PH3102: QM Assignment 10

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Q1. Degenerate Perturbation Theory on 2D Harmonic Oscillator

Here, we consider a 2D harmonic oscillator with Hamiltonian given as

$$H = \frac{1}{2m}(p_x^2 + p_y^2) + \frac{1}{2}m\omega^2(x^2 + y^2) = H_x + H_y \tag{1}$$

so that it is the sum of two 1D harmonic oscillators.

Answer 1.1

We want to show $[H, H_x] = 0$. This can be done by just showing $\big[H_x, H_y\big] = 0$. We have $[x, p_x] = \frac{i}{\hbar}$, $\big[y, p_y\big] = \frac{i}{\hbar}$, $\big[x, p_y\big] = 0$ and $[y, p_x] = 0$. Thus, we have

$$\begin{aligned}
\big[H_x, H_y\big] &= \frac{1}{2}m\omega^2\left[x^2 + \frac{p_x^2}{\omega^2 m^2}, y^2 + \frac{p_y^2}{\omega^2 m^2}\right] \\
\Rightarrow \big[H_x, H_y\big] &= \frac{1}{2}m\omega^2[x^2, y^2] + \frac{1}{2}m\omega^2\left[\frac{p_x^2}{\omega^2 m^2}, y^2\right] + \left[\frac{p_x^2}{\omega^2 m^2}, x^2\right] + \frac{1}{2}m\omega^2\left[\frac{p_x^2}{\omega^2 m^2}, \frac{p_y^2}{\omega^2 m^2}\right] \\
\Rightarrow \big[H_x, H_y\big] &= 0
\end{aligned} \tag{2}$$

Thus $[H, H_x] = \big[H_x + H_y, H_x\big] = \big[H_y, H_x\big] = 0$. Thus the eigenstates of H are also eigenstates of H_x. Similarly, we can show that the eigenstates of H are also eigenstates of H_y, because $\big[H, H_y\big] = \big[H_x + H_y, H_y\big] = \big[H_x, H_y\big] = 0$.

Thus we can write the eigenstates of H as $\big|n_x, n_y\big\rangle = |n_x\rangle \otimes \big|n_y\big\rangle$, where n_x and n_y are the quantum numbers which represent the eigenvalues of the Number operators for the 1D harmonic oscillators in the x and y directions respectively.

Answer 1.2

The angular momentum operators are given by $L = xp_y - yp_x$. We want to show that $[H, L] = 0$. Let us calculate $[H_x, L]$ and $\big[H_y, L\big]$. Let us rewrite L is terms of the raising and lowering operators. We have $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ and $y = \sqrt{\frac{\hbar}{2m\omega}}(b + b^\dagger)$ and $p_x = -i\sqrt{\frac{m\omega\hbar}{2}}(a - a^\dagger)$ and $p_y = -i\sqrt{\frac{m\omega\hbar}{2}}(b - b^\dagger)$. Thus, we have $L = xp_y - yp_x = i\hbar\big(a^\dagger b - ab^\dagger\big)$. We will use this expression to calculate $[H_x, L]$ and $[H_y, L$. Here $H_x = \hbar\omega\big(a^\dagger a + \frac{1}{2}\big)$ and $H_y = \hbar\omega\big(b^\dagger b + \frac{1}{2}\big)$. Let us have

$$\begin{aligned}
[H_x, L] &= i\hbar^2\omega\left[a^\dagger a + \frac{1}{2}, a^\dagger b - ab^\dagger\right] \\
&= i\hbar^2\omega\big[a^\dagger a, a^\dagger b\big] - i\hbar^2\omega\big[a^\dagger a, ab^\dagger\big] + i\hbar^2\omega\left[\frac{1}{2}, a^\dagger b\right] - i\hbar^2\omega\left[\frac{1}{2}, ab^\dagger\right] \\
&= -i\hbar^2\omega\big(ab^\dagger + ba^\dagger\big)
\end{aligned} \tag{3}$$

Similarly, we can calculate $\big[H_y, L\big]$. We have $\big[H_y, L\big] = i\hbar^2\omega\big(ab^\dagger + ba^\dagger\big)$. Thus, we have $[H, L] = [H_x, L] + \big[H_y, L\big] = 0$. Thus the eigenstates of H are also eigenstates of L.

Thus we can also label the eingenstates of H using H and L, instead of H_x, H_y. Thus we have found two Complete Set of Commuting Observables (CSCO) for the 2D harmonic oscillator, namely $\{H_x, H_y\}$ and $\{H, L\}$. Thus we can recast the problem into eigenstates of H and L.

Answer 1.3

The first excited states are doubly degenerate because the first excited state of H_x is degenerate with the first excited state of H_y. This is because the first excited state of H_x is $|1,0\rangle$ and the first excited state of H_y is $|0,1\rangle$. These two states have the same energy. The ground state is not degenerate since $|0,0\rangle$ can only be constructed from both the oscillators in the ground state i.e. $|0,0\rangle = |0\rangle_x \otimes |0\rangle_y$. We can also see that $|0,0\rangle$ is an eigenstate of L. But the first excited direct product states $|1,0\rangle, |0,1\rangle$ are not eigenstates of L.

Answer 1.4

We add a small perturbation $H_1 = \lambda xy$ to the Hamiltonian. We want to find the first order correction to the energy of the ground state. The ground state of the unperturbed Hamiltonian is $|0,0\rangle$. The first order correction to the energy of the ground state is given by $E_0^1 = \langle 0,0|H_1|0,0\rangle = 0$.

Let us rewrite the perturbation in terms of raising and lowering operators. We have $x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger)$ and $y = \sqrt{\frac{\hbar}{2m\omega}}(b + b^\dagger)$. Thus, $H_1 = \lambda xy = \lambda\frac{\hbar}{2m\omega}(a + a^\dagger)(b + b^\dagger)$. The first order correction to the energy of the ground state is given by

$$\begin{aligned} E_0^1 &= \lambda\frac{\hbar}{2m\omega}\langle 0,0|(a + a^\dagger)(b + b^\dagger)|0,0\rangle \\ &= \lambda\frac{\hbar}{2m\omega}\langle 0,0|(ab + ab^\dagger + a^\dagger b + a^\dagger b^\dagger)|0,0\rangle \\ &= \lambda\frac{\hbar}{2m\omega}\left[\langle 0,0|ab|0,0\rangle + \langle 0,0|ab^\dagger|0,0\rangle + \langle 0,0|a^\dagger b|0,0\rangle + \langle 0,0|a^\dagger b^\dagger|0,0\rangle\right] \\ &= \lambda\frac{\hbar}{2m\omega}[\langle 0,0|1,1\rangle] \\ &= 0 \end{aligned} \quad [4]$$

Thus the first order correction to the energy of the ground state is zero.

Answer 1.5

We will use degenerate perturbation theory and calculate the first order correction to the energy of the first excited states. The first excited states are $|1,0\rangle$ and $|0,1\rangle$. Let us write down the matrix for the first excited state subspace.

$$H_1 = \begin{bmatrix} \langle 1,0|H_1|1,0\rangle & \langle 1,0|H_1|0,1\rangle \\ \langle 0,1|H_1|1,0\rangle & \langle 0,1|H_1|0,1\rangle \end{bmatrix} = \frac{\lambda\hbar}{2m\omega}\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & v \\ v & 0 \end{bmatrix}; v = \frac{\lambda\hbar}{2m\omega} \quad [5]$$

Thus the energy corrections to the first excited states are given by the eigenvalues of the matrix H_1. The eigenvalues are λ_+ and λ_-, which are given using the characteristic equation

$$\begin{aligned} (\lambda - v^2) &= 0 \\ \Rightarrow \lambda &= \pm v \end{aligned} \quad [6]$$

Thus the first order correction to the energy of the first excited states are

$$E_{1+}^{(1)} = v = \frac{\lambda\hbar}{2m\omega} \quad ; \quad E_{1-}^{(1)} = -v = -\frac{\lambda\hbar}{2m\omega} \quad [7]$$

Since this subspace is a two state system with the state space $\{|0,1\rangle, |1,0\rangle\}$. We can represent the states as

$$|0,1\rangle = \begin{pmatrix}1\\0\end{pmatrix} \quad ; \quad |1,0\rangle = \begin{pmatrix}0\\1\end{pmatrix} \tag{8}$$

The eigenvectors of the matrix H_1 are given by the eigenvectors of the matrix $\begin{bmatrix}0 & v\\ v & 0\end{bmatrix}$. The eigenvectors are given by $\begin{pmatrix}1\\1\end{pmatrix}$ and $\begin{pmatrix}1\\-1\end{pmatrix}$. Thus the normalized eigenvectors are given by

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}(|1,0\rangle + |0,1\rangle) \quad ; \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}(|1,0\rangle - |0,1\rangle) \tag{9}$$

Thus the corrected eigenstates are given by $|1,0\rangle + |0,1\rangle$ and $|1,0\rangle - |0,1\rangle$. The corrected energies are

$$E_{1+} = E_1 + \lambda\frac{\hbar}{2m\omega} \quad ; \quad E_{1-} = E_1 - \frac{\lambda\hbar}{2m\omega} \tag{10}$$

We see that the degeneracy of the first excited states is lifted by the perturbation H_1.

Answer 1.6

We want to now show that $[H_x, H_1] \neq 0$ and $[H_1, L] \neq 0$. Let us first show that $[H_x, H_1] \neq 0$.

$$\begin{aligned}
[H_x, H_1] &= \left[\hbar\omega\left(a^\dagger a + \frac{1}{2}\right), \frac{\lambda\hbar}{2m\omega}(a + a^\dagger)(b + b^\dagger)\right] \\
&= \frac{\lambda\hbar^2}{2m}\left[\left(a^\dagger a + \frac{1}{2}\right), (a + a^\dagger)(b + b^\dagger)\right] \\
&= \frac{\lambda\hbar^2}{2m}\left[a^\dagger a, a + a^\dagger\right](b + b^\dagger) \\
&= \frac{\lambda\hbar^2}{2m}(-a + a^\dagger)(b + b^\dagger) \neq 0
\end{aligned} \tag{11}$$

We now want to show that $[H_1, L] \neq 0$

$$\begin{aligned}
[H_1, L] &= \left[\frac{\lambda\hbar}{2m\omega}(a + a^\dagger)(b + b^\dagger), i\hbar(ab^\dagger - ba^\dagger)\right] \\
&= \frac{i(\lambda\hbar^2)}{2m\omega}\left[(a + a^\dagger)(b + b^\dagger), ab^\dagger - ba^\dagger\right] \\
&= i\lambda\hbar(y^2 - x^2) \neq 0
\end{aligned} \tag{12}$$

Thus the perturbed states are not eigenstates of the angular momentum operator. Thus neither the eigenbasis of H_x and L will diagonalise the perturbed Hamiltonian.

Let us now define the reflection operator S which is reflection about $y = x$. The reflection operator commutes with the perturbation

$$\begin{aligned}
[H_1, S] &= [\lambda xy, S] = \lambda[xy, S] \\
&= \lambda(xyS - Sxy) \\
&= \lambda(yxS - ySy) \\
&= \lambda(ySy - ySy) = 0
\end{aligned} \tag{13}$$

Thus the perturbed Hamiltonian does not have a symmetry under reflection about $y = x$. The reflection operator swaps x and y. Let consider the action of the reflection operator on the position representation of the eigenkets.

$$S\phi_0(x) = \phi_0(y) \quad S\phi_1(x) = \phi_1(y) \tag{14}$$

Using these we see that

$$\begin{aligned} S\Phi_{00}(x,y) &= \Phi_{00}(y,x) = \Phi_{00}(x,y) \\ S\Phi_{01}(x,y) &= \Phi_{01}(y,x) = \Phi_{10}(x,y) \\ S\Phi_{10}(x,y) &= \Phi_{10}(y,x) = \Phi_{01}(x,y) \end{aligned}$$

Thus the degenerate eigenkets under operation of S is given by

$$\begin{aligned} S\Big(\frac{1}{\sqrt{2}}\big(\Phi_{01(x,y)} + \Phi_{10}(x,y)\big)\Big) &= \frac{1}{\sqrt{2}}\big(\Phi_{10(x,y)} + \Phi_{01}(x,y)\big) \\ S\Big(\frac{1}{\sqrt{2}}\big(\Phi_{01(x,y)} - \Phi_{10}(x,y)\big)\Big) &= -\frac{1}{\sqrt{2}}\big(\Phi_{01(x,y)} - \Phi_{10}(x,y)\big) \end{aligned}$$

We can see that swapping the x and the y values of the perturbed eigenkets just returns the eigenkets with a ± 1 eigenvalues. Thus, the perturbed eigenkets are also the eigenkets of the reflection operator S.

Q2. Variational method for a Bouncing Ball potential

The potential is given as

$$V(x) = \begin{cases} mgx & x > 0 \\ 0 & x < 0 \end{cases} \tag{15}$$

Answer 2.1

We want to figure out the boundary conditions for $x = 0$ and $x \longrightarrow \infty$. Now the since the potential is infinite at $x < 0$, $\psi(0_+) = 0$ and by the continuity of $\psi(x)$ we get

$$\lim_{x \longrightarrow 0+} \psi(x) = \lim_{x \longrightarrow 0-} \psi(x) = 0$$

Now, we want the wavefunction $\psi(x)$ should be normalizable. Thus we want the wavefunction to vanish at $x \longrightarrow \infty$. Thus we get

$$\lim_{x \longrightarrow \infty} \psi(x) = 0$$

The variational method uses a trial wavefunction as ansatz to determine the energy of the gorund state. The trial wavefunction is given by

$$\psi(x) = \begin{cases} xe^{-ax} & x > 0 \\ 0 & x < 0 \end{cases}$$

The wavefunction also satisfies the boundary conditions at $x = 0$ and $x \longrightarrow \infty$.

$$\lim_{x \longrightarrow 0} xe^{-ax} = 0 \qquad \lim_{x \longrightarrow \infty} xe^{-ax} = 0$$

Let us now normalize the wavefunction

$$\begin{aligned} 1 &= \int_{-\infty}^{\infty} \psi^*(x)\psi(x)dx = \int_0^{\infty} |N|^2 \; x^2 e^{-2ax} dx = |N|^2 \; \frac{2}{8a^3} = |N|^2 \; \frac{1}{4a^3} \\ \Rightarrow |N| &= \sqrt{4a^3} \end{aligned} \tag{16}$$

We will now calculate the expectation value of the energy. The expectation value of the energy is given by

$$\begin{aligned}\langle H\rangle = \langle T\rangle + \langle V\rangle = E &= \int_{-\infty}^{\infty}\psi^*(x)\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x)\right)dx \\ &= |N|^2\int_{\infty}^{\infty} xe^{-ax}\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}xe^{-ax}\right)dx + mg\int_0^{\infty}|N|^2\ x^3e^{-2ax}dx \\ &= \frac{-\hbar^2|N|^2}{2m}\int_{\infty}^{\infty} xe^{-2ax}(a^2x-2a)dx + |N|^2\ \frac{\Gamma(4)}{(2a)^4} \\ &= \frac{-\hbar^2}{2m}\ |N|^2\ \left(a^2\frac{\Gamma(3)}{(2a)^3} - 2a\frac{\Gamma(2)}{(2a)^2}\right) + |N|^2\ \frac{\Gamma(4)}{(2a)^4} \\ &= \frac{a^2\hbar^2}{2m} + \frac{3mg}{2a}\end{aligned} \tag{17}$$

The expectation value of the energy of the trial wavefunction is given by

$$E = \frac{a^2\hbar^2}{2m} + \frac{3mg}{2a}$$

Answer 2.2

We want to minimize the energy with respect to the parameter a. We can do this by setting the derivative of the energy with respect to a to zero. We get

$$\frac{dE}{da} = \frac{a\hbar^2}{m} - \frac{3mg}{2a^2} = 0 \Rightarrow a_0^3 = \frac{3m^2g}{2\hbar^2} \Rightarrow a_0 = \left(\frac{3m^2g}{2\hbar^2}\right)^{\frac{1}{3}} \tag{18}$$

We want to verify that the energy is a minimum. We can do this by calculating the second derivative of the energy with respect to a. We get

$$\frac{d^2E}{dx^2} = \frac{\hbar^2}{m} + \frac{3m^2g}{a_0^2\hbar^2} > 0 \tag{19}$$

Let us now calculate the $\langle H\rangle_{\min}$

$$\langle H\rangle_{\min} = \frac{1}{2a_0}\left[\frac{a_0^3\hbar^2}{m} + 3mg\right] = \frac{1}{2a_0}\frac{9mg}{2} = 3\left(\frac{9mg^2\hbar^2}{32}\right)^{\frac{1}{3}} \tag{20}$$

We know from the variational method that the ground state energy is always lower than the energy of the trial wavefunction.

$$E_0 < \langle H\rangle_{\min} = 3\left(\frac{9mg^2\hbar^2}{32}\right)^{\frac{1}{3}}$$