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

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

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

   (a) Let's say

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

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

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

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

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

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

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

1.1.2 Matrix diagonalization and unitary transformation

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

   Within S^z representation, we have

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

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

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

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

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

   In the S^z representation, we have

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

   So

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

   So the basis vectors in the S^x representation are

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

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

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

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

   So we have

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

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

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

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

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

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

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

   So we have

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

   For the other term, we have

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

Thus we have

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

□

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

(a) $[L_i, K_j]$

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

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

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

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

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

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

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

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

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

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

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

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

So we have

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

Combine the above results, and we have

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

□

1.3.2 1D tight-binding model

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

   We have

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

   So

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

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

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

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

We have the definition

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

So

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

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

We have known that

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

So the commutator

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

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

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** $\langle n_{i\sigma}\rangle = \dfrac{1}{2}$**.**

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

   (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

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

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

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

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

   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.