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

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

   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

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

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

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

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

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

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

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

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

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

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

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

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

   So the basis vectors in the S^x representation are

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

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

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

So we have

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

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 $f(x, y, z, w)$, wo we have

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

So we have

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

For the other term, we have

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

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

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

For the other term, we have

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

Combining the terms we derived, we have

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

(b) $[K_i, K_j]$.

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

So combine the terms we derived, we have

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

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

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

   And the energy eigenvalues E_n are given by

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

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

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

   where $H_n(x)$ are the Hermite polynomials.

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

   We have known that the position operator x and the momentum operator p could be expressed by the creation $a^\dagger$ and annihilation a operators:

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

   which is governed by

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

   Apply the calculating formula to the matrix elements, and we have

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

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

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

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

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

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

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

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

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

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

The coherent states are given by

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

So the inner product could be derived as

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

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

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

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. $a=\dfrac{1}{\sqrt{2}}(x+ip_x)$, $b=\dfrac{1}{\sqrt{2}}(y+ip_y)$. They satisfy the commutation relations

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

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

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

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

   So we have

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

   We have commutation formula that

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

   So we have

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

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

   Define

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

   So the angular momentum operator is

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

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

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

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

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

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

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

We have known that

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

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

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

□

1.3.2 1D tight-binding model

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

   We have

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

   So

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

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

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

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

We have the definition

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

So

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

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

We have known that

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

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

So the commutator

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

$$\begin{aligned}
\left[a_n^\dagger a_{n+1}, b_k^\dagger \right] &= a_n^\dagger \left[a_{n+1}, b_k^\dagger \right] = a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \left[a_{n+1}, a_m^\dagger \right] \\
&= a_n^\dagger \frac{1}{\sqrt{L}} \sum_{m=1}^{L} e^{ikm} \delta_{n+1,m} = a_n^\dagger \frac{1}{\sqrt{L}} e^{ik(n+1)}
\end{aligned}$$

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

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

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:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\langle n_{1\uparrow}\rangle = \langle n_{2\uparrow}\rangle = \langle n_{1\downarrow}\rangle = \langle n_{2\downarrow}\rangle = \frac{1}{2}$$

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

   (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

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

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

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

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

   and the self-consistent equation is

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

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

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

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

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

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

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

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

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

The self-consistent equation is

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

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

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

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

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

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

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

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

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

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

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

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

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

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

So the corrected energy level is

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

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

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

so the degeneracy of the energy levels remains unlifted.

第二章 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 Tr$[\rho]$ 应满足?**

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

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

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

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

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

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

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

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

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

展开变换前的薛定谔方程:

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

展开变换后的薛定谔方程:

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

$(②)-(①)\cdot e^{if(\vec{r},t)}$, 得到

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

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

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

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

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

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

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

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

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

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

密度矩阵为

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

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

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

计算 ρ_A 的纠缠熵:

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

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

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

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

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

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

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

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

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

   (a) $\boxed{\text{距离}}$. $\dfrac{\text{kg}\cdot\text{m}^2/\text{s}^2}{\text{kg}\cdot\text{m}^2/\text{s}} = \dfrac{1}{\text{s}}$, 是时间的倒数, 因此和能量同单位.

   (b) $\boxed{\text{动量}}$. $E = pc$

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

   (d) $\boxed{\text{质量}}$. $E = mc^2$.

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

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

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

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

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

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

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

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

   (b)

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

   (c)

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

   (d)

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

   (e)

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

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

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

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

2. **考虑一阶近似, 当 $i \neq f$ 时, 跃迁概率为**

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

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

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

跃迁概率为?

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

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

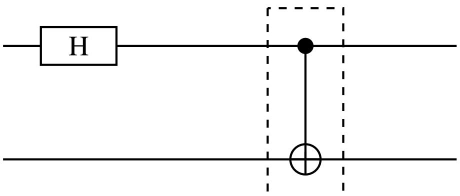
$$\begin{aligned}
(E - \vec{\sigma}\cdot\vec{p})\,\chi_+(\vec{p}) &= m\chi_-(\vec{p}) \\
(E + \vec{\sigma}\cdot\vec{p})\,\chi_-(\vec{p}) &= m\chi_+(\vec{p})
\end{aligned}$$

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

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

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

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,

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

$$\textbf{CNOT} = e^{\frac{\mathrm{i}\pi}{4}(\mathbb{I}-\sigma_1^z)\otimes(\mathbb{I}-\sigma_2^x)}$$

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

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

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

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

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

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

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

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

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

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

在 S^z 表象下有

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

从前文中可知, $\sigma^x_{(z)}$ 的本征矢为:

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

用以将 S^z 表象转换为 S^x 表象的幺正矩阵为

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

在 S^z 表象中有

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

因此

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

在 S^x 表象中的基矢为

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

2. 谐振子问题

一维谐振子的哈密顿量为

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

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

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

注意新的坐标算符 Q 和动量算符 P 是无量纲的, 哈密顿量重新写为

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

引入玻色子产生和湮灭算符, $a^\dagger$ 和 a.

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

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

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

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

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

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

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

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

(c) 在能量表象中, 计算 a 和 $a^\dagger$ 的矩阵元.

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

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

3. 角动量耦合

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

4. 自旋-1 模型

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

(a) 写出 S^x 和 S^z 的矩阵表示.

(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.

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:

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

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,

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

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

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

这里我们考虑短程势, 也就是说 $v(q=0)$ 不发散.

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

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

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

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

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

6. 量子转子模型

量子转子的角度坐标 $\theta\in[0,2\pi)$, 注意 $\theta\pm2\pi$ 和 θ 是等价的. 用 $|\theta\rangle$ 表现 $\hat{\theta}$ 算符的本征态, $|\theta\pm2\pi\rangle$ 和 $|\theta\rangle$ 是相同的态. 定义量子转子的转动算符为 $\hat{R}(\alpha)$,

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

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

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

考虑一个特定的量子转子模型, 它的哈密顿量为

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

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

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

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

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

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

因此为了保持 θ 转动 2π 后的不变性, N 应当是整数.

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

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

这意味着对于任意整数 N, 都对应存在着 $N'=1-N$ 使得能级简并.

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

$$\begin{aligned}\cos2\hat{\theta}&=\frac{1}{2}\left(e^{i2\hat{\theta}}+e^{-i2\hat{\theta}}\right)\\ e^{i2\hat{\theta}}|N\rangle&=e^{i2\hat{\theta}}\left(\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta e^{iN\theta}|\theta\rangle\right)=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta e^{iN\theta}e^{i2\hat{\theta}}|\theta\rangle\\ &=\frac{1}{\sqrt{2\pi}}\int_0^{2\pi}\mathrm{d}\theta e^{i(N+2)\theta}|\theta\rangle=|N+2\rangle\\ \Rightarrow\cos2\hat{\theta}|N\rangle&=\frac{1}{2}\left(e^{i2\hat{\theta}}+e^{-i2\hat{\theta}}\right)|N\rangle=\frac{1}{2}\left(|N+2\rangle+|N-2\rangle\right)\\ \Rightarrow\langle N|\hat{V}|N'\rangle&=-g\langle N|\cos2\hat{\theta}|N'\rangle=-\frac{g}{2}\left(\langle N|N'+2\rangle+\langle N|N'-2\rangle\right)\\ &=-\frac{g}{2}(\delta_{N,N'+2}+\delta_{N,N'-2})\end{aligned}$$

和前文一致, 如果 $|N\rangle$ 和 $|N'\rangle$ 简并, 那么 $N+N'=1$ 使得只要 $N\in\mathbb{Z}$, 那么$\delta\neq0$. 所以仍然可以使用非简并微扰论.

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

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

微扰修正后的能级为

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

代入 $N' = 1 - N$ 以检查能级简并性:

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

所以简并度未变化.