ADVANCED QUANTUM MECHANICS

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Contents

第一章 Homework

1.1 Homework 1

1.1.1 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

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

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

$$A|v\rangle = \lambda|v\rangle,$$
$$AB|v\rangle = BA|v\rangle = B\lambda|v\rangle = \lambda\left(B|v\rangle\right),$$

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. $\square$

1.1.2 Matrix diagonalization and unitary transformation

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

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

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

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

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

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

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

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

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

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 $\vec{S} = \dfrac{\hbar}{2}\vec{\sigma}$, 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

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

   So the basis vectors in the S^x representation are

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

1.2   Homework 2

1.2.1   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

$$[L_i, x_j] = \left[\sum_{kl} \epsilon_{ikl} x_k p_l, x_j \right] = \sum_{kl} \epsilon_{ikl} [x_k p_l, x_j]$$

$$= \sum_{kl} \epsilon_{ikl} (x_k [p_l, x_j] + \cancel{[x_k, x_j]} p_l) = \sum_{kl} \epsilon_{ikl} x_k (-i\hbar \delta_{lj})$$

$$= \sum_k \epsilon_{ikj} x_k (-i\hbar) = \boxed{i\hbar \sum_k \epsilon_{ijk} x_k}.$$

So we have

$$[L_i, R^2] = [L_i, x^2 + y^2 + z^2 + w^2] = [L_i, x^2] + [L_i, y^2] + [L_i, z^2] + [L_i, w^2],$$

$$[L_i, x_j^2] = [L_i, x_j x_j] = x_j [L_i, x_j] + [L_i, x_j] x_j = x_j \left[i\hbar \sum_k \epsilon_{ijk} x_k \right] + \left[i\hbar \sum_k \epsilon_{ijk} x_k \right] x_j$$

$$= 2i\hbar \sum_k \epsilon_{ijk} x_j x_k$$

$$\left[L_i, \sum_j^3 x_j^2 \right] = \sum_j^3 [L_i, x_j^2] = 2i\hbar \sum_{jk} \epsilon_{ijk} x_j x_k = 0, \quad \text{since } j \leftrightarrow k \text{ symmetry}$$

$$[L_i, w^2] = [L_i, ww] = w[L_i, w] + [L_i, w]w = 0.$$

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:

$$[K_i, R^2] = [K_i, x^2 + y^2 + z^2 + w^2] = \sum_j^3 [K_i, x_j^2] + [K_i, w^2]$$

$$[K_i, w^2] = [K_i, w]w + w[K_i, w]$$

$$[K_i, w] = [w p_i - x_i p_w, w] = \left[w \left(-i\hbar \frac{\partial}{\partial x_i} \right) - x_i \left(-i\hbar \frac{\partial}{\partial w} \right), w \right]$$

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

$$\left[w \left(-i\hbar \frac{\partial}{\partial x_i} \right) - x_i \left(-i\hbar \frac{\partial}{\partial w} \right), w \right] f = (-i\hbar) \left[w \frac{\partial}{\partial x_i} - x_i \frac{\partial}{\partial w}, w \right] f$$

$$= (-i\hbar) \left\{ \left(w \frac{\partial}{\partial x_i} - x_i \frac{\partial}{\partial w} \right) (wf) - w \left(w \frac{\partial f}{\partial x_i} - x_i \frac{\partial f}{\partial w} \right) \right\}$$

$$= (-i\hbar)(-x_i) f$$

$$\Rightarrow \boxed{[K_i, w] = i\hbar x_i}$$

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

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

Thus we have

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

$\square$

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

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

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

For the other term, we have

$$[L_i, x_j p_w] = x_j[L_i, p_w] + [L_i, x_j]p_w$$

$$[L_i, x_j] = \left[\sum_{kl} \epsilon_{ikl} x_k p_l, x_j\right] = \sum_{kl} \epsilon_{ikl}[x_k p_l, x_j]$$

$$= \sum_{kl} \epsilon_{ikl}(x_k[p_l, x_j] + \cancel{[x_k, x_j]p_l}) = \sum_{kl} \epsilon_{ikl} x_k(-i\hbar\delta_{lj})$$

$$= \sum_k \epsilon_{ikj} x_k(-i\hbar) = i\hbar\sum_k \epsilon_{ijk} x_k,$$

$$[L_i, p_w] = \sum_{jk} \epsilon_{ijk}[x_j p_k, p_w] = \sum_{jk} \epsilon_{ijk}(x_j[p_k, p_w] + [x_j, p_w]p_k) = \epsilon_{ijk}(x_j \cdot 0 + 0 \cdot p_k) = 0$$

$$\Rightarrow [L_i, x_j p_w] = x_j \cdot 0 + i\hbar\sum_k \epsilon_{ijk} x_k \cdot p_w = \boxed{i\hbar\sum_k \epsilon_{ijk} x_k p_w}$$

Combining the terms we derived, we have

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

(b) $[K_i, K_j]$.

$$[K_i, K_j] = [wp_i - x_i p_w, wp_j - x_j p_w] = [wp_i, wp_j] - [wp_i, x_j p_w] - [x_i p_w, wp_j] + [x_i p_w, x_j p_w]$$

$$[wp_i, wp_j] = w^2[p_i, p_j] = 0;$$

$$[wp_i, x_j p_w] = x_j(w\cancel{[p_i, p_w]} + [w, p_w]p_i) + (w[p_i, x_j] + \cancel{[w, x_j]p_i})p_w = x_j i\hbar p_i + w(-i\hbar)\delta_{ij} p_w$$

$$= i\hbar(x_j p_i - \delta_{ij} wp_w)$$

$$[x_i p_w, wp_j] = w(x_i\cancel{[p_w, p_j]} + [x_i, p_j]p_w) + (x_i[p_w, w] + \cancel{[x_i, w]p_w})p_j = wi\hbar\delta_{ij} p_w + x_i(-i\hbar)p_j$$

$$= i\hbar(wp_w\delta_{ij} - x_i p_j)$$

$$[x_i p_w, x_j p_w] = 0$$

So combine the terms we derived, we have

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

1.2.2　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

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

And the energy eigenvalues E_n are given by

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

The corresponding wave functions $\psi_n(x)$ are given by

$$\psi_n(x) = \frac{1}{\sqrt{2^n n!}} \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}} H_n \left(\sqrt{\frac{m\omega}{\hbar}} x \right)$$

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:

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}} \left(a + a^\dagger \right), \quad \hat{p} = i\sqrt{\frac{\hbar m\omega}{2}} \left(a^\dagger - a \right)$$

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(a + a^\dagger)^2 = \frac{\hbar}{2m\omega}(a^2 + a^{\dagger 2} + a^\dagger a + a a^\dagger)$$

$$\hat{p}^2 = -\frac{\hbar m\omega}{2}(a^\dagger - a)^2 = -\frac{\hbar m\omega}{2}(a^{\dagger 2} - a^\dagger a - a a^\dagger + a^2)$$

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

$$\langle m|\hat{x}|n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \left(\langle m|a|n \rangle + \langle m|a^\dagger|n \rangle \right) = \sqrt{\frac{\hbar}{2m\omega}} \left(\langle m|\sqrt{n}|n-1 \rangle + \langle m|\sqrt{n+1}|n+1 \rangle \right)$$

$$= \boxed{\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1})}$$

$$\langle m|\hat{p}|n \rangle = i\sqrt{\frac{\hbar m\omega}{2}}(\langle m|a^\dagger|n \rangle - \langle m|a|n \rangle) = i\sqrt{\frac{\hbar m\omega}{2}}(\langle m|\sqrt{n+1}|n+1 \rangle - \langle m|\sqrt{n}|n-1 \rangle)$$

$$= \boxed{i\sqrt{\frac{\hbar m\omega}{2}}(\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1})}$$

$$\langle m|\hat{x}^2|n \rangle = \frac{\hbar}{2m\omega}(\langle m|a^2|n \rangle + \langle m|a^{\dagger 2}|n \rangle + \langle m|a^\dagger a|n \rangle + \langle m|a a^\dagger|n \rangle)$$

$$= \frac{\hbar}{2m\omega}(\langle m|\sqrt{n(n-1)}|n-2 \rangle + \langle m|\sqrt{(n+1)(n+2)}|n+2 \rangle + \langle m|n|n \rangle + \langle m|n+1|n \rangle)$$

$$= \boxed{\frac{\hbar}{2m\omega}(\sqrt{n(n-1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + n\delta_{m,n} + (2n+1)\delta_{m,n})}$$

$$\langle m|\hat{p}^2|n \rangle = -\frac{\hbar m\omega}{2} \left(\langle m|a^{\dagger 2}|n \rangle - \langle m|2a^\dagger a|n \rangle + \langle m|a^2|n \rangle - \langle m|1|n \rangle \right)$$

$$= \boxed{-\frac{\hbar m\omega}{2}(\sqrt{(n+1)(n+2)}\delta_{m,n+2} - (2n+1)2n\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2})}$$

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

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

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

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

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

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

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

$$= -\left(-\frac{1}{2}\hbar\omega - \frac{1}{1-e^{-\beta\hbar\omega}}(-e^{-\beta\hbar\omega})(-\hbar\omega)\right)$$

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

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

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

The coherent states are given by

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

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

So the inner product could be derived as

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

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

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

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

1.3　Homework 3

1.3.1　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

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

$$= \frac{1}{4i}[a^\dagger a - b^\dagger b, a^\dagger b + b^\dagger a]$$

We have commutation formula that

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$
$$[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$
$$[\hat{A}, \hat{B}\hat{C}] = \hat{B}[\hat{A}, \hat{C}] + [\hat{A}, \hat{B}]\hat{C}$$
$$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}$$
$$\Rightarrow [\hat{A}\hat{B}, \hat{C}\hat{D}] = \hat{A}\hat{C}[\hat{B}, \hat{D}] + \hat{A}[\hat{B}, \hat{C}]\hat{D} + \hat{C}[\hat{A}, \hat{D}]\hat{B} + [\hat{A}, \hat{C}]\hat{D}\hat{B}$$

So we have

$$S^y = \frac{1}{4i}\left[a^\dagger a, a^\dagger b\right] + \frac{1}{4i}\left[a^\dagger a, b^\dagger a\right] - \frac{1}{4i}\left[b^\dagger b, a^\dagger b\right] - \frac{1}{4i}\left[b^\dagger b, b^\dagger a\right]$$

$$[a^\dagger a, a^\dagger b] = a^\dagger a^\dagger [a, b] + a^\dagger [a, a^\dagger] b + a^\dagger [a^\dagger, b] a + [a^\dagger, a^\dagger] b a = a^\dagger b$$

$$[a^\dagger a, b^\dagger a] = a^\dagger b^\dagger [a, a] + a^\dagger [a, b^\dagger] a + b^\dagger [a^\dagger, a] a + [a^\dagger, b^\dagger] a a = -b^\dagger a$$

$$[b^\dagger b, a^\dagger b] = b^\dagger a^\dagger [b, b] + b^\dagger [b, a^\dagger] b + a^\dagger [b^\dagger, b] b + [b^\dagger, a^\dagger] b b = -a^\dagger b$$

$$[b^\dagger b, b^\dagger a] = b^\dagger b^\dagger [b, a] + b^\dagger [b, b^\dagger] a + b^\dagger [b^\dagger, a] b + [b^\dagger, b^\dagger] a b = b^\dagger a$$

$$\Rightarrow S^y = \frac{1}{4i}\left(a^\dagger b - b^\dagger a + a^\dagger b - b^\dagger a\right) = \boxed{\frac{1}{2i}\left(a^\dagger b - b^\dagger a\right)}$$

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

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

So the angular momentum operator is

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

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

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

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

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

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

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

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

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

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

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

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

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

So we have

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

Combine the above results, and we have

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

$\square$

1.3.2　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

   $$\{b_k, b_{k'}^\dagger\} = \frac{1}{L} \sum_{n,n'} e^{-ikn} e^{ik'n'} \{a_n, a_{n'}^\dagger\} = \frac{1}{L} \sum_{n,n'} e^{-ikn} e^{ik'n'} \delta_{nn'}$$

   $$= \frac{1}{L} \sum_{n=1}^{L} e^{-ikn} e^{ik'n} = \frac{1}{L} \sum_{n=1}^{L} e^{i(k'-k)n} = \boxed{\delta_{kk'}}$$

   $$\{b_k, b_{k'}\} = \frac{1}{L} \sum_{n,n'} e^{-ikn} e^{-ik'n'} \{a_n, a_{n'}\} = \boxed{0}$$

   $$\{b_k^\dagger, b_{k'}^\dagger\} = \frac{1}{L} \sum_{n,n'} e^{ikn} e^{ik'n'} \{a_n^\dagger, a_{n'}^\dagger\} = \boxed{0}$$

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

   $$\frac{1}{\sqrt{L}} \sum_k e^{-ikn} b_k^\dagger = \frac{1}{\sqrt{L}} \sum_k e^{-ikn} \left(\frac{1}{\sqrt{L}} \sum_{n'} e^{ikn'} a_{n'}^\dagger \right)$$

   $$= \frac{1}{L} \sum_{n'} \sum_k e^{ik(n'-n)} a_{n'}^\dagger = \sum_{n'} \left(\frac{1}{L} \sum_k e^{ik(n'-n)} \right) a_{n'}^\dagger$$

   $$= \sum_{n'} (\delta_{nn'}) a_{n'}^\dagger = a_n^\dagger. \quad \square$$

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

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

$$\left[a_n^\dagger a_{n+1}, b_k^\dagger \right] = a_n^\dagger \left[a_{n+1}, b_k^\dagger \right] = a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \left[a_{n+1}, a_m^\dagger \right]$$

$$= a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \delta_{n+1,m} = a_n^\dagger \frac{1}{\sqrt{L}} e^{ik(n+1)}$$

$$\left[a_{n+1}^\dagger a_n, b_k^\dagger \right] = a_{n+1}^\dagger \left[a_n, b_k^\dagger \right] = a_{n+1}^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \left[a_n, a_m^\dagger \right]$$

$$= a_{n+1}^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \delta_{n,m} = a_{n+1}^\dagger \frac{1}{\sqrt{L}} e^{ikn}$$

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

$$= -t \left(e^{ik} \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ikn} a_n^\dagger + e^{-ik} \frac{1}{\sqrt{L}} \sum_{n=1}^{L} e^{ik(n+1)} a_{n+1}^\dagger \right)$$

$$= -t \left(e^{ik} b_k^\dagger + e^{-ik} b_k^\dagger \right) = \boxed{-2t \cos k} \, b_k^\dagger$$

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

1.4　Homework 4

1.4.1　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

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

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

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

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

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

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

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

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

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

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

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

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

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

13

(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 $E_{\text{MF}} = -2t + \dfrac{U}{2} + V$.

(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

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

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

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

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

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

and the self-consistent equation is

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

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

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

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

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

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

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

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

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

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

1.5　Homework 5

1.5.1　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

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

   $$\iff \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta - 2\pi)}|\theta\rangle = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} \mathrm{d}\theta e^{iN(\theta - 2\pi)}|\theta\rangle$$

   $$\iff e^{iN\theta} = e^{iN(\theta - 2\pi)} = e^{iN\theta}e^{-i2\pi N}$$

   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.**

$$\hat{H}_0|N\rangle = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2|N\rangle = \frac{1}{2}\left(N - \frac{1}{2}\right)^2|N\rangle \Rightarrow E_N^{(0)} = \frac{1}{2}\left(N - \frac{1}{2}\right)^2$$

$$\Rightarrow N_\pm - \frac{1}{2} = \pm\sqrt{2E_N^{(0)}} \Rightarrow N_\pm = \frac{1}{2} \pm \sqrt{2E_N^{(0)}}$$

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.**

$$\cos 2\hat{\theta} = \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)$$

$$e^{i2\hat{\theta}}|N\rangle = e^{i2\hat{\theta}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta\, e^{iN\theta}|\theta\rangle\right) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta\, e^{iN\theta}e^{i2\hat{\theta}}|\theta\rangle$$

$$= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta\, e^{i(N+2)\theta}|\theta\rangle = |N+2\rangle$$

$$\Rightarrow \cos 2\hat{\theta}|N\rangle = \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)|N\rangle = \frac{1}{2}\left(|N+2\rangle + |N-2\rangle\right)$$

$$\Rightarrow \langle N|\hat{V}|N'\rangle = -g\langle N|\cos 2\hat{\theta}|N'\rangle = -\frac{g}{2}\left(\langle N|N'+2\rangle + \langle N|N'-2\rangle\right)$$

$$= -\frac{g}{2}(\delta_{N,N'+2} + \delta_{N,N'-2})$$

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.**

$$E_N^{(1)} = \langle N|\hat{V}|N\rangle = -\frac{g}{2}\left(\langle N|N+2\rangle + \langle N|N-2\rangle\right) = 0$$

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

$$= \boxed{\frac{g^2}{(2N-3)(2N+1)}}$$

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

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

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

so the degeneracy of the energy levels remains unlifted.

第二章 2022秋高等量子力学期末考核

2.1 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 $\text{Tr}[\rho]$ 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 $\text{Tr}[\rho] = \sum_i p_i = \boxed{1}$

4. 如果 ρ 是混态的密度矩阵, 那么 $\text{Tr}[\rho^2]$ 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($p_n^2 = p_n$) $\text{Tr}[\rho^2] = \text{Tr}[\rho] = 1$, 而混态($p_n^2 \neq p_n$)则是 $\text{Tr}[\rho^2]\boxed{< 1}$.

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**?**

$$\frac{\mathrm{d}A_H(t)}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}Ae^{-iHt/\hbar}\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(e^{iHt/\hbar}\right)Ae^{-iHt/\hbar} + e^{iHt/\hbar}\frac{\mathrm{d}}{\mathrm{d}t}\left(Ae^{-iHt/\hbar}\right)$$

$$= \frac{iH}{\hbar}e^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}A\frac{iH}{\hbar}e^{-iHt/\hbar} = \frac{i}{\hbar}\left(He^{iHt/\hbar}Ae^{-iHt/\hbar} - e^{iHt/\hbar}Ae^{-iHt/\hbar}H\right)$$

$$= \frac{i}{\hbar}\left[H, A_H(t)\right] = \boxed{\frac{1}{i\hbar}\left[A_H(t), H\right]}$$

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:

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

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

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

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

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

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

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

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

展开变换前的薛定谔方程:

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

展开变换后的薛定谔方程:

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

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

$$+ \frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f) + \frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi - \frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi$$

$$+ \frac{i\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi) - \frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi + \frac{q^2}{2m}(\vec{A}-\vec{\nabla}\Lambda)^2\psi$$

$$\left. + q\left(\phi + \frac{\partial\Lambda}{\partial t}\right)\psi\right] \qquad \text{②}$$

② − ① · $e^{if(\vec{r},t)}$, 得到

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

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

$$+ \frac{-i\hbar^2}{2m}(\vec{\nabla}\psi)\cdot(\vec{\nabla}f) + \frac{\hbar^2}{2m}(\vec{\nabla}f)^2\psi - \frac{\hbar q}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi$$

$$+ \frac{i\hbar q}{2m}(\cancel{\vec{A}}-\vec{\nabla}\Lambda)(\vec{\nabla}\psi) - \frac{q\hbar}{2m}(\vec{A}-\vec{\nabla}\Lambda)\cdot(\vec{\nabla}f)\psi + \frac{q^2}{2m}\left(\cancel{A^2} + (\vec{\nabla}\Lambda)^2 - 2\vec{A}\cdot(\vec{\nabla}\Lambda)\right)\psi$$

$$\left. + q\left(\cancel{\phi} + \frac{\partial\Lambda}{\partial t}\right)\psi\right]$$

18

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

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

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

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

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

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

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

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

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

密度矩阵为

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

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

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

计算 ρ_A 的纠缠熵:

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

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

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

$$E[\Psi] = \left(\sum_m \langle\Psi|m\rangle\langle m|\right) \hat{H} \left(\sum_n |n\rangle\langle n|\Psi\rangle\right) = \sum_{m,n} \langle\Psi|m\rangle\langle m|\hat{H}|n\rangle\langle n|\Psi\rangle$$

$$= \sum_{m,n} c_m^* E_n \delta_{mn} c_n = \sum_n |c_n|^2 E_n \geq \sum_n |c_n|^2 E_0 = E_0$$

2.2　多项选择

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

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

$$[J^2, J_l] = [\sum_i^3 J_i^2, J_l] = \sum_i^3 [J_i^2, J_l] = \sum_i^3 \left(J_i[J_i, J_l] + [J_i, J_l]J_i\right)$$

$$= \sum_i^3 \left(J_i i\hbar\epsilon_{ilk}J_k + i\hbar\epsilon_{ilk}J_k J_i\right)$$

$$= i\hbar \sum_i^3 (\epsilon_{ilk}J_i J_k - \epsilon_{kli}J_k J_i) = 0.$$

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·m²/s², 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·m²/s. 现在要求 kg·m²/s=m/s=1, 即寻找如何通过除以 $\hbar(\text{kg}\cdot\text{m}^2/\text{s}), c(\text{m/s})$ 来进行量纲变换

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

(b) 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) 质量. $E = mc^2$.

(e) 角动量. 角动量的量纲正好是 kg·m²/s, 即无量纲数, 而能量无法通过除以 $\hbar$ 或 c 来变成角动量的量纲, 所以角动量和能量不同单位.

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

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

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

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

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

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

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

(b)

$$
\boxed{[N, b_\alpha^\dagger b_\alpha]} = \sum_i \left[b_i^\dagger b_i, b_\alpha^\dagger b_\alpha \right] = \sum_i \left\{ b_i^\dagger [b_i, b_\alpha^\dagger b_\alpha] + \left[b_i^\dagger, b_\alpha^\dagger b_\alpha \right] b_i \right\}
$$

$$
= \sum_i \left\{ b_i^\dagger \left(b_\alpha^\dagger [b_i, b_\alpha] + [b_i, b_\alpha^\dagger] b_\alpha \right) + \left(b_\alpha^\dagger [b_i^\dagger, b_\alpha] + [b_i^\dagger, b_\alpha^\dagger] b_\alpha \right) b_i \right\}
$$

$$
= \sum_i \left\{ b_i^\dagger (b_\alpha^\dagger \cdot 0 + \delta_{i\alpha} b_\alpha) + (b_\alpha^\dagger(-\delta_{i\alpha}) + 0 \cdot b_\alpha) b_i \right\}
$$

$$
= \sum_i \delta_{i\alpha}(b_i^\dagger b_\alpha - b_\alpha^\dagger b_i) = 0
$$

(c)

$$
\boxed{[N, b_\alpha^\dagger b_\beta]} = \sum_i \left[b_i^\dagger b_i, b_\alpha^\dagger b_\beta \right] = \sum_i \left\{ b_i^\dagger [b_i, b_\alpha^\dagger b_\beta] + \left[b_i^\dagger, b_\alpha^\dagger b_\beta \right] b_i \right\}
$$

$$
= \sum_i \left\{ b_i^\dagger (b_\alpha^\dagger [b_i, b_\beta] + [b_i, b_\alpha^\dagger] b_\beta) + (b_\alpha^\dagger [b_i^\dagger, b_\beta] + [b_i^\dagger, b_\alpha^\dagger] b_\beta) b_i \right\}
$$

$$
= \sum_i \left\{ b_i^\dagger (b_\alpha^\dagger \cdot 0 + \delta_{i\alpha} b_\beta) + (b_\alpha^\dagger(-\delta_{i\beta}) + 0 \cdot b_\beta) b_i \right\}
$$

$$
= \sum_i \left(b_i^\dagger b_\beta \delta_{i\alpha} - b_\alpha^\dagger b_i \delta_{i\beta} \right) = 0.
$$

(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.

2.3　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

$$
[\vec{L}, H] = \left[\sum_{ijk} \epsilon_{ijk} \hat{x}_i x_j p_k, \sum_\alpha \frac{p_\alpha^2}{2m} + r^n \right] = \frac{1}{2m} \sum_{ijk\alpha} \epsilon_{ijk} \hat{x}_i [x_j p_k, p_\alpha^2] + \sum_{ijk} \epsilon_{ijk} \hat{x}_i [x_j p_k, r^n]
$$

$$
= \frac{1}{2m} \sum_{ijk\alpha} \hat{x}_i \epsilon_{ijk} \left\{ x_j p_\alpha \cancel{[p_k, p_\alpha]} + x_j [p_k, p_\alpha] p_\alpha + p_\alpha [x_j, p_\alpha] p_k + [x_j, p_\alpha] p_\alpha p_k \right\} + \sum_{ijk} \epsilon_{ijk} \hat{x}_i x_j [-i\hbar \frac{\partial}{\partial x_k}, r^n]
$$

$$
= \frac{1}{2m} \sum_{ijk\alpha} 2i\hbar \delta_{j\alpha} p_\alpha p_k + \sum_{ijk} \epsilon_{ijk} \hat{x}_i x_j \left(-i\hbar n r^{n-1} r^{-\frac{1}{2}} x_k \right)
$$

$$
= \sum_{ijk} \epsilon_{ijk} \hat{x}_i \left\{ \frac{i\hbar}{m} p_j p_k + (-i\hbar n r^{n-\frac{3}{2}}) x_j x_k \right\}
$$

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**

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

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?

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

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

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

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

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

- $U_0(t) = e^{-\mathrm{i}H_0 t/\hbar}$ 是自由系统 H_0 的时间演化算符;
- $U(t) = e^{-\mathrm{i}Ht/\hbar}$ 是短程势散射系统的时间演化算符.

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

4. **动量空间中自由粒子的 Dirac 方程可以写为**

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

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

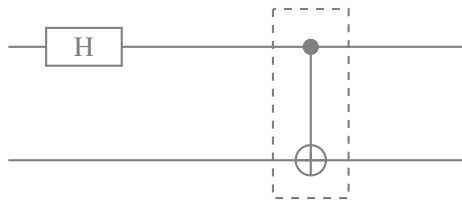$$(E - \vec{\sigma}\cdot\vec{p})\,\chi_+ = 0, \quad (E + \vec{\sigma}\cdot\vec{p})\,\chi_- = 0$$

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

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

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

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

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,

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

$$\mathrm{CNOT} = \exp\left\{\mathrm{i}\pi\frac{1}{4}(\mathbb{I} - \sigma_1^z)\otimes(\mathbb{I} - \sigma_2^x)\right\}$$

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

注意到

$$A = \frac{1}{4}(\mathbb{I} - \sigma_1^z) \otimes (\mathbb{I} - \sigma_2^x) = \frac{1}{4} \begin{pmatrix} & \\ & 2 \end{pmatrix} \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} & & & \\ & & & \\ & & \frac{1}{2} & -\frac{1}{2} \\ & & -\frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

$$A^2 = A$$

$$e^{i\alpha A} = \sum_{n=0}^{\infty} \frac{1}{n!}(i\alpha A)^n = \mathbb{I} + \sum_{n=1}^{\infty} \frac{1}{n!}(i\alpha)^n (A)^n = \mathbb{I} + A\left(\sum_{n=0}^{\infty} \frac{1}{n!}(i\alpha)^n - 1\right)$$

$$= \mathbb{I} + A(e^{i\alpha} - 1)$$

$$\Rightarrow \mathrm{CNOT} = \mathbb{I} - 2A = \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & & 1 \\ & & 1 & \end{pmatrix}.$$

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.

$$\left(\hat{H}_{(1)} \otimes \mathbb{I}_{(2)}\right) |\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} = \hat{H}_{(1)}|\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} = \left[\frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right] \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)} + |\downarrow\rangle_{(1)}) \otimes |\uparrow\rangle_{(2)} = \frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} + |\downarrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)}).$$

$$\mathrm{CNOT}\frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} + |\downarrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)}) = \frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} + \mathrm{CNOT}|\downarrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)})$$

$$= \frac{1}{\sqrt{2}}(|\uparrow\rangle_{(1)} \otimes |\uparrow\rangle_{(2)} + |\downarrow\rangle_{(1)} \otimes |\downarrow\rangle_{(2)}) = \boxed{\frac{1}{\sqrt{2}}(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)}, \quad \text{for simplicity.}$$

2.4　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 $|-\rangle^x_{(z)} = \dfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$. 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 $V = [|+\rangle^x_{(z)}, |-\rangle^x_{(z)}] = \dfrac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. 对角矩阵 Λ 对角线上依次是本征值, 即

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

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 $\vec{S} = \dfrac{\hbar}{2}\vec{\sigma}$, 其中 $\vec{\sigma}$ 的三个分量为 **Pauli** 矩阵 $\sigma^x, \sigma^y, \sigma^z$. 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

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

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

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

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.

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

(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;

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

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

$$\Rightarrow H = \frac{1}{2}\hbar\omega(P^2 + Q^2) = \frac{1}{2}\hbar\omega\left\{\left[\frac{1}{\sqrt{2}i}(a - a^\dagger)\right]^2 + \left[\frac{1}{\sqrt{2}}(a + a^\dagger)\right]^2\right\}$$

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

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

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

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

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

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

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

概率即为 $P(m_1 = m, m_2 = -m) = |C_{j,j,m,-m}^{0,0}|^2$. 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

$$\langle j_1, m_1; j_2, m_2 | J, M; j_1, j_2\rangle$$

$$= \sqrt{\frac{(2J+1)(J+j_1-j_2)!(J-j_1+j_2)!(j_1+j_2-J)!}{(j_1+j_2+J+1)!}}$$

$$\times \sqrt{(J+M)!(J-M)!(j_1+m_1)!(j_1-m_1)!(j_2+m_2)!(j_2-m_2)!}$$

$$\times \sum_{k_{\min}}^{k_{\max}} \frac{(-1)^k}{k!(j_1+j_2-J-k)!(j_1-m_1-k)!(j_2+m_2-k)!(J-M-k)!}$$

$$\times \frac{1}{(J-j_2+m_1+k)!(J-j_1-m_2+k)!}$$

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

所以代入 $j_1 = j_2 = j$, $m_1 = -m_2 = m$, 即有 $C_{j,m,j,-m}^{0,0} = \dfrac{(-1)^{j-m}}{\sqrt{2j+1}}$, 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.

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

(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.**

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

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:

$$V_{\text{sub}} = \begin{pmatrix} \langle 1,1|V|1,1 \rangle & \langle 1,1|V|1,-1 \rangle \\ \langle 1,-1|V|1,1 \rangle & \langle 1,-1|V|1,-1 \rangle \end{pmatrix}$$

$$\langle 1,1|V|1,1 \rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = 1,$$

$$\langle 1,1|V|1,-1 \rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & \frac{1}{\sqrt{2}} & \\ \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0,$$

$$\langle 1,-1|V|1,1 \rangle = 0,$$

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

$$\Rightarrow V_{\text{sub}} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

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

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

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

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

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

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

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

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

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 $|m\rangle^{(1)} = \sum\limits_{n \neq m} |n\rangle \dfrac{\langle n|V|m\rangle}{E_m^{(0)} - E_n^{(0)}}$ 给出:

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

$$= \boxed{\frac{1}{\sqrt{2}} |1,0\rangle}$$

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

$$= \boxed{\frac{1}{\sqrt{2}} (-|1,1\rangle + |1,-1\rangle)}$$

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

$$= \boxed{-\frac{1}{\sqrt{2}} |1,0\rangle}$$

总结:

$$E_1 = 1 + 1\lambda + \frac{1}{2}\lambda^2 + o(\lambda^2)$$

$$E_0 = 0 + 0\lambda - \frac{1}{2}\lambda^2 + o(\lambda^2)$$

$$E_{-1} = 1 - 1\lambda - \frac{1}{2}\lambda^2 + o(\lambda^2)$$

$$|1,1\rangle = |1,1\rangle + \frac{\lambda}{\sqrt{2}} |1,0\rangle + o(\lambda)$$

$$|1,0\rangle = |1,0\rangle + \frac{\lambda}{\sqrt{2}} (-|1,1\rangle + |1,-1\rangle) + o(\lambda)$$

$$|1,-1\rangle = |1,-1\rangle - \frac{\lambda}{\sqrt{2}} |1,0\rangle + o(\lambda)$$

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, $\vec{k} = \dfrac{2\pi}{L}(n_x, n_y, n_z)$, 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 $\varepsilon_{\vec{k}} = \dfrac{\hbar^2 \vec{k}^2}{2m}$ 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

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

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

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

$$\langle \mathrm{HF} | H_I | \mathrm{HF} \rangle = \frac{1}{2V} \frac{4\pi}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \sum_{\sigma, \sigma'} \frac{1}{q^2} \langle \mathrm{HF} | \underbrace{c^\dagger_{\vec{k}_1 + \vec{q}, \sigma} c^\dagger_{\vec{k}_2 - \vec{q}, \sigma'} c_{\vec{k}_2, \sigma'} c_{\vec{k}_1, \sigma}}_{c^\dagger_\lambda c^\dagger_\mu c_\rho c_\nu} | \mathrm{HF} \rangle$$

$$= \frac{1}{2V} \frac{4\pi}{V} \sum_{\vec{k}_1, \vec{k}_2, \vec{q}} \sum_{\sigma, \sigma'} \frac{1}{q^2} (\delta_{\vec{k}_1 + \vec{q}, \vec{k}_1} \cancel{\delta_{\vec{k}_2 - \vec{q}, \vec{k}_2}} - \delta_{\vec{k}_1 + \vec{q}, \vec{k}_2} \delta_{\sigma, \sigma'} \delta_{\vec{k}_2 - \vec{q}, \vec{k}_1} \delta_{\sigma', \sigma}), \quad v(\vec{q} = 0) \text{不发散}$$

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

$$= -\frac{1}{2V} \frac{4\pi}{V} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \sum_{\vec{q}} \sum_{\sigma} \frac{1}{q^2} \delta_{\vec{k}_1 + \vec{q}, \vec{k}_2} \delta_{\vec{k}_2 - \vec{q}, \vec{k}_1}$$

$$= -\frac{1}{V} \frac{4\pi}{V} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \sum_{\vec{q}} \frac{1}{q^2} \delta_{\vec{k}_1 + \vec{q}, \vec{k}_2} \delta_{\vec{k}_2 - \vec{q}, \vec{k}_1}$$

$$= -\frac{1}{V} \frac{4\pi}{V} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \int \mathrm{d}\vec{q} \frac{V}{(2\pi)^3} \frac{1}{q^2} \delta_{\vec{q}, \vec{k}_2 - \vec{k}_1} \delta_{\vec{q}, \vec{k}_2 - \vec{k}_1}$$

$$= -\frac{1}{V} \sum_{\vec{k}_1} \sum_{\vec{k}_2} \frac{4\pi}{|\vec{k}_1 - \vec{k}_2|^2}$$

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:

$$\langle \mathrm{HF} | H_I | \mathrm{HF} \rangle = -\frac{k_F^3 V}{4\pi^3} = -\frac{3}{4} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} n^{\frac{4}{3}} V$$

$$\Rightarrow E = \frac{(3n)^{\frac{5}{3}} \pi^{\frac{4}{3}} V}{10} - \frac{3}{4} \left(\frac{3}{\pi} \right)^{\frac{1}{3}} n^{\frac{4}{3}} V$$

6. 量子转子模型

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

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

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

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

考虑一个特定的量子转子模型, 它的哈密顿量为

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

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

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

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

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

$$\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN(\theta-2\pi)}|\theta - 2\pi\rangle = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN\theta}|\theta\rangle$$

$$\Longleftrightarrow \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN(\theta-2\pi)}|\theta\rangle = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN(\theta-2\pi)}|\theta\rangle$$

$$\Longleftrightarrow e^{iN\theta} = e^{iN(\theta-2\pi)} = e^{iN\theta}e^{-i2\pi N}$$

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.

$$\hat{H}_0|N\rangle = \frac{1}{2}\left(\hat{N} - \frac{1}{2}\right)^2|N\rangle = \frac{1}{2}\left(N - \frac{1}{2}\right)^2|N\rangle \Rightarrow E_N^{(0)} = \frac{1}{2}\left(N - \frac{1}{2}\right)^2$$

$$\Rightarrow N_\pm - \frac{1}{2} = \pm\sqrt{2E_N^{(0)}} \Rightarrow N_\pm = \frac{1}{2} \pm \sqrt{2E_N^{(0)}}$$

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.

$$\cos 2\hat{\theta} = \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)$$

$$e^{i2\hat{\theta}}|N\rangle = e^{i2\hat{\theta}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN\theta}|\theta\rangle\right) = \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{iN\theta}e^{i2\hat{\theta}}|\theta\rangle$$

$$= \frac{1}{\sqrt{2\pi}}\int_0^{2\pi} d\theta e^{i(N+2)\theta}|\theta\rangle = |N + 2\rangle$$

$$\Rightarrow \cos 2\hat{\theta}|N\rangle = \frac{1}{2}\left(e^{i2\hat{\theta}} + e^{-i2\hat{\theta}}\right)|N\rangle = \frac{1}{2}\left(|N+2\rangle + |N-2\rangle\right)$$

$$\Rightarrow \langle N|\hat{V}|N'\rangle = -g\langle N|\cos 2\hat{\theta}|N'\rangle = -\frac{g}{2}\left(\langle N|N'+2\rangle + \langle N|N'-2\rangle\right)$$

$$= -\frac{g}{2}(\delta_{N,N'+2} + \delta_{N,N'-2})$$

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.

$$E_N^{(1)} = \langle N|\hat{V}|N\rangle = -\frac{g}{2}\left(\langle N|N+2\rangle + \langle N|N-2\rangle\right) = 0$$

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

$$= \boxed{\frac{g^2}{(2N-3)(2N+1)}}$$

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:

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

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

所以简并度未变化.