Quantum Mechanics III — Michaelmas Term 2008

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Homework 3 – due 4 December 2008

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 $\alpha = m\omega/\hbar$:

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

A useful integral:

$$\int_{-\infty}^{\infty} e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}} \quad (\mathrm{Re}(\alpha) > 0) \tag{5}$$

1. For the eigenstate $|N\rangle$, calculate the average momentum $\mathbb{E}(P)$, the variance of the momentum $\sqrt{\mathbb{E}(P^2) - \mathbb{E}(P)^2}$, the average kinetic energy $\mathbb{E}(P^2/2m)$, the average position $\mathbb{E}(X)$ and the variance of the position $\sqrt{\mathbb{E}(X^2) - \mathbb{E}(X)^2}$.

2. (a) Normalise the wave function $\psi(x) = Ae^{-kx^2}$ (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 $3\hbar\omega/2$?

   (b) Normalise the vector $|\psi\rangle = A(3|0\rangle + 4|2\rangle)$. In this state, what is the probability density of finding the particle at position x? What is the probability of finding the position to be in the range $[0, \infty]$?

3. Any operator $\hat{B}$ can be written in the basis of the hamiltonian eigenstates, in the form

$$\hat{B} = \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} b_{m,n}|m\rangle\langle n| \tag{6}$$

   for some (generally complex) coefficients $b_{M,N}$. Write down the hamiltonian $\hat{H}$, the momentum $\hat{P}$ and the position $\hat{X}$ in this form.

Answers

1. We must write the momentum and position operators in terms of the ladder operators, whose action on all states we know:

$$\hat{X} = \frac{\hat{a} - \hat{a}^\dagger}{i\omega\sqrt{2m}}, \quad \hat{P} = \sqrt{\frac{m}{2}}(\hat{a} + \hat{a}^\dagger) \tag{7}$$

Then we can evaluate all averages using the orthonormality relation $\langle N|N'\rangle = \delta_{N,N'}$. First,

$$\begin{aligned}\mathbb{E}(P) &= \langle N|\hat{P}|N\rangle \\ &= \langle N|\sqrt{\frac{m}{2}}(\hat{a} + \hat{a}^\dagger)|N\rangle \\ &= \sqrt{\frac{m}{2}}\langle N|\left(\sqrt{(N+1)\hbar\omega}|N+1\rangle + \sqrt{N\hbar\omega}|N-1\rangle\right) \\ &= 0\end{aligned} \tag{8}$$

Hence the average momentum is 0, which is in agreement with the intuition that the particle "goes back an forth" but overall stays in the same region (it does not escape to infinity). This is a statement that stays true for energy eigenstates associated to any confining potential. Second,

$$\begin{aligned}\mathbb{E}(P^2) &= \langle N|\hat{P}^2|N\rangle \\ &= \langle N|\frac{m}{2}(\hat{a} + \hat{a}^\dagger)^2|N\rangle \\ &= \frac{m}{2}\langle N|(\hat{a}^2 + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a} + (\hat{a}^\dagger)^2)|N\rangle \\ &= \frac{m}{2}\langle N|(\hat{a}^2 + (\hat{a}^\dagger)^2 + 2\hat{a}\hat{a}^\dagger + \hbar\omega)|N\rangle\end{aligned} \tag{9}$$

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

$$\hat{a}\hat{a}^\dagger|N\rangle = \hat{a}\sqrt{N\hbar\omega}|N-1\rangle = \sqrt{N\hbar\omega}\sqrt{N\hbar\omega}|N\rangle = N\hbar\omega|N\rangle \tag{10}$$

as well as the fact that $\hat{a}^2|N\rangle \propto |N+2\rangle$ and $(\hat{a}^\dagger)^2|N\rangle \propto |N-2\rangle$, to get

$$\mathbb{E}(P^2) = \frac{m}{2}\langle N|(2N+1)\hbar\omega)|N\rangle = m\hbar\omega\left(\frac{1}{2} + N\right) \tag{11}$$

Hence the variance of the momentum is

$$\sqrt{\mathbb{E}(P^2) - \mathbb{E}(P)^2} = \sqrt{m\hbar\omega\left(\frac{1}{2} + N\right)} \tag{12}$$

We see that for higher energies, the variance is higher; the momentum is more spread around its average 0, because the particle goes faster in general. Third, this directly gives us the average kinetic energy operator

$$\mathbb{E}(P^2/2m) = \frac{\hbar\omega}{2}\left(\frac{1}{2} + N\right) \tag{13}$$

Interestingly, this is exactly *half* of the total energy for the state $|N\rangle$, $E_N = \hbar\omega(1/2+N)$. This means that for the harmonic oscillator, half of the total energy is in the kinetic energy; so 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". Fourth,

$$\begin{aligned}\mathbb{E}(X) &= \langle N|\hat{X}|N\rangle \\ &= \langle N|\frac{\hat{a}-\hat{a}^\dagger}{i\omega\sqrt{2m}}|N\rangle \\ &= 0 \end{aligned} \tag{14}$$

That is, the average position is 0, which is after all expected from the symmetry $X \to -X$ of the quadratic potential. Finally,

$$\begin{aligned}\mathbb{E}(X^2) &= \langle N|\hat{X}^2|N\rangle \\ &= -\frac{1}{2m\omega^2}\langle N|(\hat{a}-\hat{a}^\dagger)^2|N\rangle \\ &= -\frac{1}{2m\omega^2}\langle N|(\hat{a}^2-\hat{a}\hat{a}^\dagger-\hat{a}^\dagger\hat{a}+(\hat{a}^\dagger)^2)|N\rangle \\ &= -\frac{1}{2m\omega^2}\langle N|(\hat{a}^2+(\hat{a}^\dagger)^2-2\hat{a}\hat{a}^\dagger-\hbar\omega)|N\rangle \\ &= \frac{\hbar}{m\omega}\left(\frac{1}{2}+N\right)\end{aligned} \tag{15}$$

using again (10). Hence the variance of the position is

$$\sqrt{\mathbb{E}(X^2)-\mathbb{E}(X)^2} = \sqrt{\frac{\hbar}{m\omega}\left(\frac{1}{2}+N\right)} \tag{16}$$

Again, we see that it increases with N, which means that for higher energy states, the particles can go further away from the origin $X=0$. It is interesting to confirm that the average potential energy

$$\mathbb{E}(m\omega^2X^2/2) = \frac{\hbar\omega}{2}\left(\frac{1}{2}+N\right) \tag{17}$$

is indeed also half of the total energy.

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

$$1 = \int_{-\infty}^{\infty} dx\,|A|^2e^{-2kx^2} = \sqrt{\frac{\pi}{2k}}|A|^2 \tag{18}$$

so that $A = (2k/\pi)^{\frac{1}{4}}$ 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 $\psi(x)$:

$$P(E=\hbar\omega/2) = P(N=0) = \left|\left(\frac{2k\alpha}{\pi^2}\right)^{\frac{1}{4}}\int_{-\infty}^{\infty} dx\,e^{-(\alpha/2+k)x^2}\right|^2 = \left(\frac{8k\alpha}{(\alpha+2k)^2}\right)^{\frac{1}{2}}. \tag{19}$$

Note that for $k = \alpha/2$, we indeed recover a probability 1, since in this case the wave function $\psi(x)$ is exactly the ground state wave function. For $k \to 0$, where $\psi(x)$ tends to a constant, the probability goes to zero proportionally to $k^{1/2}$. When $k \to \infty$, where the wave function becomes a Dirac delta-function supported at $x = 0$, the probability tends to zero also, proportionally to $k^{-1/2}$. The probability to be in the state with energy $3\hbar\omega/2$, or the level $N = 1$, is

$$P(E = 2\hbar\omega/2) = P(N = 1) = \left| \left(\frac{8k\alpha}{\pi^2}\right)^{\frac{1}{4}} \int_{-\infty}^{\infty} dx\, \sqrt{\alpha} x\, e^{-(\alpha/2+k)x^2} \right|^2 = 0 \tag{20}$$

where we used the fact that the integrand is anti-symmetric (odd) under $x \to -x$. A more fundamental explanation is that the state $|1\rangle$ 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.

(b) The normalisation condition now reads

$$1 = \langle\psi|\psi\rangle = |A|^2(9 + 16) = 25|A|^2 \tag{21}$$

using $\langle 0|2\rangle = \langle 2|0\rangle = 0$ and $\langle 0|0\rangle = \langle 2|2\rangle = 1$. Hence we can take $A = 1/5$. The probability density of finding the particle at position x is simply given by

$$\begin{aligned} |\langle x|\psi\rangle|^2 &= |A|^2 |3\langle x|0\rangle + 4\langle x|2\rangle|^2 \\ &= \frac{1}{25}\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} e^{-\alpha x^2}(3 + 2\sqrt{2} - 4\sqrt{2}\alpha x^2)^2. \end{aligned} \tag{22}$$

With a little bit of work, one can check that this integrates to 1:

$$\langle\psi|\psi\rangle = \int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2 = 1 \tag{23}$$

but this is just a check that there was no mistake in the computation, since we know that $\langle\psi|\psi\rangle = 1$. The probability of finding the position in the range $[0, \infty]$ is simply

$$\int_0^{\infty} |\langle x|\psi\rangle|^2 = \frac{1}{2}\int_{-\infty}^{\infty} |\langle x|\psi\rangle|^2 = \frac{1}{2} \tag{24}$$

where we used the fact that the function $|\langle x|\psi\rangle|^2$ is symmetric (even) under $x \to -x$.

3. Note that from the expansion of the operator $\hat{B}$ in general, we have

$$\begin{aligned} \langle M|\hat{B}|N\rangle &= \langle M| \left(\sum_{m=0}^{\infty}\sum_{n=0}^{\infty} b_{m,n}|m\rangle\langle n|\right)|N\rangle \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} b_{m,n}\langle M|m\rangle\langle n|N\rangle \\ &= \sum_{m=0}^{\infty}\sum_{n=0}^{\infty} b_{m,n}\delta_{M,m}\delta_{N,n} \\ &= b_{M,N} \end{aligned} \tag{25}$$

The left-hand side can be computed easily. We have

$$\begin{aligned}
\langle M|\hat{H}|N\rangle &= \langle M|E_N|N\rangle = E_N\delta_{M,N} \\
\langle M|\hat{P}|N\rangle &= \langle M|\sqrt{\frac{m}{2}}(\hat{a}+\hat{a}^\dagger)|N\rangle \\
&= \sqrt{\frac{m}{2}}\langle M|\left(\sqrt{(N+1)\hbar\omega}|N+1\rangle + \sqrt{N\hbar\omega}|N-1\rangle\right) \\
&= \sqrt{\frac{m\hbar\omega}{2}}(\sqrt{N+1}\delta_{M,N+1} + \sqrt{N}\delta_{M,N-1}) \\
\langle M|\hat{X}|N\rangle &= \langle M|\frac{\hat{a}-\hat{a}^\dagger}{i\omega\sqrt{2m}}|N\rangle \\
&= \frac{1}{i\omega\sqrt{2m}}\langle M|\left(\sqrt{(N+1)\hbar\omega}|N+1\rangle - \sqrt{N\hbar\omega}|N-1\rangle\right) \\
&= -i\sqrt{\frac{\hbar}{2m\omega}}(\sqrt{N+1}\delta_{M,N+1} - \sqrt{N}\delta_{M,N-1}) \qquad (26)
\end{aligned}$$

These give the following expansions

$$\begin{aligned}
\hat{H} &= \sum_{N=0}^{\infty} E_N|N\rangle\langle N| \\
\hat{P} &= \sqrt{\frac{m\hbar\omega}{2}}\sum_{N=0}^{\infty}\left(\sqrt{N+1}\,|N+1\rangle\langle N| + \sqrt{N}\,|N-1\rangle\langle N|\right) \\
\hat{X} &= -i\sqrt{\frac{\hbar}{2m\omega}}\sum_{N=0}^{\infty}\left(\sqrt{N+1}\,|N+1\rangle\langle N| - \sqrt{N}\,|N-1\rangle\langle N|\right) \qquad (27)
\end{aligned}$$

(where we must remember that in these expression, when we see the vector $|N-1\rangle$ with $N=0$, we must replace this by 0 – that is, the term does not appear). These expansions can be seen as expressions of these operators as infinite matrices. Indeed, we can represent $|m\rangle\langle n|$ as a matrix $\mathcal{E}(m,n)$ where every element is zero except onyl one element, the element at the $(m+1)^{\text{th}} row$ and the $(n+1)^{\text{th}}$ column, which is just 1. This reproduces the correct multiplication law $\mathcal{E}(m,n)\mathcal{E}(m',n') = |m\langle\rangle n||m'\langle\rangle n'| = |m\langle\rangle n'|\delta_{n,m'} = \mathcal{E}(m,n')\delta_{n,m'}$ (you can check that these matrices indeed satisfy these identities). Hence, we can write

$$
\begin{aligned}
\hat{H} &= \begin{pmatrix} E_0 & 0 & 0 & \cdots \\ 0 & E_1 & 0 & \cdots \\ 0 & 0 & E_2 & \cdots \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} \\
\hat{P} &= \sqrt{\frac{m\hbar\omega}{2}} \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots \\ 1 & 0 & \sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & \sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix} \\
\hat{X} &= -i\sqrt{\frac{\hbar}{2m\omega}} \begin{pmatrix} 0 & -1 & 0 & 0 & \cdots \\ 1 & 0 & -\sqrt{2} & 0 & \cdots \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & \cdots \\ 0 & 0 & \sqrt{3} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}
\end{aligned} \tag{28}
$$