Quantum Mechanics III | Michaelmas Term 2009

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Homework 3 – due 8 December 2009

The hamiltonian of the harmonic oscillator is

$$\hat{H} = \frac{\hat{P}^2}{2m} + \frac{m\omega^2}{2}\hat{X}^2 \tag{1}$$

Its eigenvalues are

$$E_N = \hbar\omega\left(\frac{1}{2} + N\right) \tag{2}$$

For its normalised eigenstates $|N\rangle$, we know the action of the ladder operators $\hat{a} = (\hat{P} + im\omega\hat{X})/\sqrt{2m}$ and $\hat{a}^\dagger = (\hat{P} - im\omega\hat{X})/\sqrt{2m}$:

$$\hat{a}|N\rangle = \sqrt{(N+1)\hbar\omega}|N+1\rangle, \quad \hat{a}^\dagger|N\rangle = \sqrt{N\hbar\omega}|N-1\rangle, \tag{3}$$

and we know the explicit form of the eigenfunctions, which are for the first few states, with $\alpha = m\omega/\hbar$:

$$\begin{aligned}
\langle x|0\rangle &= \left(\frac{\alpha}{\pi}\right)^{\frac{1}{4}} e^{-\frac{\alpha x^2}{2}} \\
\langle x|1\rangle &= i\left(\frac{4\alpha}{\pi}\right)^{\frac{1}{4}} \left(\sqrt{\alpha}\, x\right) e^{-\frac{\alpha x^2}{2}} \\
\langle x|2\rangle &= -\left(\frac{4\alpha}{\pi}\right)^{\frac{1}{4}} \left(\alpha x^2 - \frac{1}{2}\right) e^{-\frac{\alpha x^2}{2}}
\end{aligned} \tag{4}$$

Some integrals (for $\mathrm{Re}(\alpha) > 0$ and in general $x_0 \in \mathbb{C}$):

$$\int_{-\infty}^{\infty} dx\, e^{-\alpha(x-x_0)^2} = \sqrt{\frac{\pi}{\alpha}}, \quad \int_{-\infty}^{\infty} dx\, (x-x_0)^2\, e^{-\alpha(x-x_0)^2} = -\frac{d}{d\alpha}\sqrt{\frac{\pi}{\alpha}}, \quad \text{etc.} \tag{5}$$

1. Derive the explicit form of the wave function for the third and fourth energy levels, $\langle x|3\rangle$ and $\langle x|4\rangle$, using the ladder operators and the wave function $\langle x|2\rangle$ given above.

2. For the eigenstate $|N\rangle$, calculate explicitly, using the ladder operators, the averages $\mathbb{E}(X)$, $\mathbb{E}(X^2)$ and $\mathbb{E}(X^3)$. Calculate also the average kinetic energy $\mathbb{E}(P^2/2m)$ (**hint:** it can be deduced immediately from knowing the total energy and the average potential energy).

3. Normalise the wave function $\psi(x) = A\, x\, e^{-kx^2}$ (for $k > 0$). What is the probability, in this state, of finding the energy of the harmonic oscillator to be $\hbar\omega/2$? To be $3\hbar\omega/2$?

4. Normalise the vector $|\psi\rangle = A(2|0\rangle + |1\rangle)$. In this state, what is the probability of finding the position to be in the range $[-\infty, 0]$? What is the probability density of finding the momentum of the particle to be p?

Answers

1. We use the action of $\hat{a}$ on wave functions obtained from that of $\hat{P}$ and $\hat{X}$:
$$\langle x|\hat{a}|\psi\rangle = \frac{1}{\sqrt{2m}}\left(-i\hbar\frac{d}{dx} + im\omega x\right)\langle x|\psi\rangle$$
so that
$$\begin{aligned}\langle x|3\rangle &= \frac{1}{\sqrt{3\hbar\omega}}\langle x|\hat{a}|2\rangle \\ &= \frac{i}{\sqrt{6\alpha}}\left(-\frac{d}{dx} + \alpha x\right)\langle x|2\rangle \\ &= -\frac{i}{\sqrt{6\alpha}}\left(\frac{4\alpha}{\pi}\right)^{\frac{1}{4}}\left(2\alpha^2 x^3 - 3\alpha x\right) e^{-\frac{\alpha x^2}{2}} \\ &= -i\left(\frac{16\alpha}{9\pi}\right)^{\frac{1}{4}}\left((\sqrt{\alpha}x)^3 - \frac{3}{2}\sqrt{\alpha}x\right) e^{-\frac{\alpha x^2}{2}}.\end{aligned}$$
Then also,
$$\begin{aligned}\langle x|4\rangle &= \frac{1}{\sqrt{4\hbar\omega}}\langle x|\hat{a}|3\rangle \\ &= \frac{i}{\sqrt{8\alpha}}\left(-\frac{d}{dx} + \alpha x\right)\langle x|3\rangle \\ &= \frac{1}{\sqrt{8}}\left(\frac{16\alpha}{9\pi}\right)^{\frac{1}{4}}\left(2(\sqrt{\alpha}x)^4 - 6(\sqrt{\alpha}x)^2 + \frac{3}{2}\right) e^{-\frac{\alpha x^2}{2}} \\ &= \left(\frac{4\alpha}{9\pi}\right)^{\frac{1}{4}}\left(\alpha^2 x^4 - 3\alpha x^2 + \frac{3}{4}\right) e^{-\frac{\alpha x^2}{2}}.\end{aligned}$$
We observe that we always have polynomials of parity $(-1)^N$ and degree N, as it should. We can also observe that the number of zeros of the polynomials on the real x-line is equal to N. This is quite a general phenomenon of quantum mechanics: the number of nodes (zeroes) of a one-dimensional wave function increases with the energy level. It essentially means that as the energy is increased, the wave function becomes more oscillating, so it has more zeroes.

2. We must write the momentum and position operators in terms of the ladder operators, whose action on all states we know:
$$\hat{X} = \frac{\hat{a} - \hat{a}^\dagger}{i\omega\sqrt{2m}}, \quad \hat{P} = \sqrt{\frac{m}{2}}(\hat{a} + \hat{a}^\dagger). \tag{6}$$
Then we can evaluate all averages using the orthonormality relation $\langle N|N'\rangle = \delta_{N,N'}$.

First,
$$\begin{aligned}\mathbb{E}(X) &= \langle N|\hat{X}|N\rangle \\ &= \langle N|\frac{\hat{a} - \hat{a}^\dagger}{i\omega\sqrt{2m}}|N\rangle \\ &= \frac{1}{i\omega\sqrt{2m}}\langle N|\left(\sqrt{(N+1)\hbar\omega}|N+1\rangle - \sqrt{N\hbar\omega}|N-1\rangle\right) \\ &= 0.\end{aligned}$$

That is, the average position is 0, which is after all expected from the symmetry $X \to -X$ of the quadratic potential, and which is in agreement with the physical intuition that the particle, as it "oscillates", spends as much time on one side as it does on the other. Second

$$\begin{aligned}
\mathbb{E}(X^2) &= \langle N|\hat{X}^2|N\rangle \\
&= -\frac{1}{2m\omega^2}\langle N|(\hat{a}-\hat{a}^\dagger)^2|N\rangle \\
&= -\frac{1}{2m\omega^2}\langle N|(\hat{a}^2-\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}+(\hat{a}^\dagger)^2)|N\rangle \\
&= -\frac{1}{2m\omega^2}\langle N|(\hat{a}^2+(\hat{a}^\dagger)^2-2\hat{a}\hat{a}^\dagger-\hbar\omega)|N\rangle
\end{aligned}$$

In the last line, we used the commutator $[\hat{a}^\dagger,\hat{a}]=\hbar\omega$ in the relation $\hat{a}^\dagger\hat{a}=\hat{a}\hat{a}^\dagger+[\hat{a}^\dagger,\hat{a}]$. This is useful, because we can use the result

$$\hat{a}\hat{a}^\dagger|N\rangle = \hat{a}\sqrt{N\hbar\omega}|N-1\rangle = N\hbar\omega|N\rangle \tag{7}$$

which expresses the fact that the operator $\hat{a}\hat{a}^\dagger$ "counts" the number of excitations in the state $|N\rangle$ (giving each of them an energy $\hbar\omega$; note that the Hamiltonian is just $\hat{a}\hat{a}^\dagger+\hbar\omega/2$; this is the excitation energy plus the ground-state energy). Then, using the fact that $\hat{a}^2|N\rangle \propto |N+2\rangle$ and that $(\hat{a}^\dagger)^2|N\rangle \propto |N-2\rangle$, we immediately find

$$\mathbb{E}(X^2) = \frac{\hbar}{m\omega}\left(\frac{1}{2}+N\right).$$

This increases with N, which means that although the average position is always 0, the particle becomes more and more spread around 0 as the energy increases. This is again in agreement with physical intuition, that the particle goes further away from its equilibrium position as it oscillates with higher energy. Third, we have

$$\begin{aligned}
\mathbb{E}(X^3) &= \langle N|\hat{X}^3|N\rangle \\
&= i\frac{1}{(2m)^{3/2}\omega^3}\langle N|(\hat{a}-\hat{a}^\dagger)^3|N\rangle \\
&= i\frac{1}{(2m)^{3/2}\omega^3}\langle N|(\hat{a}^3-\hat{a}^2\hat{a}^\dagger-\hat{a}\hat{a}^\dagger\hat{a}-\hat{a}^\dagger\hat{a}^2+\hat{a}(\hat{a}^\dagger)^2+\hat{a}^\dagger\hat{a}\hat{a}^\dagger+(\hat{a}^\dagger)^2\hat{a}-(\hat{a}^\dagger)^3)|N\rangle \\
&= 0
\end{aligned} \tag{8}$$

where the last line is obtained by noticing that every term has different numbers of raising operators and lowering operators, so that from $|N\rangle$ one always gets a state proportional to $|N'\rangle$ with $N' \neq N$. Of course, this result is again natural considering the symmetry of the potential.

For the average kinetic energy $\mathbb{E}(P^2/2m)$, we may use

$$E_N = \hbar\omega\left(\frac{1}{2}+N\right) = \langle N|\hat{H}|N\rangle = \langle N|\frac{\hat{P}^2}{2m}|N\rangle + \langle N|\frac{m\omega^2 X^2}{2}|N\rangle$$

and our previous result. We find, for the average potential energy,

$$\langle N|\frac{m\omega^2 X^2}{2}|N\rangle = \frac{\hbar\omega}{2}\left(\frac{1}{2}+N\right)$$

so that

$$\mathbb{E}(P^2/2m) = \langle N|\frac{\hat{P}^2}{2m}|N\rangle = \frac{\hbar\omega}{2}\left(\frac{1}{2}+N\right).$$

Interestingly, each of the average kinetic and potential energies take exactly *half* of the total average energy E_N for the state $|N\rangle$. This means that for the quantum harmonic oscillator, half of the total energy is in the kinetic energy, the other half is in the potential energy. The same thing happens in the classical statistical mechanics of many oscillators, where it is the "virial theorem".

3. We need to impose that $\int_{-\infty}^{\infty} dx\, \bar{\psi}(x)\psi(x) = 1$. That is,

$$1 = \int_{-\infty}^{\infty} dx\, |A|^2 x^2 e^{-2kx^2} = \frac{1}{2}\sqrt{\frac{\pi}{(2k)^3}}|A|^2 \tag{9}$$

so that $A = (32k^3/\pi)^{\frac{1}{4}}$ up to a phase, which we can take as we wish (for instance, to be 1) since this wave function represents a physical state. The probability that we find the energy to be $\hbar\omega/2$, or the level to be $N = 0$ (i.e. the ground state), is given by the absolute-value-squared of the overlap between the wave function $\langle x|0\rangle$ and the wave function $\psi(x)$:

$$P(E=\hbar\omega/2) = P(N=0) = \left|\left(\frac{32k^3\alpha}{\pi^2}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} dx\, x e^{-(\alpha/2+k)x^2}\right|^2 = 0 \tag{10}$$

where we used the fact that the integrand is anti-symmetric (odd) under $x \to -x$. A more fundamental explanation is that the state $|0\rangle$ is an eigenvector of the *parity* operator $\hat{Q}$, defined by $\hat{Q}|x\rangle = |-x\rangle$, with eigenvalue 1; whereas $\psi(x)$ represents an eigenvector with eigenvalue -1. Hence they must be orthogonal. The probability of observing energy $3\hbar\omega/2$ is

$$\begin{aligned} P(E=3\hbar\omega/2) = P(N=1) &= \left|\left(\frac{128k^3\alpha}{\pi^2}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} dx\, \sqrt{\alpha}x^2\, e^{-(\alpha/2+k)x^2}\right|^2 \\ &= \left(\frac{8k^3\alpha^3}{\pi^2}\right)^{\frac{1}{2}} \frac{\pi}{(\alpha/2+k)^3} \\ &= \left(\frac{\sqrt{2k\alpha}}{\alpha/2+k}\right)^3 \end{aligned} \tag{11}$$

4. The normalisation condition reads

$$1 = \langle\psi|\psi\rangle = |A|^2(4+1) = 5|A|^2 \tag{12}$$

using $\langle 0|1\rangle = \langle 1|0\rangle = 0$ and $\langle 0|0\rangle = \langle 1|1\rangle = 1$. Hence we can take $A = 1/\sqrt{5}$. The probability density of finding the particle at position x is simply given by

$$
\begin{aligned}
|\langle x|\psi\rangle|^2 &= |A|^2 \, |2\langle x|0\rangle + \langle x|1\rangle|^2 \\
&= \frac{1}{5}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\alpha x^2} |2 + i\sqrt{2\alpha}\, x|^2 \\
&= \frac{2}{5}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\alpha x^2} (2 + \alpha x^2),
\end{aligned}
$$

so that the probability is

$$
\int_{-\infty}^{0} |\langle x|\psi\rangle|^2 = \frac{1}{2}\int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2 = \frac{1}{2}
$$

where we used the normalisation $\langle\psi|\psi\rangle$ and the fact that the function $|\langle x|\psi\rangle|^2$ is symmetric (even) under $x \to -x$. That the probability be 1/2 is not a generic result; for instance, with $|\psi\rangle = A(2|0\rangle + i|1\rangle)$, we would obtain a different result.

For the probability density of finding the particle to have momentum p, this is given by

$$
\begin{aligned}
|\langle p|\psi\rangle|^2 &= \left| \int_{-\infty}^{\infty} dx\, \langle p|x\rangle\langle x|\psi\rangle \right|^2 \\
&= \frac{1}{10\pi\hbar}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \left| \int_{-\infty}^{\infty} dx\, e^{-ipx/\hbar - \alpha x^2/2} (2 + i\sqrt{2\alpha}\, x) \right|^2 \\
&= \frac{1}{10\pi\hbar}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \left| \int_{-\infty}^{\infty} dx\, e^{-\frac{\alpha}{2}\left(x^2 + \frac{2ipx}{m\omega}\right)} (2 + i\sqrt{2\alpha}\, x) \right|^2 \\
&= \frac{1}{10\pi\hbar}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \left| \int_{-\infty}^{\infty} dx\, e^{-\frac{\alpha}{2}\left(\left(x + \frac{ip}{m\omega}\right)^2 + \frac{p^2}{(m\omega)^2}\right)} (2 + i\sqrt{2\alpha}\, x) \right|^2 \\
&= \frac{1}{10\pi\hbar}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\frac{\alpha p^2}{(m\omega)^2}} \left| \int_{-\infty}^{\infty} dx\, e^{-\frac{\alpha x^2}{2}} \left(2 + i\sqrt{2\alpha}\left(x - \frac{ip}{m\omega}\right)\right) \right|^2 \\
&= \frac{1}{10\pi\hbar}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\frac{\alpha p^2}{(m\omega)^2}} \left(\frac{2\pi}{\alpha}\right) \left| 2 + \frac{\sqrt{2\alpha}\, p}{m\omega} \right|^2 \\
&= \frac{4}{5m\omega}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\frac{\alpha p^2}{(m\omega)^2}} \left(1 + \frac{\sqrt{2\alpha}\, p}{m\omega} + \frac{\alpha\, p^2}{2(m\omega)^2}\right).
\end{aligned}
$$

Hence, it is decaying as $|p| \to \infty$ like a Gaussian (times a polynomial), in the same way as the position density $|\langle x|\psi\rangle|^2$ does as $|x| \to \infty$. The momentum, like the position, is essentially concentrated around 0