QUALIFYING EXAMINATION, Part 3

Solutions

Problem 1: Quantum Mechanics I

(a) The eigenvalues λ of $\hat{L}_x$ are determined by

$$\begin{vmatrix} -\lambda & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -\lambda & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -\lambda \end{vmatrix} = 0 \; .$$

The determinant is given by $-\lambda(\lambda^2 - 1)$ and the eigenvalues are

$$\lambda = 1, 0, -1 \; .$$

The eigenvector corresponding to $\lambda = 1$ is determined from

$$\begin{pmatrix} -1 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & -1 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & -1 \end{pmatrix} \begin{pmatrix} \zeta_1 \\ \zeta 2 \\ \zeta_3 \end{pmatrix} = 0 \; .$$

Using, e.g., the first and third equations, we find $\zeta_2 = \sqrt{2}\zeta_1$ and $\zeta_3 = \frac{1}{\sqrt{2}}\zeta_2$. The normalized $\hat{L}_x$ eigenvector with the highest eigenvalue $L_x = 1$ is then found to be

$$|L_x = 1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} \; .$$

(b)

$$\langle \hat{L}_x \rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0 \; .$$

$$\langle \hat{L}_x^2 \rangle = \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \hat{L}_x \hat{L}_x \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2} \; .$$

where we have used the hermiticity of $\hat{L}_x$.

A simpler method is to use $\langle \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \rangle = 2$ (spin 1). Since $\langle \hat{L}_z^2 \rangle = 1$ and $\langle \hat{L}_x^2 \rangle = \langle \hat{L}_y^2 \rangle$ from rotational symmetry around z, we find

$$\langle \hat{L}_x^2 \rangle = (2 - 1)/2 = 1/2 \; .$$

(c) The components of the $\hat{L}_x$ eigenvector with $L_x = 1$ found in part (a) are the expansion amplitudes of this eigenvector in the $\hat{L}_z$ eigenstates. Therefore

$$P(L_z = \pm 1) = \left(\frac{1}{2}\right)^2 = \frac{1}{4}\,, \quad P(L_z = 0) = \left(\frac{1}{\sqrt{2}}\right)^2 = \frac{1}{2}\,.$$

(d) The variance of x is given by $(\Delta x)^2 = \langle n|\hat{x}^2|n\rangle - \langle n|\hat{x}|n\rangle^2$. The expectation value $\langle n|\hat{x}|n\rangle = 0$ because

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger).$$

Next we use

$$\hat{x}^2 = \frac{\hbar}{2m\omega}(a^2 + {a^\dagger}^2 + aa^\dagger + a^\dagger a)\,,$$

which has non-vanishing diagonal matrix elements due to the third and fourth terms. Using the hints we get

$$(\Delta x)^2 = \langle n|\hat{x}^2|n\rangle = \frac{\hbar}{m\omega}\left(n + \frac{1}{2}\right)$$

or $\Delta x = \sqrt{\frac{\hbar}{m\omega}(n + \frac{1}{2})}$.

(e) In coordinate space $\hat{p} = \frac{\hbar}{i}\frac{d}{dx}$, and, using the hint, $a|0\rangle = 0$ becomes

$$\left(\sqrt{\frac{m\omega}{2\hbar}}x + \sqrt{\frac{\hbar}{2m\omega}}\frac{d}{dx}\right)\psi_0(x) = 0$$

or

$$\frac{d}{dx}\ln\psi_0 = -\frac{m\omega}{\hbar}x\,,$$

which is easily integrated to give

$$\psi_0(x) = A\exp\left(-\frac{m\omega x^2}{2\hbar}\right)\,.$$

(f) In momentum space $\hat{p} = p, \hat{x} = i\hbar\frac{d}{dp}$ (which ensures $[\hat{x},\hat{p}] = i\hbar$) and we find similarly

$$\psi_0(p) = A\exp\left(-\frac{p^2}{2m\omega\hbar}\right)\,.$$

One can also calculate $\psi_0(p)$ by taking the Fourier transform of $\psi_0(x)$ (which keeps its Gaussian form).

Problem 2: Quantum Mechanics II

(a) The energies E of H are determined from

$$\det\begin{pmatrix} E_0 - E & A \\ A & E_0 - E \end{pmatrix} = 0\ .$$

We find $E = E_0 \pm A$. The two normalized eigenstates are given by

$$\psi_\pm = \frac{1}{\sqrt{2}}\left[\binom{1}{0} \pm \binom{0}{1}\right]\ .$$

(b) The new Hamiltonian matrix is given by

$$H = \begin{pmatrix} E_0 + \epsilon_1 & A \\ A & E_0 + \epsilon_2 \end{pmatrix}\ ,$$

and its exact eigenvalues E are determined from

$$\det\begin{pmatrix} E_0 + \epsilon_1 - E & A \\ A & E_0 + \epsilon_2 - E \end{pmatrix} = 0\ .$$

We find

$$E_\pm = E_0 + \frac{\epsilon_1 + \epsilon_2}{2} \pm \sqrt{\left(\frac{\epsilon_1 - \epsilon_2}{2}\right)^2 + A^2}\ .$$

(c) When $|\epsilon_1|, |\epsilon_2| \ll |A|$, we consider H'' as a perturbation to $H_0 + H'$. In first-order perturbation theory, we have

$$E_\pm = E_0 \pm A + \langle\psi_\pm|H''|\psi_\pm\rangle = E_0 \pm A + \frac{\epsilon_1 + \epsilon_2}{2}\ .$$

Expanding the exact result to first order in ϵ_i, we find

$$E_\pm = E_0 + \frac{\epsilon_1 + \epsilon_2}{2} \pm A + \ldots$$

which coincides with the first-order perturbation theory result.

(d) When $|A| \ll |\epsilon_2 - \epsilon_1|$, we can treat H' as a perturbation to $H_0^\epsilon = H_0 + H''$. The Hamiltonian matrix H_0^ϵ is given by

$$H_0^\epsilon = \begin{pmatrix} E_0 + \epsilon_1 & 0 \\ 0 & E_0 + \epsilon_2 \end{pmatrix}\ ,$$

with eigenvectors $\psi_1 = \binom{1}{0}$ and $\psi_2 = \binom{0}{1}$. The correction to the energies in first-order perturbation theory vanishes

$$\langle\psi_{1,2}|H'|\psi_{1,2}\rangle = 0\ .$$

In second-order perturbation theory

$$E_{\pm} = E_0 + \epsilon_{1,2} + \frac{|\langle\psi_{2,1}|H'|\psi_{1,2}\rangle|^2}{(E_0 + \epsilon_{1,2}) - (E_0 + \epsilon_{2,1})} = E_0 + \epsilon_{1,2} + \frac{A^2}{\epsilon_{1,2} - \epsilon_{2,1}} \ .$$

Expanding the exact result in (b) to second order in $A/(\epsilon_2 - \epsilon_1)$, we find

$$\begin{aligned} E_{\pm} &= E_0 + \frac{\epsilon_1 + \epsilon_2}{2} \pm \frac{\epsilon_1 - \epsilon_2}{2}\sqrt{1 + \left(\frac{2A}{\epsilon_1 - \epsilon_2}\right)^2} = E_0 + \frac{\epsilon_1 + \epsilon_2}{2} \pm \frac{\epsilon_1 - \epsilon_2}{2}\left[1 + 2\frac{A^2}{(\epsilon_1 - \epsilon_2)^2}\right] \\ &= E_0 + \epsilon_{1,2} \pm \frac{A^2}{\epsilon_1 - \epsilon_2} = E_0 + \epsilon_{1,2} + \frac{A^2}{\epsilon_{1,2} - \epsilon_{2,1}} \ , \end{aligned}$$

which coincides with the second-order perturbation theory result.