Quantum Mechanics III — Epiphany Term 2009

Lecturer: Dr. Benjamin Doyon

Homework 1 – due 10 February 2009

1. A quantum system has an observable $\hat{A}$ that can take values -1, 0 and 1. The corresponding orthonormal eigenstates are $|-1\rangle$, $|0\rangle$ and $|1\rangle$. The system evolves in time with the hamiltonian $\hat{H}$ whose action on these states is given by

$$\begin{aligned}\hat{H}|-1\rangle &= -|-1\rangle + 2i|1\rangle \\ \hat{H}|0\rangle &= 2|0\rangle \\ \hat{H}|1\rangle &= -2i|-1\rangle + |1\rangle\end{aligned}$$

   (a) Find the stationary state-vectors and their energies.

   (b) Initially $\hat{A}$ is measured and found to be 1. The system then evolves for a time t. At that time, if a measure of $\hat{A}$ is performed, what values may be obtained and with what probabilities? What are the expectation value $\langle\hat{A}\rangle$ and standard deviation $\Delta\hat{A}$ of $\hat{A}$? If, instead, a measure of the energy is performed at the time t, what values may be obtained and with what probabilities? Do they depend on time? Why?

2. Given the solution of the free-particle problem (in one dimension) as

$$\psi(x,t) = \int_{-\infty}^{\infty} dx' \psi_0(x') f_t(x-x')$$

with the integral kernel given by

$$f_t(x-x') = \sqrt{\frac{m}{2i\pi\hbar t}}\, e^{\frac{im(x-x')^2}{2\hbar t}},$$

evaluate $|\psi(x,t)|^2$ for the initial condition (which is here properly normalised)

$$\psi_0(x) = \frac{1}{\sqrt{a_0\sqrt{\pi}}} e^{-\frac{x^2}{2a_0^2}}$$

(**hint**: no need to keep track of the constant pre-factors all the time; just the x-dependence of the exponential suffices, since we know that the wave function always is normalised, so that we can re-calculate the modulus-squared of the normalisation constant at the end). Observe the increase of the width of the Gaussian with time.

Answer

1. (a) In matrix form:

$$|-1\rangle = \begin{pmatrix}1\\0\\0\end{pmatrix}, \quad |0\rangle = \begin{pmatrix}0\\1\\0\end{pmatrix}, \quad |1\rangle = \begin{pmatrix}0\\0\\1\end{pmatrix}$$

the hamiltonian is

$$\hat{H} = \left(\begin{array}{ccc} -1 & 0 & -2i \\ 0 & 2 & 0 \\ 2i & 0 & 1 \end{array} \right) \tag{1}$$

The characteristc polynomial equation that gives the eigenvalues E is

$$0 = \det(H - E\mathbf{1}) = (-1-E)(2-E)(1-E) - 2i(-2i)(2-E) = (2-E)(E^2-5)$$

We find $E = 2$ and $E = \pm\sqrt{5}$. For the eigenstates (the stationary states), consider $|v\rangle = v_1|-1\rangle + v_2|0\rangle + v_3|1\rangle$. The eigenvalue equation $\hat{H}|v\rangle = E|v\rangle$ gives:

$$\begin{aligned} -v_1 - 2iv_3 &= Ev_1 \\ 2v_2 &= Ev_2 \\ 2iv_1 + v_3 &= Ev_3 \end{aligned}$$

In the case $E = 2$, we find from the first and last equation $v_1 = v_3 = 0$ so that $|E = 2\rangle = |0\rangle$. In the case $E = \sqrt{5}$, we must have $v_2 = 0$ and we find $v_1 = (\sqrt{5}-1)/(2i)v_3 = -2i/(\sqrt{5}+1)$. In the case $E = -\sqrt{5}$, we again have $v_2 = 0$ and we find $v_1 = -(\sqrt{5}+1)/(2i)$. Normalising to $\langle v|v\rangle = 1$, we find:

$$\begin{aligned} E = 2 \quad &: \quad |E = 2\rangle = |0\rangle \\ E = \sqrt{5} \quad &: \quad |E = \sqrt{5}\rangle = \sqrt{\frac{2}{5-\sqrt{5}}}\left(\frac{\sqrt{5}-1}{2i}|-1\rangle + |1\rangle\right) \\ E = -\sqrt{5} \quad &: \quad |E = -\sqrt{5}\rangle = \sqrt{\frac{2}{5+\sqrt{5}}}\left(-\frac{\sqrt{5}+1}{2i}|-1\rangle + |1\rangle\right) \end{aligned} \tag{2}$$

(b) When a measurement is performed, the state of the system just after the measurement is the state corresponding to the value observed – this is the collapse of the wave function. Hence, here we have $|\Psi(0)\rangle = |1\rangle$. We have to write this initial state in the basis of the hamiltonian eigenstates, in order to be able to evolve it in time. With the decomposition of the identity operator in the energy basis, $\mathbf{1} = |E = 2\rangle\langle E = 2| + |E = \sqrt{5}\rangle\langle E = \sqrt{5}| + |E = -\sqrt{5}\rangle\langle E = -\sqrt{5}|$, we have

$$|1\rangle = |E = 2\rangle\langle E = 2|1\rangle + |E = \sqrt{5}\rangle\langle E = \sqrt{5}|1\rangle + |E = -\sqrt{5}\rangle\langle E = -\sqrt{5}|1\rangle$$

so that

$$|\Psi(0)\rangle = \sqrt{\frac{2}{5-\sqrt{5}}}|E = \sqrt{5}\rangle + \sqrt{\frac{2}{5+\sqrt{5}}}|E = -\sqrt{5}\rangle \tag{3}$$

Evolving this state for a time t, we just have to multiply by $e^{-i\hat{H}t/\hbar}$, giving

$$|\Psi(t)\rangle = \sqrt{\frac{2}{5-\sqrt{5}}}e^{-i\sqrt{5}t/\hbar}|E = \sqrt{5}\rangle + \sqrt{\frac{2}{5+\sqrt{5}}}e^{i\sqrt{5}t/\hbar}|E = -\sqrt{5}\rangle$$

The values of $\hat{A}$ that can be obtained are just those stated in the question: -1, 0 and 1. In order to find their respective probabilities, we must re-write the evolved state in the basis of the $\hat{A}$-eigenstates, $|-1\rangle$, $|0\rangle$ and $|1\rangle$, using the explicit expressions we found for the energy eigenstates. This can be written in column vector, and gives

$$|\Psi(t)\rangle = \begin{pmatrix} -\frac{2}{\sqrt{5}}\sin(\sqrt{5}t/\hbar) \\ 0 \\ \cos(\sqrt{5}t/\hbar) - \frac{i}{\sqrt{5}}\sin(\sqrt{5}t/\hbar) \end{pmatrix}$$

The probability for measuring a value n is just $P(n) = |\langle n|\Psi(t)\rangle|^2$, for $n = -1, 0, 1$. Hence, the probabilities are as follows:

$$\begin{aligned} P(-1) &= \frac{4}{5}\sin^2(\sqrt{5}t/\hbar) \\ P(0) &= 0 \\ P(1) &= \cos^2(\sqrt{5}t/\hbar) + \frac{1}{5}\sin^2(\sqrt{5}t/\hbar) = 1 - \frac{4}{5}\sin^2(\sqrt{5}t/\hbar) \end{aligned}$$

Note that they add up to 1 for any t, as it should. Also, at $t = 0$, we have $P(-1) = P(0) = 0$ and $P(1) = 1$, as it should also, since the initial state was just after measuring the value 1. The expectation value of $\hat{A}$ is just $-P(-1) + P(1)$, that is

$$\langle\hat{A}\rangle = \cos^2(\sqrt{5}t/\hbar) - \frac{3}{5}\sin^2(\sqrt{5}t/\hbar) = 1 - \frac{8}{5}\sin^2(\sqrt{5}t/\hbar)$$

The standard deviation is $\sqrt{\langle\hat{A}^2\rangle - \langle\hat{A}\rangle^2} = \sqrt{P(-1) + P(1) - \langle\hat{A}\rangle^2}$, and we find $\langle\hat{A}^2\rangle = 1$ giving

$$\Delta\hat{A} = \frac{4}{5}\left|\sin(\sqrt{5}t/\hbar)\right|\sqrt{1 + 4\cos^2(\sqrt{5}t/\hbar)}$$

Note that $\Delta\hat{A}$ is zero periodically, at the times when $P(-1) = 0$, because at these times, we have a sure value of 1 (i.e. $P(1) = 1$), so a these times the variance of $\hat{A}$ must be zero.

Finally, if we measure the energy instead, the values we can obtain are 2, $\sqrt{5}$ or $-\sqrt{5}$, and the probabilities are just given by the modulus squared of each the coefficients in the decomposition (3) (time evolution doesn't affect these probabilities, because $\hat{H}$ is a conserved quantity):

$$\begin{aligned} P(E = 2) &= 0 \\ P(E = \sqrt{5}) &= \frac{2}{5 - \sqrt{5}} \\ P(E = -\sqrt{5}) &= \frac{2}{5 + \sqrt{5}} \end{aligned}$$

which add up to 1 as it should.

2. We have

$$\psi(x,t) \propto \int_{-\infty}^{\infty} dx' \exp\left[-\frac{(x')^2}{2a_0^2} + \frac{im(x-x')^2}{2\hbar t}\right]$$

where proportionality constants do not depend on x. Doing the integral, we get the exact x dependence, and the proportionality constant can always be recovered by normalising the wave function (the normalisation is always 1, at all times, since time evolution is a unitary transformation of states). Doing the integral, we have to complete the square. In the exponential, we have

$$\frac{im}{2t\hbar}x^2 - \frac{im}{t\hbar}xx' + \left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right)(x')^2$$

We change variable $x' \mapsto x' + A$, and look at the resulting *linear* terms in x', which we must set to zero:

$$\left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right) 2Ax' - \frac{im}{t\hbar}xx' = 0$$

This gives

$$A = \frac{imx}{2t\hbar\left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right)} = \frac{x}{1 - \frac{t\hbar}{ima_0^2}}$$

Then, in the exponential we have only the terms in $(x')^2$ and in $(x')^0$, and this gives

$$\frac{im}{2t\hbar}x^2 - \frac{im}{t\hbar}xA + \left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right)A^2 + \left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right)(x')^2$$

We see that the term in $(x')^2$ does not depend on x; hence the integral over x' only gives another proportionality constant that is x independent. Hence, we find

$$\psi(x,t) \propto \exp\left[\frac{im}{2t\hbar}x^2 - \frac{im}{t\hbar}xA + \left(\frac{im}{2t\hbar} - \frac{1}{2a_0^2}\right)A^2\right]$$

The last term in this exponential may be simplified to $\frac{im}{2t\hbar}xA$, which gives

$$\begin{aligned}
\psi(x,t) &\propto \exp\left[\frac{im}{2t\hbar}x^2 - \frac{im}{t\hbar}xA + \frac{im}{2t\hbar}xA\right] \\
&= \exp\left[\frac{im}{2t\hbar}x^2 - \frac{im}{2t\hbar}xA\right] \\
&= \exp\left[\frac{im}{2t\hbar}x(x-A)\right] \\
&= \exp\left[-\frac{x^2}{2a_0^2\left(1 - \frac{t\hbar}{ima_0^2}\right)}\right]
\end{aligned}$$

Finally, we then find

$$|\psi(x,t)|^2 = |A|^2 \exp\left[-\frac{x^2}{a_0^2 - \frac{t^2\hbar^2}{m^2a_0^2}}\right] \equiv |A|^2 e^{-\frac{x^2}{a_t^2}}$$

and since we know how to normalise such an exponential, we know that

$$|A|^2 = \frac{1}{a_t\sqrt{\pi}}$$