D_t^2 - \vec{D}^2, \quad \begin{cases} D_t = \partial_t + iq\phi \\ \vec{D} = \vec{\nabla} - iq\vec{A} \end{cases}
\end{aligned}$$

为了求解二阶方程, 使用共轭展开引入两个新函数降阶:

$$\begin{aligned}
\phi(\vec{x},t) &= \frac{1}{2}\left[\psi(\vec{x},t) + \frac{i}{m}D_t\psi(\vec{x},t)\right] \\
\chi(\vec{x},t) &= \frac{1}{2}\left[\psi(\vec{x},t) - \frac{i}{m}D_t\psi(\vec{x},t)\right]
\end{aligned}$$

满足

$$\begin{aligned}
iD_t\phi &= -\frac{1}{2m}\vec{D}^2(\phi+\chi) + m\phi \\
iD_t\chi &= +\frac{1}{2m}\vec{D}^2(\phi+\chi) - m\phi \\
\Rightarrow iD_t\begin{bmatrix}\phi\\\chi\end{bmatrix} &= -\frac{1}{2m}\vec{D}^2\begin{bmatrix}+\phi+\chi\\-\phi-\chi\end{bmatrix} + m\begin{bmatrix}+\phi\\-\phi\end{bmatrix} \\
&= -\frac{1}{2m}\vec{D}^2\begin{bmatrix}1 & 1\\-1 & -1\end{bmatrix}\begin{bmatrix}\phi\\\chi\end{bmatrix} + m\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix}\begin{bmatrix}\phi\\\chi\end{bmatrix}
\end{aligned}$$

使用 Pauli 矩阵合成公式中出现的以若干 1 和 −1 为元素的矩阵, 即 $\begin{bmatrix}1 & 1\\-1 & -1\end{bmatrix} = \begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} + \begin{bmatrix}0 & 1\\-1 & 0\end{bmatrix} = \sigma^z + i\sigma^y$, 以及 $\begin{bmatrix}1 & 0\\0 & -1\end{bmatrix} = \sigma^z$, 所以最后 K-G 方程化为

$$iD_t\begin{bmatrix}\phi\\\chi\end{bmatrix} = -\frac{1}{2m}\vec{D}^2\left[\sigma^z + i\sigma^y\right]\begin{bmatrix}\phi\\\chi\end{bmatrix} + m\left[\sigma^z\right]\begin{bmatrix}\phi\\\chi\end{bmatrix}$$

4-矢量概率流 $j^\mu = \dfrac{i}{2m}\left[\psi^* D^\mu\psi - \psi(D^\mu\psi)^*\right]$, 概率密度 $\rho = j^0 = \dfrac{i}{2m}\left[\psi^* D_t\psi - (D_t\psi)^*\psi\right] = \phi^*\phi - \chi^*\chi$, 其中 ϕ 为正粒子波函数, χ 为反粒子波函数.

1.7.3 Dirac 方程

K-G 是 ∂_t^2 的, Dirac 为了化为传统的 ∂_t^1, 推广 Pauli 矩阵为 4×4 的 γ 矩阵, 使得∇ 为一阶. Dirac 方程描述自旋 $\frac{1}{2}$, $g=2$ 的粒子.

1.7.3.1 自由粒子的 Dirac 方程

$$K\to K', \text{则} \begin{cases} t' = +t\cosh\zeta - z\sinh\zeta \\ x' = x \\ y' = y \\ z' = -t\sinh\zeta + z\cosh\zeta \end{cases}, \quad \tanh\zeta = v, \text{其中有 } \frac{p_z}{m} = v_z\gamma = -\sinh\zeta(*).$$

存在两种方法 $\Omega_\pm$ 使得 (*) 成立, 定义 Weyl 旋量来体现着这种区别:

$$\begin{aligned} \chi_\pm(p_z) &= e^{\mp\frac{1}{2}\zeta\sigma_z}\xi \\ \Rightarrow \chi_-(p_z) &= e^{\zeta\sigma_z}\chi_+(p_z) \end{aligned} \tag{**}$$

由于 $me^{\zeta\sigma_z} = m(\cosh\zeta + \sigma_z\sinh\zeta) = E - \sigma_z p_z$, 所以 ** 展开为

$$\begin{cases} (E-\sigma_z p_z)\chi_+(p_z) = m\chi_-(p_z) \\ (E+\sigma_z p_z)\chi_-(p_z) = m\chi_+(p_z) \end{cases} \Rightarrow \begin{cases} (E-\vec\sigma\cdot\vec p)\chi_+(\vec p) = m\chi_-(\vec p) \\ (E+\vec\sigma\cdot\vec p)\chi_-(\vec p) = m\chi_+(\vec p) \end{cases}$$

1. 0 质量粒子. 此时 $\chi_\pm$ 去耦合, 即 $(E\mp\vec\sigma\cdot\vec p)\,\chi_\pm = 0$. 根据能动关系, $m=0$ 时 $E=|\vec p|$, 所以同除 $|\vec p|$ 进行归一化:

$$\begin{aligned} &\left(1\mp\hat{\vec p}\cdot\vec\sigma\right)\chi_\pm(\vec p) = 0, \quad \hat{\vec p} = \frac{\vec p}{|\vec p|}, \quad \text{螺旋度算符: } \frac{1}{2}\hat{\vec p}\cdot\vec\sigma \\ &\Rightarrow \frac{1}{2}\hat{\vec p}\cdot\vec\sigma\chi_\pm(\vec p) = \pm\frac{1}{2}\chi_\pm(\vec p) \end{aligned}$$

2. 一次量子化 $\vec p\to -i\nabla$, $E = i\partial_t$, 得到坐标表象的 Dirac 方程:

$$\begin{aligned} \left(\partial_t \pm \vec\sigma\cdot\vec\nabla\right)\varphi_\pm(\vec r,t) + im\varphi_\mp(\vec r,t) &= 0 \\ \varphi_\pm(\vec r,t) = \int \mathrm{d}^3\vec p e^{-iEt}e^{i\vec p\cdot\vec r}\chi_\pm(\vec p), &\quad E = \sqrt{p^2+m^2} \end{aligned}$$

3. Dirac 方程的协变性. Dirac 旋量定义为 $\psi = \begin{pmatrix}\varphi_+\\ \varphi_-\end{pmatrix} = \begin{pmatrix}\varphi_{+1}\\ \varphi_{+2}\\ \varphi_{-1}\\ \varphi_{-2}\end{pmatrix} \equiv \begin{pmatrix}\psi_1\\ \psi_2\\ \psi_3\\ \psi_4\end{pmatrix}$. 现在引入 γ 矩阵以进行后续讨论, 它被定义为

$$\gamma^i = \begin{pmatrix}0 & \sigma^i\\ -\sigma^i & 0\end{pmatrix} \equiv -\gamma_i, \quad \gamma^0 = \begin{pmatrix}I & 0\\ 0 & -I\end{pmatrix}.$$

定义 $\Sigma^i = \sigma^{3i}, \quad i = \{1,2,3\}$, 则 Dirac 旋量满足的方程为

$$\left(\frac{\partial}{\partial t} - \Sigma^i\frac{\partial}{\partial x^i}\cdot\vec\nabla + im\gamma^0\right)\psi = 0$$

利用协变 4-梯度 $\frac{\partial}{\partial x^\mu} \equiv \partial_\mu = (\partial_t,\nabla)$ 和逆变 4-梯度 $\frac{\partial}{\partial x_\mu} \equiv \partial^\mu = (\partial_t,-\nabla)$, 将 Dirac 化为协变形式

$$(i\gamma^\mu\partial_\mu - m)\,\psi = 0$$

(a) Dirac 方程与 Klein-Gordon 方程. 通过左乘 $(-i\gamma^\mu\partial_{mu} - m)$, 将方程化为 $(\partial^\mu\partial_\mu + m^2)\psi = 0$. 代入平面波解, 即有

$$\begin{aligned} \gamma^\mu p_\mu - m = 0 &\Rightarrow E = \gamma^0\vec\gamma\cdot\vec p + \gamma^0 m \\ &\Rightarrow \hat H = \vec\alpha\cdot\vec p + \beta m, \quad \alpha_i \equiv \gamma^0\gamma^i, \quad \beta\equiv\gamma^0 \end{aligned}$$

(b) 电磁场. 引入 $\begin{cases} p_\mu \to p_\mu - qA_\mu \\ i\partial_\mu \to i\partial_\mu - qA_\mu \\ D_\mu \equiv \partial_\mu + iqA_\mu \end{cases}$, 有电磁场中的 Dirac 方程为

$$(i\gamma^\mu D_\mu - m)\psi = 0$$

通过约定 $(P_0, \vec{P}) \equiv i\partial^\mu - qA^\mu = (i\partial_t - q\phi, -i\nabla - q\vec{A})$ 分离时空导数, 得到 Weyl 旋量形式的 Dirac 方程:

$$(P^0 \mp \vec{P} \cdot \vec{\sigma})\varphi_\pm = m\varphi_\mp$$

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 $\lambda_1 \neq \lambda_2$).$\square$

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

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

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

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

   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 $L_i = \epsilon_{ijk}x_jp_k$ and $K_i = wp_i - x_ip_w$ 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) $K_i = w p_i - x_i p_w$.

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

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

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) $[K_i, K_j]$.

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

So combine the terms we derived, we have

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

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 $\dfrac{1}{k_B T}$ as β for simplicity. Since the energy eigenvalues are given by $E_n = \left(n + \dfrac{1}{2}\right)\hbar\omega$, 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

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

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 $S^x = \frac{1}{2}(a^\dagger b + b^\dagger a)$, $S^z = \frac{1}{2}(a^\dagger a - b^\dagger b)$.

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

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:

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

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

$$H_{\text{chain}} = -t\sum_{n=1}^{L}\left(\hat{a}_n^\dagger \hat{a}_{n+1} + \hat{a}_{n+1}^\dagger \hat{a}\right), \quad \hat{a}_{L+1} = \hat{a}_1$$

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

   So the commutator

$$[H_{\text{chain}}, b_k^\dagger] = -t\sum_{n=1}^{L}\left(\left[a_n^\dagger a_{n+1}, b_k^\dagger\right] + \left[a_{n+1}^\dagger a_n, b_k^\dagger\right]\right)$$

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

   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:

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

where:

- $c_{i\sigma}^\dagger$ **and** $c_{i\sigma}$ **are the fermionic creation and annihilation operators for an eletron with spin** σ **at site** i**.**
- $n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}$ **is the number operator for electrons with spin** σ **at site** i**.**
- $n_i = \sum_\sigma c_{i\sigma}^\dagger c_{i\sigma}$ **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

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

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

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

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

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 $E_{\text{MF}} \approx -\frac{4t^2}{U}+V$. 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:

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

$$i\hbar\frac{\partial}{\partial t}\left[\psi e^{if(\vec{r},t)}\right] = \left[i\hbar\frac{\partial\psi}{\partial t} - \hbar\psi\frac{\partial f}{\partial t}\right]e^{if(\vec{r},t)}$$

$$\vec{\nabla}\left(\psi e^{if(\vec{r},t)}\right) = \left(\vec{\nabla}\psi + \psi i\vec{\nabla}f\right)e^{if(\vec{r},t)}$$

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

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

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 $f = \dfrac{-q\Lambda}{\hbar}$, 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 $\hat{H} = \hbar\omega\left(\hat{n}_1 + \hat{n}_2 + \dfrac{1}{2}\right)$, 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 $|\psi\rangle = \dfrac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)$, 计算可得量子比特 A 的纠缠熵为?**

密度矩阵为

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

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

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

由于 ρ_A 已经是对角阵, 所以对角线上元素即为特征值 $\lambda_{A,i}$. 计算 ρ_A 的纠缠熵:

$$
\begin{aligned}
S(A) &= -\mathrm{Tr}[\rho_A\ln\rho_A] = -\sum_i^{\uparrow,\downarrow}\lambda_{A,i}\ln\lambda_{A,i} \\
&= -\left(\frac{1}{2}\ln\frac{1}{2} + \frac{1}{2}\ln\frac{1}{2}\right) = \boxed{\ln 2 = 1\text{ bit}}
\end{aligned}
$$

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

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

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

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

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 $\hbar(\mathrm{kg\cdot m^2/s}),c(\mathrm{m/s})$ 来进行量纲变换

(a) 距离. $\dfrac{E}{\hbar c}=\dfrac{\mathrm{kg\cdot m^2/s^2}}{\mathrm{kg\cdot m^2/s\cdot m/s}}=\dfrac{1}{\mathrm{m}}$, 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 $\lambda=\pm1$. 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 $N=\sum_\alpha b_\alpha^\dagger b_\alpha$ 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 $[N,A]=\sum_i\left[b_i^\dagger b_i,A\right]=\sum_i\left\{b_i^\dagger[b_i,A]+\left[b_i^\dagger,A\right]b_i\right\}$, 代入以上各算符 A 判断是否对易.

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

(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

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

   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?

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

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

$$\left|\left|\int_0^t \mathrm{d}t' e^{\mathrm{i}\Delta\omega t'}\right|\right|^2=\left|\left|\frac{e^{\mathrm{i}\Delta\omega t}-1}{\mathrm{i}\omega}\right|\right|^2=\frac{(e^{\mathrm{i}\Delta\omega t}-1)(e^{-\mathrm{i}\Delta\omega t}-1)}{(\Delta\omega)^2}=\frac{2-2\cos\Delta t}{(\Delta\omega)^2}=\frac{4}{(\Delta\omega)^2}\sin^2\left(\frac{\Delta\omega t}{2}\right)$$

$$P_{i\to f}(t)=\boxed{\frac{4\left|\langle f|V|i\rangle\right|^2}{\hbar^2(\Delta\omega)^2}\sin^2\left(\frac{\Delta\omega t}{2}\right)}$$

3. *算符 $\Omega(t)\equiv U^{-1}(t)U_0(t)$, 算符 $\Omega_\pm\equiv\lim\limits_{t\to\mp\infty}\Omega(t)$, 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

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

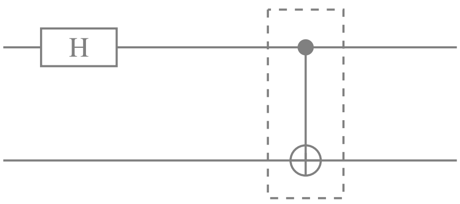
   定义螺旋度算符为 $\dfrac{1}{2}\hat{\vec p}\cdot\vec\sigma$, 其中 $\hat{\vec p}=\dfrac{\vec p}{|\vec p|}$, 那么可知 Weyl 旋量 $\chi_\pm$ 恰好是螺旋度算符的本征态, 本征值分别为?

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

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

   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,

   $$H=\frac{1}{\sqrt2}\begin{pmatrix}1&1\\1&-1\end{pmatrix},$$
   $$\mathrm{CNOT}=\exp\left\{\mathrm{i}\pi\frac{1}{4}(\mathbb{I}-\sigma_1^z)\otimes(\mathbb{I}-\sigma_2^x)\right\}$$

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

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

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.

根据 $J=0$, 而 $-|J|\le M\le |J|$, 夹逼定理得到 $M=0$. 而磁量子数守恒, 所以 $J_{1,z}+J_{2,z}=J_z=0$. 已知 C-G 系数可以用于将 $|J,M;j_1,j_2\rangle$ 以基矢 $|j_1,m_1;j_2,m_2\rangle$ 展开, 代入上述讨论结果有

$$|0,0;j,j\rangle=\sum_{m,-m}^{-j\le m\le j} C^{0,0}_{j,j,m,-m}|j,m;j,-m\rangle$$

概率即为 $P(m_1=m,m_2=-m)=|C^{0,0}_{j,j,m,-m}|^2$. 那么问题就来到如何计算这个特殊的 C-G 系数. 根据 C-G 系数的递推定义, 可以得到其解析表达式

$$
\begin{aligned}
& \langle j_1,m_1;j_2,m_2|J,M;j_1,j_2\rangle \\
& =\sqrt{\frac{(2J+1)(J+j_1-j_2)!(J-j_1+j_2)!(j_1+j_2-J)!}{(j_1+j_2+J+1)!}} \\
& \times\sqrt{(J+M)!(J-M)!(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!} \\
& \times\sum_{k_{\min}}^{k_{\max}}\frac{(-1)^k}{k!(j_1+j_2-J-k)!(j_1-m_1-k)!(j_2+m_2-k)!(J-M-k)!} \\
& \times\frac{1}{(J-j_2+m_1+k)!(J-j_1-m_2+k)!}
\end{aligned}
$$

$$k_{\min}=\max\{0,j_2-m_1-J,j_1+m_2-J\}, \quad k_{\max}=\min\{j_1+j_2-J,j_1-m_1,j_2+m_2\}$$

所以代入 $j_1 = j_2 = j$, $m_1 = -m_2 = m$, 即有 $C^{0,0}_{j,m,j,-m} = \frac{(-1)^{j-m}}{\sqrt{2j+1}}$, 显然因为平方消去了可能存在的负号, 使得 $|j,m;j,-m\rangle$, $\quad \forall m \in \{-j,-j+1,\cdots,j-1,j\}$ 等概率, 所以得到

$$\boxed{P(m_1 = m, m_2 = -m) = \frac{1}{2j+1}}$$

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.**

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

注意到 m^2 会带来 $m = \pm 1$ 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 $E_m^{(n)} = \sum_{n\neq m} \frac{|\langle n|V|m\rangle|^2}{E_m^{(0)} - E_n^{(0)}}$ 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.**

分离变量法求解薛定谔方程 $\frac{\hbar^2\hat{k}^2}{2m}\psi = E\psi$. 于是能量本征值为 $\frac{\hbar^2 k^2}{2m} = \sum_i \frac{\hbar^2 k_i^2}{2m}$, 其中 $k_i = \frac{\sqrt{2mE_i}}{\hbar}$. 由于使用了箱归一化, 即有边界条件 $k_i l_i = n_i\pi (n_i \in \mathbb{N}^*)$, 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 $\prod_i^3 \frac{\pi}{l_i} = \frac{\pi^3}{l_x l_y l_z} = \frac{\pi^3}{V}$, 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 $|k| \le k_F$. 由于前面讨论 $k_i \in \mathbb{N}^*$, 因此 $k \le k_F$ 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

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

接下来计算总能量. 假设 N 充分大, 使得电子可存在的状态遍布整个半径为 k_F 的 $\frac{1}{8}$ 费米球, 于是求和化为积分形式, 即有 $E_{\text{tot}} = \sum_i^{k\le k_F} \frac{\hbar^2 k^2}{2m} \Rightarrow \int_0^{k_F} \frac{\hbar^2 k^2}{2m} f(k)\mathrm{d}k$, 其中 $f(k)$ 是态密度, 表示在同一能量 $\frac{\hbar^2 k^2}{2m}$ 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

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

因此总能量为

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

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:

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

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

(b) **计算能量的一阶修正 $E^{(1)} = \langle \mathbf{FS}|H_I|\mathbf{FS}\rangle$.**
题目中定义的傅里叶变换是非幺正的, 代入结论的时候需要注意系数.

$$v(\vec{q}) = \frac{1}{V}\int \frac{1}{|\vec{x}|}e^{i\vec{q}\cdot\vec{x}}\mathrm{d}\vec{x} = \frac{1}{V}\frac{4\pi}{q^2}$$

代 $v(\vec{q})$ 入两体相互作用部分, 有

$$H_I = \frac{1}{2V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}}\sum_{\sigma,\sigma'}\frac{1}{V}\frac{4\pi}{q^2}c^\dagger_{\vec{k}_1+\vec{q},\sigma}c^\dagger_{\vec{k}_2-\vec{q},\sigma'}c_{\vec{k}_2,\sigma'}c_{\vec{k}_1,\sigma}$$

(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.**
代 $|\mathrm{HF}\rangle = \prod_{k\le k_F,\sigma}c^\dagger_{\vec{k},\sigma}|0\rangle$ 入能量一阶修正, 有

$$\langle\mathrm{HF}|H_0|\mathrm{HF}\rangle = \sum_{\vec{k},\sigma}\langle\mathrm{HF}|\frac{k^2}{2}c^\dagger_{\vec{k},\sigma}c_{\vec{k},\sigma}|\mathrm{HF}\rangle$$

$$\begin{aligned}
\langle\mathrm{HF}|H_I|\mathrm{HF}\rangle &= \frac{1}{2V}\frac{4\pi}{V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}}\sum_{\sigma,\sigma'}\frac{1}{q^2}\langle\mathrm{HF}|\underbrace{c^\dagger_{\vec{k}_1+\vec{q},\sigma}c^\dagger_{\vec{k}_2-\vec{q},\sigma'}c_{\vec{k}_2,\sigma'}c_{\vec{k}_1,\sigma}}_{c^\dagger_\lambda c^\dagger_\mu c_\rho c_\nu}|\mathrm{HF}\rangle \\
&= \frac{1}{2V}\frac{4\pi}{V}\sum_{\vec{k}_1,\vec{k}_2,\vec{q}}\sum_{\sigma,\sigma'}\frac{1}{q^2}(\cancel{\delta_{\vec{k}_1+\vec{q},\vec{k}_1}\delta_{\vec{k}_2-\vec{q},\vec{k}_2}} - \delta_{\vec{k}_1+\vec{q},\vec{k}_2}\delta_{\sigma,\sigma'}\delta_{\vec{k}_2-\vec{q},\vec{k}_1}\delta_{\sigma',\sigma}), \quad v(\vec{q}=0)\text{不发散} \\
&= -\frac{1}{2V}\frac{4\pi}{V}\sum_{\vec{k}_1}\sum_{\vec{k}_2}\sum_{\vec{q}}\sum_{\sigma}\sum_{\sigma'}\frac{1}{q^2}\delta_{\vec{k}_1+\vec{q},\vec{k}_2}\delta_{\vec{k}_2-\vec{q},\vec{k}_1}\delta_{\sigma',\sigma}\delta_{\sigma,\sigma'} \\
&= -\frac{1}{2V}\frac{4\pi}{V}\sum_{\vec{k}_1}\sum_{\vec{k}_2}\sum_{\vec{q}}\sum_{\sigma}\frac{1}{q^2}\delta_{\vec{k}_1+\vec{q},\vec{k}_2}\delta_{\vec{k}_2-\vec{q},\vec{k}_1} \\
&= -\frac{1}{V}\frac{4\pi}{V}\sum_{\vec{k}_1}\sum_{\vec{k}_2}\sum_{\vec{q}}\frac{1}{q^2}\delta_{\vec{k}_1+\vec{q},\vec{k}_2}\delta_{\vec{k}_2-\vec{q},\vec{k}_1} \\
&= -\frac{1}{V}\frac{4\pi}{V}\sum_{\vec{k}_1}\sum_{\vec{k}_2}\int\mathrm{d}\vec{q}\frac{V}{(2\pi)^3}\frac{1}{q^2}\delta_{\vec{q},\vec{k}_2-\vec{k}_1}\delta_{\vec{q},\vec{k}_2-\vec{k}_1} \\
&= -\frac{1}{V}\sum_{\vec{k}_1}\sum_{\vec{k}_2}\frac{4\pi}{|\vec{k}_1-\vec{k}_2|^2}
\end{aligned}$$

在第二行消去了一项, 这是因为它会引起 $\vec{q}=0$. 有关于最后一行的求和, 这是一个固定结论, 没有必要在考场现场计算求和, 在这里直接给出答案:

$$\begin{aligned}
\langle\mathrm{HF}|H_I|\mathrm{HF}\rangle = -\frac{k_F^3V}{4\pi^3} &= -\frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}n^{\frac{4}{3}}V \\
\Rightarrow E &= \frac{(3n)^{\frac{5}{3}}\pi^{\frac{4}{3}}V}{10} - \frac{3}{4}\left(\frac{3}{\pi}\right)^{\frac{1}{3}}n^{\frac{4}{3}}V
\end{aligned}$$

6. 量子转子模型

量子转子的角度坐标 $\theta\in[0,2\pi)$, 注意 $\theta\pm2\pi$ 和 θ 是等价的. 用 $|\theta\rangle$ 表现 $\hat{\theta}$ 算符的本征态, $|\theta\pm2\pi\rangle$ 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

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

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.