

ADVANCED QUANTUM MECHANICS

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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

$$\begin{aligned}\langle v, Av \rangle &= \langle v, \lambda v \rangle = \lambda \langle v, v \rangle = \lambda \|v\|^2. \\ \langle Av, v \rangle &= \langle \lambda v, v \rangle = \lambda^* \langle v, v \rangle = \lambda^* \|v\|^2.\end{aligned}$$

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

$$\begin{aligned}\langle v_1, Av_2 \rangle &= \langle v_1, \lambda_2 v_2 \rangle = \lambda_2 \langle v_1, v_2 \rangle, \\ \langle Av_1, v_2 \rangle &= \langle \lambda_1 v_1, v_2 \rangle = \lambda_1 \langle v_1, v_2 \rangle.\end{aligned}$$

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

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

We define the unitary matrix as $U = [v_1, v_2, \dots, v_n]$, 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

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

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

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 $\sigma_{(z)}^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$, and find the eigenvalues of $\sigma_{(z)}^x$.**

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

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

So we have $\lambda = \pm 1$. 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 $|+\rangle_{(z)}^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. 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 $|-\rangle_{(z)}^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. The eigenvectors have been normalized, so the unitary matrix V is $[|+\rangle_{(z)}^x, |-\rangle_{(z)}^x] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. 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 $\sigma_{(z)}^x$ by the unitary transformation V :

$$\sigma_{(z)}^x = V^\dagger \Lambda V = V^\dagger \sigma_{(z)}^z V$$

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 :

$$\sigma_{(z)}^x = V^\dagger \sigma_{(z)}^z V = V^\dagger \sigma_{(x)}^x V \Rightarrow \sigma_{(x)}^x = (V^\dagger)^{-1} \sigma_{(z)}^x (V)^{-1}$$

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

$$\sigma_{(x)}^x = V \sigma_{(z)}^x V$$

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

$$S_{(z)}^x = \frac{\hbar}{2} \sigma_{(z)}^x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

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

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

So

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

So the basis vectors in the S^x representation are

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

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 $L_i = \sum_{jk} \epsilon_{ijk}x_jp_k$ is defined in the usual 3-dimension subspace, so we still have

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

So we have

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

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

(b) $K_i = wp_i - x_ip_w$.

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

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

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

$$\begin{aligned} [L_i, p_j] &= \left[\sum_{lk} \epsilon_{ilk} x_l p_k, p_j \right] = \sum_{lk} \epsilon_{ilk} (\cancel{x_l [p_k, p_j]} + [x_l, p_j] p_k) = \sum_{lk} \epsilon_{ilk} i\hbar \delta_{lj} p_k = i\hbar \sum_k \epsilon_{ijk} p_k \\ \Rightarrow \quad &\boxed{w[L_i, p_j] = i\hbar \sum_k \epsilon_{ijk} w p_k} \end{aligned}$$

For the other term, we have

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

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

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

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 Hamiltonian 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

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

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:

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

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

$$\begin{aligned} \langle m|\hat{x}|n\rangle &= \sqrt{\frac{\hbar}{2m\omega}} (\langle m|a|n\rangle + \langle m|a^\dagger|n\rangle) = \sqrt{\frac{\hbar}{2m\omega}} (\langle m|\sqrt{n}|n-1\rangle + \langle m|\sqrt{n+1}|n+1\rangle) \\ &= \sqrt{\frac{\hbar}{2m\omega}} (\sqrt{n}\delta_{m,n-1} + \sqrt{n+1}\delta_{m,n+1}) \\ \langle m|\hat{p}|n\rangle &= i\sqrt{\frac{\hbar m\omega}{2}} (\langle m|a^\dagger|n\rangle - \langle m|a|n\rangle) = i\sqrt{\frac{\hbar m\omega}{2}} (\langle m|\sqrt{n+1}|n+1\rangle - \langle m|\sqrt{n}|n-1\rangle) \\ &= i\sqrt{\frac{\hbar m\omega}{2}} (\sqrt{n+1}\delta_{m,n+1} - \sqrt{n}\delta_{m,n-1}) \\ \langle m|\hat{x}^2|n\rangle &= \frac{\hbar}{2m\omega} (\langle m|a^2|n\rangle + \langle m|a^{\dagger 2}|n\rangle + \langle m|a^\dagger a|n\rangle + \langle m|a a^\dagger|n\rangle) \\ &= \frac{\hbar}{2m\omega} (\langle m|\sqrt{n(n-1)}|n-2\rangle + \langle m|\sqrt{(n+1)(n+2)}|n+2\rangle + \langle m|n|n\rangle + \langle m|n+1|n\rangle) \\ &= \frac{\hbar}{2m\omega} (\sqrt{n(n-1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} + n\delta_{m,n} + (2n+1)\delta_{m,n}) \\ \langle m|\hat{p}^2|n\rangle &= -\frac{\hbar m\omega}{2} (\langle m|a^{\dagger 2}|n\rangle - \langle m|2a^\dagger a|n\rangle + \langle m|a^2|n\rangle - \langle m|1|n\rangle) \\ &= -\frac{\hbar m\omega}{2} (\sqrt{(n+1)(n+2)}\delta_{m,n+2} - (2n+1)2n\delta_{m,n} + \sqrt{n(n-1)}\delta_{m,n-2}) \end{aligned}$$

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

Note $\frac{1}{k_B T}$ 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

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

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

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

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

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

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

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

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

Define

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

So the angular momentum operator is

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

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

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

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

3. Define the following set of states, where $s = 0, 1/2, 1, \dots$, and $m = -s, -s+1, \dots, s-1, s$ (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

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

$$\vec{S}^2 = (S^x)^2 + (S^y)^2 + (S^z)^2$$

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

$$a^\dagger a |s, m\rangle = (s+m) |s, m\rangle, \quad b^\dagger b |s, m\rangle = (s-m) |s, m\rangle$$

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

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

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

$$S^+ = a^\dagger b, \quad S^- = b^\dagger a$$

$$\Rightarrow S^2 = S^z S^z + \frac{1}{2} (S^+ S^- + S^- S^+)$$

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

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

$$= m^2 |s, m\rangle + \frac{1}{2} ((s+m)(s-m+1) + (s+m+1)(s-m)) |s, m\rangle$$

$$= \boxed{s(s+1) |s, m\rangle}$$

\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:

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

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 $\{a_n^\dagger, a_n; n=1, \dots, L\}$ 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 $n \rightarrow n+n'$ ("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 $n \rightarrow n+n'$, 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^\dagger remain invariant, so $e^{ikn'} = 1$ for any shift $n' \in \mathbb{Z}$, which means

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

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

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

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

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

We have

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

So

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

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

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

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

We have the definition

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

So

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

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

We have known that

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

So the commutator

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

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

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:

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

where:

- $c_{i\sigma}^\dagger$ and $c_{i\sigma}$ are the fermionic creation and annihilation operators for an electron 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

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

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

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 diagonal elements, this matrix is very similar to the case in the lecture. We can get

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

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

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

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

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

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

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

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

(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

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

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

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

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

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

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

$$\alpha \approx 0, \quad \langle n_{1\sigma} \rangle = 1, \quad \langle n_{2\sigma} \rangle = 0;$$

$$H_{\text{MF}} \approx U.$$

- (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 quantum 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 $\theta \pm 2\pi$ represents the same state as $|\theta\rangle$. Define the rotation operator for the quantum rotator as $\hat{R}(\alpha)$,

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

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

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

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

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

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.

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

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.

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

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 $P(S_z^+) = \|\chi_+^{\dagger} \frac{1}{\sqrt{2}}(\chi_+^z + \chi_-^z)\|^2 = \boxed{\frac{1}{2}}$

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

$$\rho = \sum_i |\phi_i\rangle p_i \langle \phi_i|, \text{ 那么 } \text{Tr}[\rho] \text{ 应满足?}$$

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 $A_H(t) = U^{\dagger}(t, 0) A U(t, 0)$, 其中 A 是薛定谔绘景中的算符, 如果 A 不显含时间, 那么 $dA_H(t)/dt$ 等于?

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

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: $\vec{A} \rightarrow \vec{A} - \nabla \Lambda$, $\phi \rightarrow \phi + \frac{\partial \Lambda}{\partial t}$, $\psi \rightarrow ?$

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

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

展开变换前的薛定谔方程:

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

展开变换后的薛定谔方程:

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

(2) - (1) · $e^{if(\vec{r},t)}$, 得到

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

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

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

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

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

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

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

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

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

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

密度矩阵为

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

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

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

计算 ρ_A 的纠缠熵:

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

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 $E[\Psi] = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}$, $E(\Psi)$ 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

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

2.2 多项选择

1. 与总角动量算符的平方 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

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

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

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

(b) 动量. $E = pc$

(c) 时间. $E = \hbar \omega = \hbar \frac{1}{\tau}$, 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 $\text{kg} \cdot \text{m}^2/\text{s}$, 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 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 $[b_\alpha^\dagger, b_\beta^\dagger] = [b_\alpha, b_\beta] = 0$, $[b_\alpha, b_\beta^\dagger] = \delta_{\alpha\beta}$, 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 $[N, A] = \sum_i [b_i^\dagger b_i, A] = \sum_i \{b_i^\dagger [b_i, A] + [b_i^\dagger, A] b_i\}$, 代入以上各算符 A 判断是否对易.

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

(b)

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

(c)

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

(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)

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

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 $H = \frac{\vec{p}^2}{2M} + V(r)$. 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

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

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

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

其中 $\hbar\omega_{fi} = E_f - E_i$. 当微扰为

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

跃迁概率为?

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

3. *算符 $\Omega(t) \equiv U^{-1}(t)U_0(t)$, 算符 $\Omega_{\pm} \equiv \lim_{t \rightarrow \mp\infty} \Omega(t)$, 其中

- $U_0(t) = e^{-iH_0 t/\hbar}$ 是自由系统 H_0 的时间演化算符;
- $U(t) = e^{-iH t/\hbar}$ 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

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

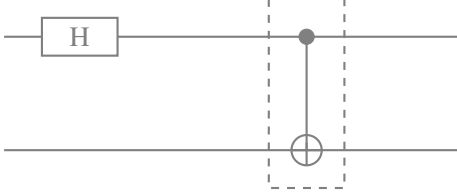
定义螺旋度算符为 $\frac{1}{2} \hat{p} \cdot \vec{\sigma}$, 其中 $\hat{p} = \frac{\vec{p}}{|\vec{p}|}$, 那么可知 Weyl 旋量 χ_{\pm} 恰好是螺旋度算符的本征态, 本征值分别为?

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

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

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

5. *一个可以制备 Bell 态的简单量子线路为



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

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

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

注意到

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

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.

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

2.4 应用题

1. 矩阵对角化和表象变换

- (a) 对角化矩阵 L 就是去找到么正变换 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 是一个么正矩阵, 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 $\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ 的么正矩阵 V , 并找到 σ^x 的本征值.

通过求解其特征方程以得到 $\sigma_{(z)}^x$ 的本征值:

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

解得 $\lambda = \pm 1$. 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 $|+\rangle_{(z)}^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$. 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 $|-\rangle_{(z)}^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$. 在求解过程中已经对这些本征矢进行了归一化, 所以可以得到么正矩阵 $V = [|+\rangle_{(z)}^x, |-\rangle_{(z)}^x] = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$. 对角矩阵 Λ 对角线上依次是本征值, 即

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

于是我们可以通过么正矩阵 V 来对 $\sigma_{(z)}^x$ 进行对角化:

$$\sigma_{(z)}^x = V^\dagger \Lambda V = V^\dagger \sigma_{(z)}^z V$$

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:

$$\sigma_{(z)}^x = V^\dagger \sigma_{(z)}^z V = V^\dagger \sigma_{(x)}^x V \Rightarrow \sigma_{(x)}^x = (V^\dagger)^{-1} \sigma_{(z)}^x (V)^{-1}$$

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

$$\sigma_{(x)}^x = V \sigma_{(z)}^x V$$

- (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 $\sigma^x, \sigma^y, \sigma^z$. 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

$$S_{(z)}^x = \frac{\hbar}{2} \sigma_{(z)}^x = \frac{\hbar}{2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

从前文中可知, $\sigma_{(z)}^x$ 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 表象的么正矩阵为

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

在 S^z 表象中有

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

因此

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

在 S^x 表象中的基矢为

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

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 $[Q, P], [a, a^\dagger], [a, a^\dagger a], [a^\dagger, a^\dagger a]$;

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

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

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

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:

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

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

(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 $\vec{J}_1^2 = \vec{J}_2^2 = j(j+1)\hbar^2$, $J^2 = J(J+1)\hbar^2$, $J = 2j, 2j-1, \dots, 1, 0$. 在总角动量量子数 $J=0$ 的状态下, 求 $J_{1,z}$ 和 $J_{2,z}$ 的可能取值及相应概率.

4. 自旋-1 模型

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

(a) 写出 S^x 和 S^z 的矩阵表示.

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

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

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.

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

(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.

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

注意到 m^2 会带来 $m = \pm 1$ 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:

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

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

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

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:

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

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

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

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

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

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

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, $\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z)$, 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, $q = |\vec{q}|$, $x = |\vec{x}|$,

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

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

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

- 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.
- 计算能量的一阶修正 $E^{(1)} = \langle \mathbf{FS} | H_I | \mathbf{FS} \rangle$.
- 利用 **Hartree 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 $\langle c_{k\sigma}^\dagger c_{k'\sigma'} \rangle = \langle c_{k\sigma}^\dagger c_{k\sigma} \rangle \delta_{k,k'} \delta_{\sigma,\sigma'}$, 以及 $\langle c_{k\uparrow}^\dagger c_{k\uparrow} \rangle = \langle c_{k\downarrow}^\dagger c_{k\downarrow} \rangle$. 计算系统总能量, 并与 $E^{(0)} + E^{(1)}$ 比较大小.

6. 量子转子模型

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

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

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 $\hat{R}(\alpha)$ 是一个么正算符, 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

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

其中 $g \cos(2\hat{\theta})$ 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

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

- 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

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

因此为了保持 θ 转动 2π 后的不变性, N 应当是整数.

- 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 $V = -g \cos(2\hat{\theta})$ 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 $\langle N|V|N'\rangle = 0$). 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.

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

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.

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

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.