Física Quântica I / Mecânica Quântica (2021/22)

Folha de Problemas 6 (consolidação dos postulados)

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— Soluções —

Problema 1 | Sistema de 3 níveis

Considere uma partícula quântica que pode ocupar apenas uma de três posições diferentes, $\{x_1, x_2, x_3\}$, e cujos estados correspondentes definem uma base ortonormal: $\{|x_1\rangle, |x_2\rangle, |x_3\rangle\}$. Sabe-se que a ação do Hamiltoniano da partícula nesta base é a seguinte:

$$\hat{H}|x_1\rangle = \hbar\omega|x_3\rangle, \quad \hat{H}|x_2\rangle = \hbar\omega|x_2\rangle, \quad \hat{H}|x_3\rangle = \hbar\omega|x_1\rangle,$$

onde $\hbar\omega > 0$ é constante e com dimensões de energia. Imediatamente *antes* do instante $t = 0$ mediu-se a posição da partícula, tendo esta sido encontrada em x_1.

1. *Calcule* o valor esperado e a incerteza na energia da partícula no instante $t = 0$.

2. *Explique* como é que o resultado anterior nos permite concluir que o vetor de estado da partícula não é um auto-estado do Hamiltoniano.

3. *Calcule* os possíveis resultados de uma medição de energia e as respetivas probabilidades.

4. *Determine* a dependência temporal do vetor de estado. Isto é, determine $\psi_1(t)$, $\psi_2(t)$ e $\psi_3(t)$ tais que:
$$|\psi(t)\rangle = \psi_1(t)\,|x_1\rangle + \psi_2(t)\,|x_2\rangle + \psi_3(t)\,|x_3\rangle.$$

5. Como varia o valor esperado da energia com o tempo, assumindo que não é efetuada nenhuma medição desde $t = 0$?

6. No instante $T = \pi/(3\omega)$ é novamente medida a posição da partícula. Onde é mais provável encontrá-la, e com que probabilidade?

7. Assuma que na medição anterior se obteve o valor mais provável da posição. Imediatamente a seguir, foi medida a energia tendo-se obtido o valor mais elevado possível. Qual é o vetor de estado após esta medição da energia, expresso na base $\{|x_i\rangle\}$?

Solution

1. We need to compute two things: the expectation value of the energy, $\langle\hat{H}\rangle_\psi \equiv \langle\psi|\hat{H}|\psi\rangle$, and the energy uncertainty, which is given by

$$\delta H \equiv \sqrt{\langle\hat{H}^2\rangle - \langle\hat{H}\rangle^2},$$

where the averages are computed in the state vector of the system $|\psi\rangle$. So, before anything else, we must know what the state vector is at $t = 0$. The text of the problem tells us that immediately before $t = 0$, the position measurement yielded $\mathcal{X} \to x_1$. According to the postulate on the reduction of the state vector (P6), immediately after this measurement we should have the reduction to

$$|\psi\rangle = \cdots \quad \xrightarrow[t=0]{\mathcal{X}\to x_1} \quad |\psi\rangle = |x_1\rangle.$$

Therefore, the state vector we must use at $t = 0$ is

$$|\psi\rangle = |x_1\rangle.$$

We can now compute the two expectation values we need:

$$\langle\hat{H}\rangle_\psi = \langle\psi|\hat{H}|\psi\rangle = \langle x_1|\hat{H}|x_1\rangle = \hbar\omega\langle x_1|x_3\rangle = 0,$$

$$\langle\hat{H}^2\rangle_\psi = \langle\psi|\hat{H}^2|\psi\rangle = \langle x_1|\hat{H}\hat{H}|x_1\rangle = \hbar\omega\langle x_1|\hat{H}|x_3\rangle = (\hbar\omega)^2\langle x_1|x_1\rangle = (\hbar\omega)^2.$$

Combining these two results, in conclusion, we obtain for the expectation value and for the uncertainty in the energy of the system at $t = 0$ the results

$$\langle\hat{H}\rangle_\psi = 0, \qquad \delta H = \sqrt{\langle\hat{H}^2\rangle_\psi - \langle\hat{H}\rangle_\psi^2} = \hbar\omega.$$

2. In an eigenstate of $\hat{H}$, the energy uncertainty *always* will be zero. Since we found in the previous question that $\delta H \neq 0$, it follows that the system cannot be in an eigenstate of $\hat{H}$.

   Note: the reason is that, if the state vector coincides with an eigenstate of $\hat{H}$ associated with the energy eigenvalue ε (in other words if $|\psi\rangle = |\varepsilon\rangle$) it follows that

   $$\hat{H}|\varepsilon\rangle = \varepsilon|\varepsilon\rangle \quad \longrightarrow \quad \langle\varepsilon|\hat{H}|\varepsilon\rangle = \varepsilon, \qquad \hat{H}^2|\varepsilon\rangle = \varepsilon^2|\varepsilon\rangle \quad \longrightarrow \quad \langle\varepsilon|\hat{H}^2|\varepsilon\rangle = \varepsilon^2,$$

   and therefore the energy uncertainty in this state is

   $$\delta H\Big|_{|\psi\rangle=|\varepsilon\rangle} = \sqrt{\langle\varepsilon|\hat{H}^2|\varepsilon\rangle - \big(\langle\varepsilon|\hat{H}|\varepsilon\rangle\big)^2} = 0.$$

   This is always verified for any energy eigenstate.

3. The possible outcomes of a measurement of energy are the eigenvalues of the Hamiltonian, which we can call ε_n and designate the associated eigenstate by $\{|\varepsilon_n\rangle$. The probabilities associated with each of the outcomes ε_n in the energy measurement are given by (probability postulate, P4):

   $$\mathcal{P}(\varepsilon_n) = |\langle\varepsilon_n|\psi\rangle|^2.$$

   Hence, in order to answer this question, we need to determine both the eigenvalues ε_n and the associated eigenvectors $|\varepsilon_n\rangle$. Let's do that in two stages.

   Eigenvalues of $\hat{H}$ — We need the matrix representation of $\hat{H}$ in the given basis. Starting from the action of $\hat{H}$ on the basis kets $|x_i\rangle$ given in the text of the problem, we find that the only non-zero matrix elements will be

   $$\langle x_3|\hat{H}|x_1\rangle = \langle x_2|\hat{H}|x_2\rangle = \langle x_1|\hat{H}|x_3\rangle = \hbar\omega,$$

and therefore the matrix representation is given by

$$\hat{H} \quad \mapsto \quad H = \hbar\omega \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}.$$

From here, we determine the eigenvalues explicitly as follows (leaving the constant $\hbar\omega$ out for a moment).

$$\det(H - \lambda\mathbf{1}) = 0 \quad \Leftrightarrow \quad \begin{vmatrix} -\lambda & 0 & 1 \\ 0 & 1-\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = 0 \quad \Leftrightarrow \quad \lambda = \begin{cases} -1, \\ +1, \quad \text{(2-degenerate)}. \end{cases}$$

Therefore, there are only two possible outcomes in a measurement of the energy. Putting back the overall factor $\hbar\omega$, those two energies are

$$\varepsilon_1 = -\hbar\omega, \qquad \varepsilon_2 = +\hbar\omega \quad \text{(2-degenerate)}.$$

Eigenvectors of $\hat{H}$ — Since there are only two distinct outcomes, we only need to calculate one of those probabilities, and it is easier to do that for the non-degenerate eigenvalue. The corresponding eigenvector is obtained from

$$\varepsilon_1 = -\hbar\omega: \qquad \begin{bmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \begin{cases} u + w = 0 \\ v = 0 \end{cases} \qquad \Leftrightarrow \quad \begin{bmatrix} u \\ v \\ w \end{bmatrix} \propto \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix},$$

so that, after normalization, we arrive at

$$|\varepsilon_1\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ -1 \end{bmatrix}.$$

The probabilities of either outcome are therefore

$$\mathcal{P}(\varepsilon_1) = |\langle\varepsilon_1|\psi\rangle|^2 = |\langle\varepsilon_1|x_1\rangle|^2 = \frac{1}{2} \qquad \text{and} \qquad \mathcal{P}(\varepsilon_2) = 1 - \mathcal{P}(\varepsilon_1) = \frac{1}{2}.$$

This completes the response to this question. For completeness, we show now how to determine a set of orthogonal eigenvectors associated with the degenerate eigenvalue as well, which will be useful in the next question:

$$\varepsilon_2 = \hbar\omega: \qquad \begin{bmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \quad u = w \quad \Leftrightarrow \quad \begin{bmatrix} u \\ v \\ w \end{bmatrix} = \begin{bmatrix} u \\ v \\ u \end{bmatrix}.$$

The freedom in choosing any u and v stems for the degeneracy of the eigenvalue ε_2. The simplest first choice is to take $v = 0$, $u \neq 0$, and set

$$|\varepsilon_2^{(1)}\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix},$$

and the second choice for $|\varepsilon_2^{(2)}\rangle$ is made by requiring that $\langle\varepsilon_2^{(1)}|\varepsilon_2^{(2)}\rangle = 0$:

$$\begin{bmatrix} 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} u \\ v \\ w \end{bmatrix} = 0 \quad \Leftrightarrow \quad u = 0 \qquad \longrightarrow \qquad |\varepsilon_2^{(2)}\rangle \mapsto \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}.$$

Therefore, a complete set of orthogonal and normalized eigenvectors of $\hat{H}$ is

$$|\varepsilon_1\rangle \mapsto \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\-1\end{bmatrix}, \qquad |\varepsilon_2^{(1)}\rangle \mapsto \frac{1}{\sqrt{2}}\begin{bmatrix}1\\0\\1\end{bmatrix}, \qquad |\varepsilon_2^{(2)}\rangle \mapsto \begin{bmatrix}0\\1\\0\end{bmatrix},$$

where we used the notation $|\varepsilon_2^{(\alpha)}\rangle$ discussed in the lectures to distinguish the two distinct eigenvectors that belong to the same eigenvalue ε_2: $|\varepsilon_2^{(1)}\rangle$ and $|\varepsilon_2^{(2)}\rangle$.

4. The time-evolved state is given, in the most general case, by

$$|\psi(t)\rangle = \sum_n e^{-iE_n t/\hbar} \sum_{\alpha=1}^{g_n} \langle \varepsilon_n^{(\alpha)}|\psi(0)\rangle |\varepsilon_n^{(\alpha)}\rangle,$$

where the second summation over α covers the distinct eigenstates belonging to the same degenerate eigenvalue. In our case, this general expression for $|\psi(t)\rangle$ becomes

$$\begin{aligned}|\psi(t)\rangle &= e^{-i\varepsilon_1 t/\hbar}\langle\varepsilon_1|\psi(0)\rangle|\varepsilon_1\rangle + e^{-i\varepsilon_2 t/\hbar}\langle\varepsilon_2^{(1)}|\psi(0)\rangle|\varepsilon_2^{(1)}\rangle + e^{-i\varepsilon_2 t/\hbar}\langle\varepsilon_2^{(2)}|\psi(0)\rangle|\varepsilon_2^{(2)}\rangle \\ &= \frac{e^{i\omega t}}{\sqrt{2}}|\varepsilon_1\rangle + \frac{e^{-i\omega t}}{\sqrt{2}}|\varepsilon_2^{(1)}\rangle,\end{aligned}$$

which we can write back in the original basis by expanding the energy eigenstates we found in the previous question:

$$\begin{aligned}|\psi(t)\rangle &= \frac{e^{i\omega t}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|x_1\rangle - \frac{1}{\sqrt{2}}|x_3\rangle\right) + \frac{e^{-i\omega t}}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}|x_1\rangle + \frac{1}{\sqrt{2}}|x_3\rangle\right) \\ &= \cos(\omega t)\,|x_1\rangle - i\sin(\omega t)\,|x_3\rangle.\end{aligned}$$

The requested amplitude functions are thus

$$\psi_1(t) = \cos(\omega t), \qquad \psi_2(t) = -i\sin(\omega t), \qquad \psi_3(t) = 0.$$

5. When the system is evolving in time and there is no measurement, the expectation value of the energy remains unchanged. This follows by a direct application of Ehrenfest's theorem to the expectation values of $\hat{H}$:

$$i\hbar\frac{\partial}{\partial t}\langle\psi(t)|\hat{H}|\psi(t)\rangle = \langle\psi(t)|[\hat{H},\,\hat{H}]|\psi(t)\rangle + i\hbar\langle\psi(t)|\frac{\partial}{\partial t}\hat{H}|\psi(t)\rangle = 0.$$

Consequently,

$$\langle\psi(t)|\hat{H}|\psi(t)\rangle = \langle\psi(0)|\hat{H}|\psi(0)\rangle = 0,$$

where we used the result of question 1, where we determined the expectation value at $t = 0$ (if you wish, you can confirm this explicitly by computing the expectation value with $|\psi(t)\rangle$ obtained in the previous question).

6. The state vector at $t = T = \pi/(3\omega)$ will be

$$|\psi(t)\rangle = \cos\frac{\pi}{3}\,|x_1\rangle - i\sin\frac{\pi}{3}\,|x_3\rangle = \frac{1}{2}\,|x_1\rangle - \frac{i\sqrt{3}}{2}\,|x_3\rangle.$$

which means that the particle is more likely to be found at position x_3 with probability

$$\mathcal{P}(x_3, T) = |\langle x_3|\psi(T)\rangle|^2 = \frac{3}{4}.$$

7. The more likely value of the position is x_3. Immediately after a measurement yields this value, the state vector is reduced/projected to the corresponding eigenstate of the position:

$$|\psi(t)\rangle \quad \xrightarrow[t=T]{\mathcal{X}\to x_3} \quad |\psi(T^+)\rangle = \hat{\mathrm{P}}_{\{x_3\}}|\psi(T)\rangle = |x_3\rangle.$$

Now, immediately after this, where the state vector of the system has been reduced to $|x_3\rangle$, we measure the energy and obtain the value $\varepsilon_2 = \hbar\omega$ (according to what we found in question 2 above, this is the highest among ε_1 and ε_2). The state vector will undergo another reduction/projection, this time into the subspace associated with the energy eigenvalue found (ε_2):

$$|x_3\rangle \quad \xrightarrow{\mathcal{H}\to\varepsilon_2} \quad |\psi\rangle = \hat{\mathrm{P}}_{\{\varepsilon_2\}}|x_3\rangle.$$

Since ε_2 is the doubly degenerate eigenvalue, the projector is given by the two terms

$$\hat{\mathrm{P}}_{\{\varepsilon_2\}} = |\varepsilon_2^{(1)}\rangle\langle\varepsilon_2^{(1)}| + |\varepsilon_2^{(2)}\rangle\langle\varepsilon_2^{(2)}|,$$

and so

$$\hat{\mathrm{P}}_{\{\varepsilon_2\}}|x_3\rangle = |\varepsilon_2^{(1)}\rangle\langle\varepsilon_2^{(1)}|x_3\rangle + |\varepsilon_2^{(2)}\rangle\langle\varepsilon_2^{(2)}|x_3\rangle = \frac{1}{\sqrt{2}}|\varepsilon_2^{(1)}\rangle.$$

This means that the normalized state vector after the energy measurement is

$$|\psi\rangle = |\varepsilon_2^{(1)}\rangle = \frac{1}{\sqrt{2}}|x_1\rangle + \frac{1}{\sqrt{2}}|x_3\rangle.$$
