0.1 Homework 5

0.1.1 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

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

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

2. **Consider the unperturbed Hamiltonian $\hat{H}_0 = \dfrac{1}{2}\left(\hat{N} - \dfrac{1}{2}\right)^2$, 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.