Quantum Physics 1 - Homework 2

Solutions

1. Quantum Harmonic Oscillator [10pt.]

A particle of mass m is trapped in the harmonic potential $V(x) = \frac{1}{2}m\omega^2 x^2$, with ω being the frequency of oscillation. The normalised wavefunction of this particle at the time $t = 0$ is given by:

$$\Psi(x,0) = \frac{1}{2}\sqrt[4]{\frac{m\omega}{\pi\hbar}}\ [b_+ + ib_-]\ e^{-\frac{m\omega}{2\hbar}x^2}\ ,$$

with $b_\pm = 1 \pm x\sqrt{\frac{2m\omega}{\hbar}}$. Note that $b_\pm$ is a function of x.

a. [2pt.] The given wavefunction $\Psi(x,0)$ can be expressed in terms of the wavefunctions ψ_n of the quantum harmonic oscillator as follows:

$$\Psi(x,0) = \sum_{n=0}^{\infty} c_n\ \psi_n(x). \tag{1}$$

The coefficients c_n can be determined using Fourier's trick:

$$c_n = \frac{1}{\sqrt{n!}}\int \psi_0\ (\hat{a}_-)^n\ \Psi(x,0)\ dx. \tag{2}$$

Calculate c_0 and c_1 explicitly using Fourier's trick.

Hint: Before trying to evaluate any integrals, check whether they're even or odd.

We will use that:

$$\hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p} + m\omega x) = \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right) \tag{3}$$

and that

$$\Psi(x,0) = \frac{1}{2}\sqrt[4]{\frac{m\omega}{\pi\hbar}}\ [b_+ + ib_-]\ e^{-\frac{m\omega}{2\hbar}x^2} \tag{4}$$

$$= \frac{1}{2}\sqrt[4]{\frac{m\omega}{\pi\hbar}}\left[1 + x\sqrt{\frac{2m\omega}{\hbar}} + i - ix\sqrt{\frac{2m\omega}{\hbar}}\right]\ e^{-\frac{m\omega}{2\hbar}x^2} \tag{5}$$

$$= \frac{1}{2}\sqrt[4]{\frac{m\omega}{\pi\hbar}}\left[(1+i) + (1-i)x\sqrt{\frac{2m\omega}{\hbar}}\right]\ e^{-\frac{m\omega}{2\hbar}x^2}. \tag{6}$$

You can recognise this as $\Psi(x,0) = \frac{1}{2}\ [(1+i)\psi_0 + (1-i)\psi_1]$, but where's the fun in that? Calculating explicitly:

$$c_0 = \int_{-\infty}^{\infty} \psi_0\ (\hat{a}_-)^0\ \Psi(x,0)\ dx \tag{7}$$

$$= \int_{-\infty}^{\infty} \psi_0 \; \Psi(x,0) \; dx \tag{8}$$

$$= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \left[(1+i) + (1-i)x\sqrt{\frac{2m\omega}{\hbar}}\right] \; e^{-\frac{m\omega}{2\hbar}x^2} \; dx \tag{9}$$

The second term in square brackets makes the integrand odd in x, and given that our integration interval is even, it integrates to zero. Only the first term survives:

$$c_0 = \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; (1+i) \; e^{-\frac{m\omega}{2\hbar}x^2} \; dx \tag{10}$$

$$= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \; (1+i) \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2} \; dx \tag{11}$$

$$= \frac{1}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \; (1+i)\sqrt{\frac{\pi\hbar}{m\omega}} \tag{12}$$

$$= \frac{1+i}{2}. \tag{13}$$

For the next coefficient, we get:

$$c_1 = \int_{-\infty}^{\infty} \psi_0 \; (\hat{a}_-)^1 \; \Psi(x,0) \; dx = \int_{-\infty}^{\infty} \psi_0 \; \hat{a}_- \; \Psi(x,0) \; dx \tag{14}$$

$$= \frac{1}{2}\frac{1}{\sqrt{2\hbar m\omega}}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \left(\hbar\frac{d}{dx} + m\omega x\right) \; \left\{\left[(1+i) + (1-i)x\sqrt{\frac{2m\omega}{\hbar}}\right] \; e^{-\frac{m\omega}{2\hbar}x^2}\right\} \; dx \tag{15}$$

$\hat{a}_-$ applied on the first term in square brackets is no good: both the $\frac{d}{dx}$ and x term will transform it to an odd function in x. So, only the second term needs to be evaluated:

$$c_1 = \frac{1}{2}\frac{1}{\sqrt{2\hbar m\omega}}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \left(\hbar\frac{d}{dx} + m\omega x\right) \; \left\{(1-i)x\sqrt{\frac{2m\omega}{\hbar}} \; e^{-\frac{m\omega}{2\hbar}x^2}\right\} \; dx \tag{16}$$

$$= \frac{1-i}{2\hbar}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \left(\hbar\frac{d}{dx} + m\omega x\right) \; \left\{x \; e^{-\frac{m\omega}{2\hbar}x^2}\right\} \; dx \tag{17}$$

$$= \frac{1-i}{2\hbar}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \left\{\hbar + \hbar \cdot x \cdot -\frac{m\omega x}{\hbar} + m\omega x^2\right\} e^{-\frac{m\omega}{2\hbar}x^2} \; dx \tag{18}$$

$$= \frac{1-i}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} \; \{\hbar\} \, e^{-\frac{m\omega}{2}x^2} \; dx \tag{19}$$

$$= \frac{1-i}{2}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{\hbar}x^2} \; dx = \frac{1-i}{2}\sqrt{\frac{m\omega}{\pi\hbar}}\sqrt{\frac{\pi\hbar}{m\omega}} \tag{20}$$

$$= \frac{1-i}{2} \tag{21}$$

Since the wavefunction is given to be normalised, and since $|c_0|^2 + |c_1|^2 = 1$, we know already now the other coefficients should be zero.

b. [1pt.] Calculate $\sum_{n=0}^{1} |c_n|^2$. Does your answer make sense? Explain why. (If you didn't manage to solve question (a), you can take $\Psi(x,0) = \frac{1}{\sqrt{2}}(\psi_0 + i\psi_1)$ for the subsequent calculations.)

Yes:

$$\sum_{n=0}^{\infty} |c_n|^2 = |c_0|^2 + |c_1|^2 = \frac{|1+i|^2}{2^2} + \frac{|1-i|^2}{2^2} = \frac{2}{4} + \frac{2}{4} = 1. \tag{22}$$

This makes sense because $|c_n|^2$ represents a probability. The sum over all configurations should hence be 1 (assuming a proper normalisation).

c. [1pt.] What happens when you try to calculate c_2 or higher coefficients?

Physically, we note that the wavefunction can be expressed in terms of ψ_0 and ψ_1 only. This means that if we apply the lowering operator $\hat{a}_-$ at least twice (for coefficients c_2 and higher), than we destroy both ψ_0 and ψ_1. In other words, all ψ_n components are annihilated and the integral for c_2 (and higher) will be zero for sure.

Mathematically, we can show this as follows (this derivation is by no means required, it's just here to show what happens mathematically). We can check c_m, $m \geq 2$ using our previous results:

$$c_m = \frac{1}{4\hbar m\omega}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2}\, (\hat{a}_-)^m \left\{\left[(1+i) + (1-i)x\sqrt{\frac{2m\omega}{\hbar}}\right]\, e^{-\frac{m\omega}{2\hbar}x^2}\right\} dx \tag{23}$$

$$= \frac{1}{4\hbar m\omega}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2}\, (\hat{a}_-)^{m-1} \left(\hbar\frac{d}{dx} + m\omega x\right) \left\{\left[(1+i) + (1-i)x\sqrt{\frac{2m\omega}{\hbar}}\right]\, e^{-\frac{m\omega}{2\hbar}x^2}\right\} dx \tag{24}$$

$$= \frac{1}{4\hbar m\omega}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} (\hat{a}_-)^{m-1} \left\{\left[(1+i)(-m\omega x + m\omega x) + (1-i)\sqrt{2m\omega\hbar}\right]\, e^{-\frac{m\omega}{2\hbar}x^2}\right\} dx \tag{25}$$

$$= \frac{1}{4\hbar m\omega}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} (\hat{a}_-)^{m-2} \left(\hbar\frac{d}{dx} + m\omega x\right) \left\{(1-i)\, \sqrt{2m\omega\hbar}\, e^{-\frac{m\omega}{2\hbar}x^2}\right\} dx \tag{26}$$

$$= \frac{1-i}{\sqrt{2\hbar m\omega}}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} (\hat{a}_-)^{m-2} \left(\hbar\frac{d}{dx} + m\omega x\right) e^{-\frac{m\omega}{2\hbar}x^2} dx \tag{27}$$

$$= \frac{1-i}{\sqrt{2\hbar m\omega}}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} (\hat{a}_-)^{m-2} \left(\hbar \cdot -\frac{m\omega x}{\hbar} + m\omega x\right) e^{-\frac{m\omega}{2\hbar}x^2} dx \tag{28}$$

$$= \frac{1-i}{\sqrt{2\hbar m\omega}}\sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\infty}^{\infty} e^{-\frac{m\omega}{2\hbar}x^2} (\hat{a}_-)^{m-2}\, (0)\, e^{-\frac{m\omega}{2\hbar}x^2} dx \tag{29}$$

$$= 0. \tag{30}$$

So, the series terminates at $m = 2$: for any integer $n \geq m = 2$, $c_n = 0$ for sure. Therefore, we have that

$$\Psi(x,0) = \frac{1}{2}\, \left[(1+i)\psi_0 + (1-i)\psi_1\right] \tag{31}$$

d. [1pt.] Construct $\Psi(x,t)$ by adding the time-dependence to $\Psi(x,0)$.

The energies of ψ_0 and ψ_1 are respectively $E_0 = \frac{1}{2}\hbar\omega$ and $E_1 = \frac{3}{2}\hbar\omega$, hence:

$$\Psi(x,t) = \frac{1}{2}\ \left[(1+i)\psi_0 e^{-\frac{i}{2}\omega t} + (1-i)\psi_1 e^{-\frac{3i}{2}\omega t}\right] \tag{32}$$

e. [2pt.] Calculate $\langle x\rangle$ for the time-dependent wavefunction.

The expectation value for position is:

$$\langle x\rangle = \int \Psi^*(x,t)\ x\ \Psi(x,t)\ dx \tag{33}$$

$$= \int \left[c_0^*\psi_0 e^{\frac{i}{2}\omega t} + c_1^*\psi_1 e^{\frac{3i}{2}\omega t}\right]\ x\ \left[c_0\psi_0 e^{-\frac{i}{2}\omega t} + c_1\psi_1 e^{-\frac{3i}{2}\omega t}\right]\ dx \tag{34}$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \int \left[c_0^*\psi_0 e^{\frac{i}{2}\omega t} + c_1^*\psi_1 e^{\frac{3i}{2}\omega t}\right]\ (\hat{a}_+ + \hat{a}_-)\ \left[c_0\psi_0 e^{-\frac{i}{2}\omega t} + c_1\psi_1 e^{-\frac{3i}{2}\omega t}\right]\ dx \tag{35}$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \int \left[c_0^*\psi_0 e^{\frac{i}{2}\omega t} + c_1^*\psi_1 e^{\frac{3i}{2}\omega t}\right]\ \left[c_0\psi_1 e^{-\frac{i}{2}\omega t} + c_1\sqrt{2}\psi_2 e^{-\frac{3i}{2}\omega t} + c_1\psi_0 e^{-\frac{3i}{2}\omega t}\right]\ dx \tag{36}$$

Here we used that $\hat{a}_+\psi_n = \sqrt{n+1}\psi_{n+1}$, $\hat{a}_-\psi_n = \sqrt{n}\psi_{n-1}$ and $\hat{a}_-\psi_0 = 0$. By the orthonormality of the wavefunctions, $\int \psi_m\psi_n\ dx = \delta_{mn}$, so this reduces to:

$$= \sqrt{\frac{\hbar}{2m\omega}} \left[c_0^* c_1 e^{-i\omega t} + c_0 c_1^* e^{i\omega t}\right] \tag{37}$$

$$= \frac{1}{4}\sqrt{\frac{\hbar}{2m\omega}} \left[(1-i)^2 e^{-i\omega t} + (1+i)^2 e^{i\omega t}\right] \tag{38}$$

$$= \frac{1}{4}\sqrt{\frac{\hbar}{2m\omega}} \left[-2ie^{-i\omega t} + 2ie^{i\omega t}\right] \tag{39}$$

$$= \frac{1}{4}\sqrt{\frac{\hbar}{2m\omega}} \left[-4sin(\omega t)\right] \tag{40}$$

$$= -\sqrt{\frac{\hbar}{2m\omega}} \sin(\omega t) \tag{41}$$

f. [2pt.] We have already seen that we can calculate the expectation value of momentum, $\langle p\rangle$, to get an idea of how the expectation value of position, $\langle x\rangle$, moves over time. Perhaps we're interested in calculating $\langle a\rangle$ today, the expectation value of acceleration:

$$\langle a\rangle = \frac{1}{m}\frac{i}{\hbar}\langle\ [V,\ \hat{p}]\ \rangle. \tag{42}$$

First, calculate the commutator $[V,\ \hat{p}]$ and substitute $V = \frac{1}{2}m\omega^2 x^2$.

Hint: Follow the same steps as in the book by introducing the 'test function' f.

We let the commutator act on a test function f:

$$\begin{aligned}
[V, \hat{p}]\, f &= V\,\hat{p} f - \hat{p} V f && (43)\\
&= -i\hbar\, V\, \frac{d}{dx} f + i\hbar \frac{d}{dx}(V f) && (44)\\
&= -i\hbar\, V\, \frac{d}{dx} f + i\hbar \frac{d}{dx}(V)\, f + i\hbar\, V\, \frac{d}{dx} f && (45)\\
&= i\hbar \frac{d}{dx}(V)\, f && (46)
\end{aligned}$$

So by dropping the test function f again, we find:

$$[V, \hat{p}] = i\hbar \frac{dV}{dx} = i\hbar m\omega^2 x. \qquad (47)$$

g. [1pt.] Calculate $\langle a \rangle$ for this wavefunction. How does your result relate to classical mechanics?

The expectation value for acceleration can now be derived as follows:

$$\begin{aligned}
\langle a \rangle &= \frac{1}{m}\frac{i}{\hbar}\langle\, [V, \hat{p}]\, \rangle && (48)\\
&= \frac{1}{m}\frac{i}{\hbar}\langle\, i\hbar m\omega^2 x\, \rangle && (49)\\
&= -\omega^2 \langle x \rangle = -\frac{k}{m}\langle x \rangle && (50)\\
&= \frac{k}{m}\sqrt{\frac{\hbar}{2m\omega}} \sin(\omega t) && (51)
\end{aligned}$$

Of course, we recognise $\langle a \rangle = -\frac{k}{m}\langle x \rangle$ as being the quantum mechanical version of Hooke's Law from classical dynamics. This shows (by Ehrenfest's Theorem) that quantum expectation values obey the classical laws.

Grade = your points rounded to the nearest integer in $\{1, 4, 7, 10\}$.