Second Year Quantum Mechanics - Classwork 1 Problems
Probability conservation

Paul Dauncey, 18 Oct 2011

In Lecture 2, we discussed the physical interpretion of the wavefunction $\psi(x,t)$, namely that $\rho(x,t) = |\psi|^2 = \psi^*\psi$ was the probability density at time t for finding the particle at the position x. Hence the total probability to find the particle anywhere in x is given by

$$P(t) = \int_{-\infty}^{\infty} \rho(x,t)\, dx$$

which in general would appear to be a function of t. However, this would mean that even if we fix $P = 1$ at $t = 0$, then it might become less than one at later times, which implies the particle might *not* be found anywhere; this is clearly unphysical. Hence, we need to show that P is in fact constant and not a function of time; P must be *conserved*.

1. Using the product rule, calculate $\partial\rho/\partial t$ in terms of derivatives of ψ and ψ^*.

2. For the special case that ψ satisfies the time-independent Schrödinger equation (TISE)
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi = E\psi \qquad \text{so} \qquad i\hbar\frac{\partial\psi}{\partial t} = E\psi$$
Rearrange the second of these to give $\partial\psi/\partial t$. Take the complex conjugate of both sides of the resulting expression to also get $\partial\psi^*/\partial t$. Substitute these into your expression for $\partial\rho/\partial t$ and show the latter is zero, which means ρ is constant with time. This clearly means P is a constant for this special case; this should not be surprising as it is a stationary state.

3. However, we must show P is constant with time for the general case, when ψ is *not* a stationary state. Here, we only know ψ satisfies the time-dependent Schrödinger equation (TDSE), not the more restrictive time-independent equation, so
$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V\psi$$
Again, rearrange to get $\partial\psi/\partial t$ and take the complex conjugate to find $\partial\psi^*/\partial t$.

4. Use your expressions for $\partial\psi/\partial t$ and $\partial\psi^*/\partial t$ to express $\partial\rho/\partial t$ in terms of J, where
$$J = \frac{i\hbar}{2m}\left[\left(\frac{\partial\psi^*}{\partial x}\right)\psi - \psi^*\left(\frac{\partial\psi}{\partial x}\right)\right]$$
Hint: Note that J contains only first derivatives of ψ with respect to x.

5. Integrate the resulting equation over all x, noting that the time derivative can be taken outside of the x integral as it operates on a different variable (see standard relation at end of page). Assuming ψ and hence J become zero for large $|x|$, what does the J term give? Deduce that P is constant for the general case.

6. Show for plane wave solutions $\psi = Ae^{-i(Et-px)/\hbar}$, then $J = v\rho$, where v is the classical particle velocity. How does this allow us to interpret the physical meaning of the equation you found in part 4?

7. *Supplementary:* For any complex number $z = x + iy$, show $(z + z^*)/2$ is always purely real and $(z - z^*)/2$ is always purely imaginary. What does this tell us about J?

Standard relation: for any function $f(x,t)$, then:

$$\frac{d}{dt}\left(\int f\, dx\right) = \int \left(\frac{\partial f}{\partial t}\right) dx$$

Second Year Quantum Mechanics - Classwork 2 Problems
Orthogonality of energy states

Paul Dauncey, 28 Oct 2011

1. As shown in the lectures, the general form for the infinite square well energy states is
$$u_n = A\cos\frac{n\pi x}{2a} \text{ for } n = 1,3,5,\dots, \qquad u_n = B\sin\frac{n\pi x}{2a} \text{ for } n = 2,4,6,\dots$$
Find expressions for the normalisation constants A and B, valid for any n.

2. In Problem Sheet 2, you calculated the probability density function for a state that was a superposition of the ground state and the first excited state of the infinite square well potential with walls at $x = -a$ and a. You found it to be a time-dependent function that "sloshed" from side to side. On the other hand, Classwork 1 and Handout 1 show that the total probability of finding the particle anywhere in the well remains constant in time, as the probability density obeys a continuity equation. From Problem Sheet 2, the total probability is given by the integral
$$\int_{-a}^{a} |\psi_s|^2\, dx = \frac{1}{2a}\left[\int_{-a}^{a}\cos^2\frac{\pi x}{2a}\, dx + \int_{-a}^{a}\sin^2\frac{\pi x}{a}\, dx + 2\cos(\Delta E t/\hbar)\int_{-a}^{a}\cos\frac{\pi x}{2a}\sin\frac{\pi x}{a}\, dx\right].$$
Check the total probability above is correctly normalised and is indeed constant.

3. The fact that this does not change in time was ensured by the third integral vanishing. That integral is the product of the ground state and first excited state. This being zero turns out to be an important and general feature of energy states. In general, we find that
$$\int_{-\infty}^{\infty} u_n^* u_m\, dx = 0$$
for all $n \neq m$ and the energy states are said to be *orthogonal.* Show that the ground state and second excited state of the infinite square well are also orthogonal.

4. As this is supposed to be a general result, it should hold for all energy states. For the simple harmonic oscillator, check the equivalent integrals both for the ground state (U_0) and first excited state (U_1), and also the ground state and the second excited state (U_2), give zero. These states are
$$U_0 = C\exp(-\alpha x^2/2), \qquad U_1 = Dx\exp(-\alpha x^2/2), \qquad U_2 = F(2\alpha x^2 - 1)\exp(-\alpha x^2/2),$$
where $\alpha = m\omega_0/\hbar$ and C, D and F are constants.

5. Show generally that the orthogonality of the energy states ensures that the total probability of finding the particle anywhere remains constant for any general wavefunction which is a superposition of energy states
$$\psi_s = \sum_n a_n u_n e^{-iE_n t/\hbar},$$
where the index n runs over any arbitrary number of integer values.

You may need the following standard relations and integrals:
$$\cos^2\alpha = \frac{1}{2}(1+\cos 2\alpha), \qquad \sin^2\alpha = \frac{1}{2}(1-\cos 2\alpha), \qquad 2\cos\alpha\cos\beta = \cos(\alpha+\beta) + \cos(\alpha-\beta).$$
$$\int_{-\infty}^{\infty}\exp(-\alpha x^2)dx = \sqrt{\frac{\pi}{\alpha}}, \qquad \int_{-\infty}^{\infty} x^2\exp(-\alpha x^2)dx = \frac{1}{2\alpha}\sqrt{\frac{\pi}{\alpha}}.$$

Second Year Quantum Mechanics - Classwork 3 Problems
Measurements and probabilities

Paul Dauncey, 8 Nov 2011

1. A particle is confined in a one-dimensional infinite square potential with "walls" at $x = \pm a$. The energy of this particle is measured and a result corresponding to the ground state energy is found.

   (a) What is the wave function that describes the particle after this measurement?

   (b) What are the possible results of subsequent energy measurements?

   (c) Following the measurement, calculate the total probability of finding the particle in the region $-a/2 < x < a/2$.

2. At $t = 0$, just after measuring the particle to have the ground state energy, the walls are suddenly removed and immediately replaced by walls at $x = \pm 2a$. The wavefunction is unchanged by the replacement of the walls. By considering the old energy eigenfunctions and potential, deduce the eigenfunctions applicable to this new situation.

3. Following the change to the walls, show that a measurement of the energy will not give an eigenvalue corresponding to an eigenstate with an even quantum number n.

4. Find an expression for the probability that an energy measurement will yield the energy of an eigenstate with an odd quantum number n. Hence evaluate:

   (a) The probability of measuring the energy of the ground state, $n = 1$.

   (b) The probability of measuring the energy of the second excited state, $n = 3$.

   (c) The sum of probabilities of measuring any energy corresponding to the values $n > 3$.

5. *If time permits:* You should have found that the probability of measuring any energy higher than the $n = 3$ value was small. Hence, an approximation to the particle's wave function following the sudden displacement of the walls can be obtained if a superposition of eigenstates no higher than $n = 3$ is considered. Write down the probability as a function of t for finding the particle in the region $-a/2 < x < a/2$. (You do not need to evaluate the integrals.) Note that this probability for $t > 0$ is never higher than the probability of finding the particle in this range at $t = 0$. Why?

The following may be useful

Normalised eigenstates for the infinite square well (walls at $\pm a$) for integer $n \geq 1$

$$u_n(x) = \frac{1}{\sqrt{a}} \cos \frac{n\pi x}{2a} \ [n \text{ odd}] \qquad u_n(x) = \frac{1}{\sqrt{a}} \sin \frac{n\pi x}{2a} \ [n \text{ even}],$$

$$2 \cos A \cos B = \cos(A + B) + \cos(A - B), \qquad \sin(A \pm B) = \sin A \cos B \pm \cos A \sin B,$$

$$|Z_1 + Z_2|^2 = |Z_1|^2 + |Z_2|^2 + 2\mathcal{R}e(Z_1^* Z_2); \qquad [Z_1, Z_2 \text{ are complex; } \mathcal{R}e \equiv \text{Real Part}].$$

Second Year Quantum Mechanics - Classwork 4 Problems
Expectation values

Paul Dauncey, 18 Nov 2011

A particle is bound in a harmonic oscillator potential

$$V(x) = \frac{1}{2} m\omega_0^2 x^2$$

where ω_0 is the angular frequency of the corresponding classical oscillator.

1. Show that $\hat{H}$ can be written in the form

$$\hat{H} = \frac{1}{2}\hbar\omega_0 \left(-\frac{d^2}{dy^2} + y^2 \right)$$

where $y = x/a$ and $a = \sqrt{(\hbar/m\omega_0)}$. We can now just use y where we would normally use x in the following.

2. The wave function of a particle in this potential is

$$\psi(y) = \left(\frac{2}{3\sqrt{\pi}} \right)^{1/2} (1 + iy)\exp(-y^2/2) \ .$$

(a) Verify that $\psi(y)$ is normalized.

(b) What is the expectation value of y^2 and hence of the potential energy V?

(c) Evaluate the expectation value of the kinetic energy, T.
Hint: Integration by parts gives

$$\left\langle \frac{d^2}{dy^2} \right\rangle = \int_{-\infty}^{\infty} \psi^* \frac{d^2\psi}{dy^2}\, dy = -\int_{-\infty}^{\infty} \left| \frac{d\psi}{dy} \right|^2 dy$$

(d) Use the results of (b) and (c) to calculate the expectation value of $\langle E \rangle$, where E is the total energy.

3. The normalized eigenstates of $\hat{H}$ corresponding to the eigenvalues $\hbar\omega_0/2$ and $3\hbar\omega_0/2$ are

$$u_0(y) = \left(\frac{1}{\sqrt{\pi}} \right)^{1/2} \exp(-y^2/2)$$

$$u_1(y) = \left(\frac{2}{\sqrt{\pi}} \right)^{1/2} y\exp(-y^2/2)$$

(a) Expand the particle wavefunction given in part 2 in terms of energy eigenstates, i.e. $\psi(y) = \sum_n a_n u_n(y)$. Hence calculate the probabilities that a measurement of the energy will give a result equal to $\hbar\omega_0/2$ and to $3\hbar\omega_0/2$.
Hint: Calculating the overlap integral will always give you a_n, but you can sometimes find the expansion directly by inspection of the wavefunction.

(b) Verify that the value of $\langle E \rangle$ obtained in part 2(d) is equal to that given by $\sum_n |a_n|^2 E_n$.

Standard integrals:

$$\int_{-\infty}^{\infty} \exp(-y^2)\, dy = \sqrt{\pi}, \qquad \int_{-\infty}^{\infty} y^2 \exp(-y^2)\, dy = \frac{\sqrt{\pi}}{2}, \qquad \int_{-\infty}^{\infty} y^4 \exp(-y^2)\, dy = \frac{3\sqrt{\pi}}{4}$$

Second Year Quantum Mechanics - Classwork 5 Problems
The Uncertainty Principle

Paul Dauncey, 29 Nov 2011

1. The operators corresponding to measurement of position $\hat{x}$ and momentum $\hat{p}$ are
$$\hat{x} = x, \qquad \hat{p} = -i\hbar \frac{d}{dx}.$$
Show that $\hat{x}$ and $\hat{p}$ satisfy the operator commutation relation
$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = i\hbar.$$
Hint: operate with the commutator on an arbitary function $\psi(x)$.

2. A particle is in the nth energy eigenstate of an infinite square-well potential with walls at $x = 0, 2a$. (The normalized eigenfunctions are given at the bottom of this page; note the walls are *not* at $x = \pm a$, which was the case in the lectures.)
   (a) Show the expectation values of x, x^2, p and p^2 are a, $a^2(4/3 - 2/n^2\pi^2)$, 0 and $n^2\hbar^2\pi^2/4a^2$, respectively.
   (b) Hence show that the Heisenberg uncertainty product is given by:
$$\Delta x \Delta p = \frac{\hbar}{2}\left[\frac{n^2\pi^2}{3} - 2\right]^{1/2}.$$
   (c) Which state has smallest uncertainty product $\Delta x \Delta p$?

3. A form of the uncertainty relation for a pair of operators $\hat{A}, \hat{B}$ is
$$\Delta A \Delta B \geq \left|\left\langle \frac{i}{2}\left[\hat{A}, \hat{B}\right]\right\rangle\right|.$$
For the case of $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$:
   (a) Calculate the right hand side of this inequality.
   (b) Hence show this uncertainty inequality is valid for all n eigenstates of the infinite square-well.
   (c) Are any of the infinite square well energy eigenstates true "minimum uncertainty" states?

The following may be useful:

Normalized energy eigenfunctions for the infinite square well with walls at $x = 0, 2a$ are
$$u_n(x) = \frac{1}{\sqrt{a}} \sin\left(\frac{n\pi x}{2a}\right) \qquad \text{for all integer } n \geq 1.$$

Some other standard results
$$\cos^2 A = \frac{1}{2}(1 + \cos 2A), \qquad \sin^2 A = \frac{1}{2}(1 - \cos 2A), \qquad \sin A \cos A = \frac{1}{2}\sin 2A.$$
$$\int_0^{2a} \sin\frac{n\pi x}{a}\,dx = \int_0^{2a} \cos\frac{n\pi x}{a}\,dx = \int_0^{2a} x\cos\frac{n\pi x}{a}\,dx = 0.$$
$$\int_0^{2a} x^2 \cos\frac{n\pi x}{a}\,dx = \frac{4a^3}{n^2\pi^2}.$$

Second Year Quantum Mechanics - Classwork 6 Problems
Angular momentum operators

Paul Dauncey, 6 Dec 2011

Angular momentum raising and lowering ("ladder") operators can be defined in terms of the operators for the angular momentum components as

$$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y.$$

Generally, these have the effect of converting an angular momentum eigenstate (i.e. a spherical harmonic) $Y_{l\,m_l}$ into a state proportional to $Y_{l\,(m_l\pm1)}$, respectively.

In spherical polars, the operators representing the components of angular momentum are

$$\begin{aligned}
\hat{L}_x &= -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)\\
\hat{L}_y &= -i\hbar\left(\ \ \cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)\\
\hat{L}_z &= -i\hbar\frac{\partial}{\partial\phi}
\end{aligned}$$

1. The $l = 0$ spherical harmonic is

$$Y_{0\,0} = \sqrt{\frac{1}{4\pi}}.$$

   (a) Verify that this is an eigenstate of $\hat{L}_z$ and find its eigenvalue.

   (b) Operate with $\hat{L}_x$ and $\hat{L}_y$ on this eigenstate and hence find the effect of the operators $\hat{L}_\pm$ on $Y_{0\,0}$.

2. The $l = 1$ spherical harmonics are

$$Y_{1\,0} = \sqrt{\frac{3}{4\pi}}\cos\theta, \qquad Y_{1\,\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}.$$

   (a) Verify that these are eigenstates of $\hat{L}_z$ and find their eigenvalues.

   (b) Operate on $Y_{1\,0}$ with $\hat{L}_x$ and $\hat{L}_y$ and hence verify that $\hat{L}_\pm Y_{1\,0}$ give states proportional to $Y_{1\,\pm1}$.

   (c) Operate on $Y_{1\,1}$ with $\hat{L}_x$ and $\hat{L}_y$. Hence, verify that $\hat{L}_- Y_{1\,1}$ gives what you would expect.

   (d) What is the result of $\hat{L}_+ Y_{1\,1}$?

3. The results you got in parts 1(b) and 2(d) are particular cases of a general property of the ladder operators. Explain why you got these results and write down the general expressions for the two cases.

Second Year Quantum Mechanics - Classwork 7 Problems
Hydrogen atom

Paul Dauncey, 16 Dec 2011

An electron in the Coulomb field of a proton is described by the normalised wavefunction

$$\psi(\boldsymbol{r}) = R(r) \times A(\theta,\phi) = \frac{1}{\sqrt{24a_0^3}}\frac{r}{a_0}e^{-r/2a_0} \times \sqrt{\frac{3}{16\pi}}\left[\sqrt{2}\cos\theta - \sin\theta e^{i\phi}\right]$$

where a_0 is the *Bohr radius*, $a_0 = 5.3 \times 10^{-11}$ m. The two parts above are the individually normalised radial (R) and angular (A) contributions to the wavefunction.

1. By considering the angular part of the wavefunction
   (a) Express the wavefunction as a sum of angular momentum eigenstates.
   (b) Hence give the possible results of a measurement of L^2 or of L_z.
   (c) Find the probability that a measurement of L_z will yield the result zero.
2. Using the full wavefunction
   (a) Assuming the spherical harmonics are orthonormal, check the overall wavefunction is normalised.
   (b) Calculate $\langle r^2 \rangle^{1/2}$, the RMS separation of the electron and proton; give your answer in metres.
   (c) Give the possible results of a measurement of the energy of the electron.

Useful information:

Some of the spherical harmonics

$$Y_{1\,0} = \sqrt{\frac{3}{4\pi}}\cos\theta, \qquad Y_{1\,\pm1} = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}$$

Standard integral

$$\int_0^\infty r^n e^{-r/a} dr = n!\, a^{n+1}$$

The radial parts of the hydrogen atom energy eigenstates go as

$$R_{nl}(r) = f_{nl}(r)e^{-r/na_0}$$

where n is the principal quantum number, l is the angular momentum quantum number which is required to satisfy $l < n$, and $f_{nl}(r)$ is a polynomial of degree $n-1$ which is proportional to r^l for small r.

Hydrogen atom energy eigenvalues: $E_n = -\dfrac{13.6}{n^2}$ eV

Second Year Quantum Mechanics - Classwork 1 Solutions
Probability conservation

Paul Dauncey, 18 Oct 2011

1. The derivative is simply

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}(\psi^* \psi) = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t}$$

2. Rearranging and taking the complex conjugate gives

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar} E\psi \qquad \text{and so} \qquad \frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar} E\psi^*$$

since E is real. Substituting into the expression for $\partial\rho/\partial t$ above gives

$$\frac{\partial \rho}{\partial t} = \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t} = \frac{i}{\hbar} E\psi^*\psi - \psi^* \frac{i}{\hbar} E\psi = 0$$

as required.

3. Rearranging gives

$$\frac{\partial \psi}{\partial t} = -\frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right]$$

Taking the complex conjugate of this equation gives

$$\frac{\partial \psi^*}{\partial t} = \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right]$$

as the potential V is always real.

4. The general expression for $\partial\rho/\partial t$ is

$$\begin{aligned}\frac{\partial \rho}{\partial t} &= \frac{\partial \psi^*}{\partial t}\psi + \psi^* \frac{\partial \psi}{\partial t} = \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi^*}{\partial x^2} + V\psi^*\right]\psi - \psi^* \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + V\psi\right] \\ &= \frac{i\hbar}{2m}\left[\psi^*\left(\frac{\partial^2 \psi}{\partial x^2}\right) - \left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi\right]\end{aligned}$$

Noting that J only contains first derivatives while the above expression contains second derivatives, then consider

$$\begin{aligned}\frac{\partial J}{\partial x} &= \frac{i\hbar}{2m}\frac{\partial}{\partial x}\left[\left(\frac{\partial \psi^*}{\partial x}\right)\psi - \psi^*\left(\frac{\partial \psi}{\partial x}\right)\right] \\ &= \frac{i\hbar}{2m}\left[\left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi + \left(\frac{\partial \psi^*}{\partial x}\right)\left(\frac{\partial \psi}{\partial x}\right) - \left(\frac{\partial \psi^*}{\partial x}\right)\left(\frac{\partial \psi}{\partial x}\right) - \psi^*\left(\frac{\partial^2 \psi}{\partial x^2}\right)\right] \\ &= \frac{i\hbar}{2m}\left[\left(\frac{\partial^2 \psi^*}{\partial x^2}\right)\psi - \psi^*\left(\frac{\partial^2 \psi}{\partial x^2}\right)\right]\end{aligned}$$

Hence

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial x}$$

5. Integrating the left hand side of the above equation gives

$$\int_{-\infty}^{\infty} \frac{\partial \rho}{\partial t}\, dx = \frac{d}{dt}\int_{-\infty}^{\infty} \rho\, dx = \frac{dP}{dt}$$

while the right hand side gives

$$-\int_{-\infty}^{\infty} \frac{\partial J}{\partial x}\, dx = -\left[J\right]_{-\infty}^{\infty} = J(-\infty) - J(\infty)$$

If $J \to 0$ for $|x| \to \infty$, then the J terms are zero and hence $dP/dt = 0$, so P is constant.

6. For the plane wave solution $\psi = Ae^{-i(Et-px)/\hbar}$

$$\frac{\partial \psi}{\partial x} = \frac{ip}{\hbar}\psi$$

Hence

$$J = \frac{i\hbar}{2m}\left[\left(\frac{\partial \psi^*}{\partial x}\right)\psi - \psi^*\left(\frac{\partial \psi}{\partial x}\right)\right] = \frac{i\hbar}{2m}\left[-\frac{ip}{\hbar}\psi^*\psi - \frac{ip}{\hbar}\psi^*\psi\right] = \frac{p}{m}\psi^*\psi = v\rho$$

This indicates that J is the *probability flux* of the particles, i.e. the velocity times density. Hence the equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial J}{\partial x}$$

is a *continuity* equation saying that the probability density can only change due to a probability flux, i.e. due to motion of the particles. This is discussed in detail in Handout 1.

7. For $z = x + iy$ with x and y real, then

$$\frac{z + z^*}{2} = \frac{x + iy + x - iy}{2} = \frac{2x}{2} = x$$

i.e. the real part of z. Similarly

$$\frac{z - z^*}{2} = \frac{x + iy - x + iy}{2} = \frac{2iy}{2} = iy$$

i.e. i times the imaginary part of z and, since y is real, this is purely imaginary.

The derivatives part of J is

$$\left(\frac{\partial \psi^*}{\partial x}\right)\psi - \psi^*\left(\frac{\partial \psi}{\partial x}\right)$$

where the two terms are clearly complex conjugates of each other. Hence, this is equivalent to $z - z^*$ and so is purely imaginary. Since J is formed by multiplying this by i (and other real factors), then this makes J purely real, as would be expected for a physical quantity such as the flux.

Second Year Quantum Mechanics - Classwork 2 Solutions
Orthogonality of energy states

Paul Dauncey, 28 Oct 2011

1. To normalise the states, we will need to use the relations given
$$\cos^2\alpha = \frac{1}{2}\left(1+\cos 2\alpha\right), \qquad \sin^2\alpha = \frac{1}{2}\left(1-\cos 2\alpha\right)$$
For the infinite square well problem it is only necessary to integrate from $-a$ to a since the wavefunction is zero outside this range. The normalisation for the cosine states is given by calculating
$$\begin{aligned}\int_{-a}^{a}\cos^2\frac{n\pi x}{2a}\,dx &= \frac{1}{2}\int_{-a}^{a}1+\cos\frac{n\pi x}{a}\,dx\\ &= \frac{1}{2}\left[x+\frac{a}{n\pi}\sin\frac{n\pi x}{a}\right]_{-a}^{a} = a\end{aligned}$$
since the sine terms are zero, so that we can set $A = 1/\sqrt{a}$ for all n. For the sine states
$$\begin{aligned}\int_{-a}^{a}\sin^2\frac{n\pi x}{2a}\,dx &= \frac{1}{2}\int_{-a}^{a}1-\cos\frac{n\pi x}{a}\,dx\\ &= \frac{1}{2}\left[x-\frac{a}{n\pi}\sin\frac{n\pi x}{a}\right]_{-a}^{a} = a\end{aligned}$$
so also $B = 1/\sqrt{a}$ for all n.

2. For the total probability, the first two integrals are as above for $n=1$ and 2, while the third integral is an odd function of x and so is zero by inspection. Hence, the total probability is
$$\int_{-a}^{a}|\psi_s|^2\,dx = \frac{1}{2a}(a+a) = 1$$
and so is normalised and constant, as required.

3. If u_1 and u_3 are orthogonal then
$$\int_{-a}^{a}u_1^* u_3\,dx = 0$$
The relevant wavefunctions are $u_1 = \cos(\pi x/2a)/\sqrt{a}$ and $u_3 = \cos(3\pi x/2a)/\sqrt{a}$.
$$\begin{aligned}\int_{-a}^{a}\frac{1}{\sqrt{a}}\cos\pi x/2a\frac{1}{\sqrt{a}}\cos 3\pi x/2a\,dx &= \frac{1}{a}\frac{2a}{\pi}\int_{-\pi/2}^{\pi/2}\cos\theta\cos 3\theta\,d\theta\\ &= \frac{1}{\pi}\int_{-\pi/2}^{\pi/2}2\cos\theta\cos 3\theta\,d\theta\end{aligned}$$
where $\theta = \pi x/2a$. Now, using the relation given
$$2\cos\theta\cos 3\theta = \cos 4\theta + \cos 2\theta$$
so that
$$\begin{aligned}\frac{1}{\pi}\int_{-\pi/2}^{\pi/2}2\cos\theta\cos 3\theta\,d\theta &= \frac{1}{\pi}\left(\int_{-\pi/2}^{\pi/2}\cos 4\theta d\theta + \int_{-\pi/2}^{\pi/2}\cos 2\theta d\theta\right)\\ &= \frac{1}{\pi}\left[\frac{1}{4}\sin 4\theta + \frac{1}{2}\sin 2\theta\right]_{-\pi/2}^{\pi/2}\\ &= 0\end{aligned}$$

so that the u_1 and u_3 are indeed orthogonal.

This is a more surprising result than for u_1 and u_2 since the integrand is not an odd function, so it is not so obvious that the relevant integral vanishes.

4. The harmonic oscillator ground and first excited state integral is

$$\int_{-\infty}^{\infty} U_0^* U_1\, dx = \int_{-\infty}^{\infty} C^* \exp(-\alpha x^2/2) D x \exp(-\alpha x^2/2)\, dx = C^* D \int_{-\infty}^{\infty} x \exp(-\alpha x^2)\, dx = 0$$

since this is again an odd integral.

For the ground and second excited state, then

$$\begin{aligned} \int_{-\infty}^{\infty} U_0^* U_2\, dx &= \int_{-\infty}^{\infty} C^* \exp(-\alpha x^2/2)\ F(2\alpha x^2 - 1) \exp(-\alpha x^2/2)\, dx \\ &= C^* F \int_{-\infty}^{\infty} (2\alpha x^2 - 1) \exp(-\alpha x^2)\, dx \\ &= C^* F \left(2\alpha \int_{-\infty}^{\infty} x^2 \exp(-\alpha x^2)\, dx - \int_{-\infty}^{\infty} \exp(-\alpha x^2)\, dx \right) \\ &= C^* F \left(2\alpha \frac{1}{2\alpha} \sqrt{\frac{\pi}{\alpha}} - \sqrt{\frac{\pi}{\alpha}} \right) = 0 \end{aligned}$$

5. For the general superposition given $|\psi_s|^2$ can be written

$$\begin{aligned} |\psi_s|^2 = \psi_s^* \psi_s &= \left(\sum_n a_n^* u_n^* e^{iE_n t/\hbar} \right) \left(\sum_m a_m u_m e^{-iE_m t/\hbar} \right) \\ &= \sum_n |a_n|^2 |u_n|^2 + \sum_{n \neq m} a_n^* u_n^* a_m u_m e^{i(E_n - E_m)t/\hbar} \end{aligned}$$

Hence

$$\begin{aligned} \int_{-\infty}^{\infty} |\psi_s|^2\, dx &= \sum_n |a_n|^2 \int_{-\infty}^{\infty} |u_n|^2\, dx + \sum_{n \neq m} a_n^* a_m e^{i(E_n - E_m)t/\hbar} \int_{-\infty}^{\infty} u_n^* u_m\, dx \\ &= \sum_n |a_n|^2 \int_{-\infty}^{\infty} |u_n|^2\, dx \end{aligned}$$

All terms in the second sum contain $u_n^* u_m$ so when these terms are integrated over all space, orthogonality ensures that they *all* vanish, leaving only the first sum, which is clearly time independent.

Second Year Quantum Mechanics - Classwork 3 Solutions
Measurements and probabilities

Paul Dauncey, 8 Nov 2011

1. (a) Following the measurement, the particle is in eigenstate u_1 of the potential, and so the wave function is $\psi(x) = u_1(x) = \cos(\pi x/2a)/\sqrt{a}$.

   (b) Since $\psi(x)$ is an eigenstate of energy, then subsequent energy measurements yield the corresponding eigenvalue, i.e. E_1 is the only possible result.

   (c) $\psi(x)$ must be normalized, since $u_1(x)$ is normalized, so the probability of $|x| < a/2$ is

$$\begin{aligned}\int_{-a/2}^{a/2} |\psi(x)|^2 dx &= \frac{1}{a}\int_{-a/2}^{a/2} \cos^2\frac{\pi x}{2a} dx = \frac{1}{2a}\int_{-a/2}^{a/2}\left(\cos\frac{\pi x}{a} + 1\right) dx \\ &= \frac{1}{2a}\left[\frac{a}{\pi}\sin\frac{\pi x}{a} + x\right]_{-a/2}^{a/2} = \frac{1}{2a}\left[\frac{2a}{\pi} + a\right] = \frac{1}{2}\left[\frac{2}{\pi} + 1\right] = 0.818\end{aligned}$$

2. After the walls are shifted suddenly at $t = 0$, the wave function is

$$\psi(x, t=0) = \begin{cases}\frac{1}{\sqrt{a}}\cos\frac{\pi x}{2a} & : \quad |x| < a \\ 0 & : \quad |x| > a\end{cases}$$

   Solutions for the energy eigenstates for the new potential, u' can be obtained simply by replacing $a \to 2a$ in the solutions for the old potential, i.e.

$$\begin{aligned} n \text{ odd}: \qquad u'_n(x) &= \frac{1}{\sqrt{2a}}\cos\frac{n\pi x}{4a} \\ n \text{ even}: \qquad u'_n(x) &= \frac{1}{\sqrt{2a}}\sin\frac{n\pi x}{4a}\end{aligned}$$

3. The probability of a measurement giving E_n is $|c_n|^2$, where c_n is given by the overlap integral between the eigenstate u'_n and the wavefunction. The integral only needs to go over $x = \pm a$ as the wavefunction is zero outside this range. For even n

$$c_n = \int_{-\infty}^{\infty} u'^*_n(x)\psi(x,0)\,dx = \frac{1}{a\sqrt{2}}\int_{-a}^{a}\sin\frac{n\pi x}{4a}\cos\frac{\pi x}{2a} dx = 0$$

   as this is an odd function. Hence the probability of measuring any eigenvalue corresponding to an even value of n is zero.

4. For odd n

$$\begin{aligned} c_n &= \int_{-a}^{a} u'^*_n(x)\psi(x,0)\,dx = \frac{1}{a\sqrt{2}}\int_{-a}^{a}\cos\frac{n\pi x}{4a}\cos\frac{\pi x}{2a}\,dx \\ &= \frac{1}{2a\sqrt{2}}\int_{-a}^{a}\left[\cos\frac{(n+2)\pi x}{4a} + \cos\frac{(n-2)\pi x}{4a}\right] dx \\ &= \frac{1}{2a\sqrt{2}}\left[\frac{4a}{(n+2)\pi}\sin\frac{(n+2)\pi x}{4a} + \frac{4a}{(n-2)\pi}\sin\frac{(n-2)\pi x}{4a}\right]_{-a}^{a} \\ &= \frac{2\sqrt{2}}{\pi}\left[\frac{1}{n+2}\sin\left(\frac{n\pi}{4} + \frac{\pi}{2}\right) + \frac{1}{n-2}\sin\left(\frac{n\pi}{4} - \frac{\pi}{2}\right)\right]\end{aligned}$$

   Noting

$$\sin\left(\frac{n\pi}{4} \pm \frac{\pi}{2}\right) = \sin\frac{n\pi}{4}\cos\frac{\pi}{2} \pm \cos\frac{n\pi}{4}\sin\frac{\pi}{2} = \pm\cos\frac{n\pi}{4}$$

then

$$c_n = \frac{2\sqrt{2}}{\pi}\left[\frac{1}{n+2}\cos\frac{n\pi}{4} - \frac{1}{n-2}\cos\frac{n\pi}{4}\right] = \frac{2\sqrt{2}}{(n^2-4)\pi}\left[(n-2)\cos\frac{n\pi}{4} - (n+2)\cos\frac{n\pi}{4}\right]$$
$$= -\frac{8\sqrt{2}\cos(n\pi/4)}{\pi(n^2-4)}$$

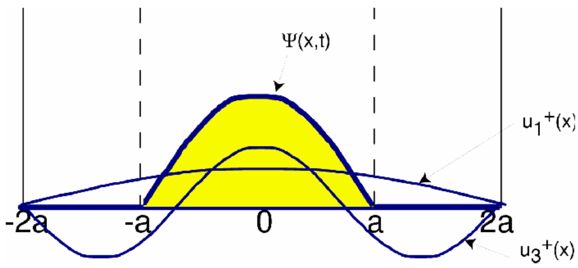
Note, $\cos(n\pi/4) = \pm 1/\sqrt{2}$ for odd n.

(a) For $n = 1$, then $c_1 = 8/3\pi$ so the probability is $P_1 = |c_1|^2 = (8/3\pi)^2 = 0.72$.

(b) For $n = 3$, then $c_3 = 8/5\pi$ so the probability is $P_3 = |c_3|^2 = (8/5\pi)^2 = 0.26$.

(c) The total probability must be one, so the sum of probabilities for all odd $n > 3$ must be $1 - 0.72 - 0.26 = 0.02$.

5. Using the suggested approximation, then the wavefunction is a superposition of only two eigenstates



Hence we can approximate the wavefunction to

$$\psi(x,t) \approx c_1 u_1(x)\exp(-iE_1 t/\hbar) + c_3 u_3(x)\exp(-iE_3 t/\hbar)$$

and using the formula given on the question sheet

$$\begin{aligned} \text{Prob}(|x| < a/2) &= \int_{-a/2}^{a/2} |\psi(x,t)|^2\, dx \\ &= \frac{|c_1|^2}{2a}\int_{-a/2}^{a/2}\cos^2\frac{\pi x}{4a}\, dx + \frac{|c_3|^2}{2a}\int_{-a/2}^{a/2}\cos^2\frac{3\pi x}{4a}\, dx \\ &+ \left\{\frac{c_1 c_3}{a}\int_{-a/2}^{a/2}\cos\frac{\pi x}{4a}\cos\frac{3\pi x}{4a}\, dx\right\}\cos\left[\frac{(E_3 - E_1)t}{\hbar}\right] . \end{aligned}$$

The first two terms are constant. When $t = 0$, the $\cos[(E_3 - E_1)t/\hbar]$ factor is at its maximum of one. For any future time, the cosine will be less than or equal to one. Since c_1 and c_3 are positive and, from the diagram above, it is clear the third integral will be positive, then the probability is at its maximum at $t = 0$. The reason that the probability of finding the particle within $\pm a/2$ is smaller for $t > 0$ than initially is because the particle is no longer confined to the original box, but can spread out into the region between $\pm 2a$.

Second Year Quantum Mechanics - Classwork 4 Solutions
Expectation values

Paul Dauncey, 18 Nov 2011

1. Changing from x to y gives

$$\begin{aligned}
\hat{H} &= \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega_0^2 x^2 : \qquad \text{Change variables} \qquad x = ay, \qquad \frac{d^2}{dx^2} = \frac{1}{a^2}\frac{d^2}{dy^2} \\
&= \frac{-\hbar^2}{2m}\frac{1}{a^2}\frac{d^2}{dy^2} + \frac{1}{2}m\omega_0^2 a^2 y^2 : \qquad \text{substitute} : \quad a = \sqrt{\frac{\hbar}{m\omega_0}} \\
&= -\frac{\hbar\omega_0}{2}\frac{d^2}{dy^2} + \frac{\hbar\omega_0}{2}y^2 = \frac{1}{2}\hbar\omega_0\left(-\frac{d^2}{dy^2} + y^2\right)
\end{aligned}$$

2. (a) Checking the normalisation

$$\begin{aligned}
\psi(y) &= \left(\frac{2}{3\sqrt{\pi}}\right)^{1/2}(1+iy)\exp(-y^2/2) \\
\int_{-\infty}^{\infty}\psi^*\psi\,dy &= \frac{2}{3\sqrt{\pi}}\int_{-\infty}^{\infty}(1+y^2)\exp(-y^2)\,dy \\
&= \frac{2}{3\sqrt{\pi}}\int_{-\infty}^{\infty}\exp(-y^2)\,dy + \frac{2}{3\sqrt{\pi}}\int_{-\infty}^{\infty}y^2\exp(-y^2)\,dy \\
&= \frac{2}{3\sqrt{\pi}}\sqrt{\pi} + \frac{2}{3\sqrt{\pi}}\frac{\sqrt{\pi}}{2} = \frac{2}{3} + \frac{1}{3} = 1
\end{aligned}$$

so ψ is normalized.

(b) The expectation value of y^2 is given by

$$\begin{aligned}
\langle y^2\rangle &= \int_{-\infty}^{\infty}\psi^*\ y^2\ \psi\,dy = \int_{-\infty}^{\infty}y^2|\psi|^2\,dy \\
&= \frac{2}{3\sqrt{\pi}}\int_{-\infty}^{\infty}y^2\exp(-y^2)\,dy + \frac{2}{3\sqrt{\pi}}\int_{-\infty}^{\infty}y^4\exp(-y^2)\,dy \\
&= \frac{2}{3\sqrt{\pi}}\frac{\sqrt{\pi}}{2} + \frac{2}{3\sqrt{\pi}}\frac{3\sqrt{\pi}}{4} = \frac{1}{3} + \frac{1}{2} = \frac{5}{6}
\end{aligned}$$

Hence, since from above $\hat{V} = (\hbar\omega_0/2)y^2$, then

$$\langle V\rangle = \frac{1}{2}\hbar\omega_0\langle y^2\rangle = \frac{5}{12}\hbar\omega_0$$

(c) For the kinetic energy, since from above $\hat{T} = -(\hbar\omega_0/2)\,d^2/dy^2$, then

$$\langle T\rangle = -\frac{\hbar\omega_0}{2}\int_{-\infty}^{\infty}\psi^*\frac{d^2\psi}{dy^2}\,dy = \frac{\hbar\omega_0}{2}\int_{-\infty}^{\infty}\left|\frac{d\psi}{dy}\right|^2\,dy$$

Since

$$\begin{aligned}
\frac{d\psi}{dy} &= \left(\frac{2}{3\sqrt{\pi}}\right)^{1/2}\left[-y\exp(-y^2/2) - iy^2\exp(-y^2/2) + i\exp(-y^2/2)\right] \\
&= \left(\frac{2}{3\sqrt{\pi}}\right)^{1/2}\left[-y\exp(-y^2/2) + i(1-y^2)\exp(-y^2/2)\right]
\end{aligned}$$

then

$$\left|\frac{d\psi}{dy}\right|^2 = \left(\frac{2}{3\sqrt{\pi}}\right)\left[y^2\exp(-y^2) + (1-y^2)^2\exp(-y^2)\right]$$
$$= \left(\frac{2}{3\sqrt{\pi}}\right)(y^4 - y^2 + 1)\exp(-y^2)$$

Hence

$$\left\langle\frac{d^2}{dy^2}\right\rangle = -\int_{-\infty}^{\infty}\left(\frac{2}{3\sqrt{\pi}}\right)(y^4 - y^2 + 1)\exp(-y^2)\,dy$$
$$= -\left(\frac{2}{3\sqrt{\pi}}\right)\left[\frac{3\sqrt{\pi}}{4} - \frac{\sqrt{\pi}}{2} + \sqrt{\pi}\right] = -\frac{5}{6}$$

so

$$\langle T\rangle = -\frac{1}{2}\hbar\omega_0\left\langle\frac{d^2}{dy^2}\right\rangle = \frac{5}{12}\hbar\omega_0$$

(d) The total energy is the sum of the kinetic and potential energies so

$$\langle E\rangle = \langle T\rangle + \langle V\rangle = \frac{5}{6}\hbar\omega_0$$

3. (a) The wavefunction is

$$\psi(y) = \left(\frac{2}{3\sqrt{\pi}}\right)^{1/2}(1+iy)\exp(-y^2/2)$$

We want $\psi = \sum_n a_n u_n$; by inspection

$$\psi = \sqrt{\frac{2}{3}}u_0 + \frac{i}{\sqrt{3}}u_1$$

so

$$a_0 = \sqrt{\frac{2}{3}}, \qquad a_1 = \frac{i}{\sqrt{3}}$$

Hence

$$P(E_0) = |a_0|^2 = \frac{2}{3}, \qquad P(E_1) = |a_1|^2 = \frac{1}{3}$$

and so $\sum_n |a_n|^2 = 1$ as required. The same result could be obtained by doing the overlap integrals

$$a_n = \int_{-\infty}^{\infty} u_n^*\psi\,dy$$

(b) A direct calculation of $\langle E\rangle$ using the above probabilities gives

$$\langle E\rangle = \sum_n |a_n|^2 E_n$$
$$= \frac{2}{3}E_0 + \frac{1}{3}E_1 = \frac{\hbar\omega_0}{3} + \frac{\hbar\omega_0}{2} = \frac{5\hbar\omega_0}{6}$$

Therefore, the calculation of the expectation value using the operator integral gives the same result as using the statistical weighted average.

Second Year Quantum Mechanics - Classwork 5 Solutions
The Uncertainty Principle

Paul Dauncey, 29 Nov 2011

1. Consider $[\hat{x},\hat{p}]$ acting on a state $\psi(x)$:

$$[\hat{x},\hat{p}]\psi = (\hat{x}\hat{p}-\hat{p}\hat{x})\psi = x\left(-i\hbar\frac{d}{dx}\right)\psi + i\hbar\frac{d}{dx}(x\psi)$$
$$= -xi\hbar\frac{d\psi}{dx} + i\hbar x\frac{d\psi}{dx} + i\hbar\psi = i\hbar\psi$$

Hence $[\hat{x},\hat{p}] = i\hbar$.

2. (a) *Terms in {} brackets in the following calculation have been substituted using the standard integrals as given.*

The particle is described by $\psi(x) = \frac{1}{\sqrt{a}}\sin\frac{n\pi x}{2a}$, so

$$\langle x\rangle = \int_{-\infty}^{\infty}\psi^* x\psi\,dx = \frac{1}{a}\int_0^{2a} x\sin^2\frac{n\pi x}{2a}\,dx$$
$$= \frac{1}{2a}\int_0^{2a} x\left[1-\cos\frac{n\pi x}{a}\right]dx = \frac{1}{2a}\left[\frac{x^2}{2}\right]_0^{2a} - \frac{1}{2a}\int_0^{2a} x\cos\frac{n\pi x}{a}\,dx$$
$$= \frac{1}{2a}\frac{4a^2}{2} - \frac{1}{2a}\{0\} = a$$

as expected by the symmetry of the potential. Also

$$\langle x^2\rangle = \int_{-\infty}^{\infty}\psi^* x^2\psi\,dx = \frac{1}{a}\int_0^{2a} x^2\sin^2\frac{n\pi x}{2a}\,dx$$
$$= \frac{1}{2a}\int_0^{2a} x^2\left[1-\cos\frac{n\pi x}{a}\right]dx$$
$$= \frac{1}{2a}\left[\frac{x^3}{3}\right]_0^{2a} - \frac{1}{2a}\int_0^{2a} x^2\cos\frac{n\pi x}{a}\,dx$$
$$= \frac{1}{2a}\frac{8a^3}{3} - \frac{1}{2a}\left\{\frac{4a^3}{n^2\pi^2}\right\} = \frac{4a^2}{3} - \frac{2a^2}{n^2\pi^2}$$

For momentum

$$\langle p\rangle = \int_{-\infty}^{\infty}\psi^*\left(-i\hbar\frac{d}{dx}\right)\psi\,dx = \frac{-i\hbar}{a}\int_0^{2a}\sin\frac{n\pi x}{2a}\left(\frac{n\pi}{2a}\right)\cos\frac{n\pi x}{2a}\,dx$$
$$= \frac{-i\hbar n\pi}{4a^2}\int_0^{2a}\sin\frac{n\pi x}{a}dx = \frac{-i\hbar n\pi}{4a^2}\{0\} = 0$$

as expected for a bound state. Finally

$$\langle p^2\rangle = \int_{-\infty}^{\infty}\psi^*\left((-i\hbar)^2\frac{d^2}{dx^2}\right)\psi\,dx = \frac{-\hbar^2}{a}\int_0^{2a}\sin\frac{n\pi x}{2a}\left(-\frac{n^2\pi^2}{4a^2}\right)\sin\frac{n\pi x}{2a}\,dx$$
$$= \frac{\hbar^2 n^2\pi^2}{4a^3}\int_0^{2a}\sin^2\frac{n\pi x}{2a}dx = \frac{\hbar^2 n^2\pi^2}{8a^3}\int_0^{2a}\left[1-\cos\frac{n\pi x}{a}\right]dx$$
$$= \frac{\hbar^2 n^2\pi^2}{8a^3}\left([x]_0^{2a} - \{0\}\right) = \frac{\hbar^2 n^2\pi^2}{4a^2}$$

(b) The mean square values are

$$(\Delta x)^2 = \langle x^2\rangle - \langle x\rangle^2 = \frac{4a^2}{3} - \frac{2a^2}{n^2\pi^2} - a^2 = a^2\left[\frac{1}{3} - \frac{2}{n^2\pi^2}\right].$$
$$(\Delta p)^2 = \langle p^2\rangle - \langle p\rangle^2 = \frac{\hbar^2 n^2\pi^2}{4a^2}$$

Hence

$$(\Delta x)^2(\Delta p)^2 = \frac{\hbar^2 n^2\pi^2}{4}\left[\frac{1}{3} - \frac{2}{n^2\pi^2}\right] = \frac{\hbar^2}{4}\left[\frac{n^2\pi^2}{3} - 2\right]$$
$$\Delta x\Delta p = \frac{\hbar}{2}\left[\frac{n^2\pi^2}{3} - 2\right]^{1/2}$$

(c) When $n = 1$, this is $\sqrt{(\pi^2/3 - 2)}(\hbar/2) = 1.14(\hbar/2)$ and so is real, i.e. the first term in the square root is larger than the second. Clearly, for bigger n, this will remain true and so for $n > 1$, the uncertainty product will always be larger than for $n = 1$. Hence the ground state has the smallest value of the uncertainty product.

3. The given uncertainty relation for $\hat{A} = \hat{x}$ and $\hat{B} = \hat{p}$ is

$$\Delta x\Delta p \geq \left|\left\langle \frac{i}{2}[\hat{x},\hat{p}]\right\rangle\right|$$

(a) Using the commutator, the expectation value on the RHS for any normalized wavefunction is
$$\left\langle \frac{i}{2}[\hat{x},\hat{p}]\right\rangle = \left\langle -\frac{\hbar}{2}\right\rangle = -\frac{\hbar}{2}\int_{-\infty}^{\infty}\psi^*\psi\,dx = -\frac{\hbar}{2}$$
so the right hand side of the uncertainty relation is $|-\hbar/2| = \hbar/2$.

(b) As shown in question 2(c), $\Delta x\Delta p = 1.14(\hbar/2)$ for $n = 1$ and is larger for $n > 1$. Hence $\Delta x\Delta p > \hbar/2$ for all n and so the inequality is always valid.

(c) The ground state ($n = 1$) has the smallest uncertainty product but it is not a true minimum uncertainty state since it has $\Delta x\Delta p > \hbar/2$, rather than $\Delta x\Delta p = \hbar/2$. Only a Gaussian function (e.g. the ground state of the SHO) is a true minimum uncertainty state.

Second Year Quantum Mechanics - Classwork 6 Solutions
Angular momentum operators

Paul Dauncey, 6 Dec 2011

1. (a) $Y_{0\,0}$ is not a function of θ or ϕ. Hence, taking a derivative of ϕ will give zero, so

$$\hat{L}_z Y_{0\,0} = 0 = 0 \times Y_{0\,0}$$

Hence, $Y_{0\,0}$ is an eigenstate of $\hat{L}_z$ with eigenvalue 0.

(b) Similarly, a derivative of θ on $Y_{0\,0}$ gives zero so

$$\hat{L}_x Y_{0\,0} = 0, \qquad \hat{L}_y Y_{0\,0} = 0$$

Hence

$$\hat{L}_\pm Y_{0\,0} = 0$$

2. (a) $Y_{1\,0}$ is not a function of ϕ so operating with $\hat{L}_z$ gives

$$\hat{L}_z Y_{1\,0} = 0 = 0 \times Y_{1\,0}$$

while

$$\begin{aligned}\hat{L}_z Y_{1\,\pm1} &= \pm i\hbar\sqrt{\frac{3}{8\pi}}\sin\theta\frac{\partial}{\partial\phi}(e^{\pm i\phi}) = \pm i\hbar\sqrt{\frac{3}{8\pi}}\sin\theta(\pm ie^{\pm i\phi}) \\ &= -\hbar\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} = (\pm\hbar)Y_{1\,\pm1}\end{aligned}$$

Hence, all three of the $l = 1$ spherical harmonics are eigenstates of $\hat{L}_z$, with eigenvalues of 0 and $\pm\hbar$, respectively.

(b) Operating with $\hat{L}_x$ and $\hat{L}_y$ on $Y_{1\,0}$ gives

$$\hat{L}_x Y_{1\,0} = i\hbar\sqrt{\frac{3}{4\pi}}\sin\phi\frac{\partial}{\partial\theta}(\cos\theta) = -i\hbar\sqrt{\frac{3}{4\pi}}\sin\phi\sin\theta$$

and

$$\hat{L}_y Y_{1\,0} = -i\hbar\sqrt{\frac{3}{4\pi}}\cos\phi\frac{\partial}{\partial\theta}(\cos\theta) = i\hbar\sqrt{\frac{3}{4\pi}}\cos\phi\sin\theta$$

Hence

$$\begin{aligned}\hat{L}_\pm Y_{1\,0} &= \hat{L}_x Y_{1\,0} \pm i\hat{L}_y Y_{1\,0} = -i\hbar\sqrt{\frac{3}{4\pi}}\sin\phi\sin\theta \mp \hbar\sqrt{\frac{3}{4\pi}}\cos\phi\sin\theta \\ &= \mp\hbar\sqrt{\frac{3}{4\pi}}\sin\theta(\cos\phi \pm i\sin\phi) = \mp\sqrt{2}\hbar\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi} = \sqrt{2}\hbar Y_{1\,\pm1}\end{aligned}$$

Hence, $\hat{L}_\pm$ changes $Y_{1\,0}$ into states proportional to $Y_{1\,\pm1}$, as expected.

(c) Operating with $\hat{L}_x$ and $\hat{L}_y$ on $Y_{1\,1}$ gives

$$\begin{aligned}\hat{L}_x Y_{1\,1} &= i\hbar\sqrt{\frac{3}{8\pi}}\left(-\sin\phi\cos\theta e^{i\phi} - i\cos\phi\cot\theta\sin\theta e^{i\phi}\right) \\ &= \hbar\sqrt{\frac{3}{8\pi}}\cos\theta e^{i\phi}(-i\sin\phi + \cos\phi) = \frac{\hbar}{\sqrt{2}}\sqrt{\frac{3}{4\pi}}\cos\theta e^{i\phi}e^{-i\phi} = \frac{\hbar}{\sqrt{2}}Y_{1\,0}\end{aligned}$$

and

$$\begin{aligned}\hat{L}_y Y_{1\,1} &= i\hbar\sqrt{\frac{3}{8\pi}}\left(\cos\phi\cos\theta e^{i\phi} - i\sin\phi\cot\theta\sin\theta e^{i\phi}\right) \\ &= i\hbar\sqrt{\frac{3}{8\pi}}\cos\theta e^{i\phi}(\cos\phi - i\sin\phi) = \frac{i\hbar}{\sqrt{2}}\sqrt{\frac{3}{4\pi}}\cos\theta e^{i\phi}e^{-i\phi} = \frac{i\hbar}{\sqrt{2}}Y_{1\,0}\end{aligned}$$

Hence

$$\hat{L}_- Y_{1\,1} = \frac{\hbar}{\sqrt{2}}Y_{1\,0} - i\frac{i\hbar}{\sqrt{2}}Y_{1\,0} = \frac{\hbar}{\sqrt{2}}Y_{1\,0} + \frac{\hbar}{\sqrt{2}}Y_{1\,0} = \sqrt{2}\hbar Y_{1\,0}$$

i.e. it is proportional to $Y_{1\,0}$, as expected.

(d) Operating with $\hat{L}_+$ gives

$$\hat{L}_+ Y_{1\,1} = \frac{\hbar}{\sqrt{2}}Y_{1\,0} + i\frac{i\hbar}{\sqrt{2}}Y_{1\,0} = \frac{\hbar}{\sqrt{2}}Y_{1\,0} - \frac{\hbar}{\sqrt{2}}Y_{1\,0} = 0$$

3. For part 1(b) when $l = 0$, the only allowed value is $m_l = 0$ so the ladder operators should not be able to create a state with any higher or lower values of m_l. Specifically, we should have $\hat{L}_+ Y_{0\,0} = 0$ and $\hat{L}_- Y_{0\,0} = 0$, as was found.

   For part 2(d) when $l = 1$, then the highest allowed value is $m_l = 1$ so we cannot raise this further, and so we expect $\hat{L}_+ Y_{1\,1} = 0$, again as found. (We would also find $\hat{L}_- Y_{1\,-1} = 0$ if we had calculated that.)

   Generally, the highest and lowest values are $m_l = \pm l$ so we should always find $\hat{L}_+ Y_{l\,l} = 0$ and $\hat{L}_- Y_{l\,-l} = 0$ for any value of l.

Second Year Quantum Mechanics - Classwork 7 Solutions
Hydrogen atom

Paul Dauncey, 16 Dec 2011

1. Angular momentum eigenstates are the spherical harmonics $Y_{l\,m_l}(\theta,\phi)$. They can be multiplied by any function of r.

   (a) The given wavefunction can be expanded in terms of the spherical harmonics by inspection. Noting

   $$Y_{1\,0} \propto \cos\theta, \qquad Y_{1\,1} \propto \sin\theta e^{i\phi}$$

   then putting

   $$\begin{aligned}\sqrt{\frac{3}{16\pi}}\left[\sqrt{2}\cos\theta - \sin\theta e^{i\phi}\right] &= \sum_{l,m_l} a_{l\,m_l} Y_{l\,m_l} = a_{1\,0}Y_{1\,0} + a_{1\,1}Y_{1\,1} \\ &= a_{1\,0}\sqrt{\frac{3}{4\pi}}\cos\theta - a_{1\,1}\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\phi}\end{aligned}$$

   gives

   $$a_{1\,0}\sqrt{\frac{3}{4\pi}} = \sqrt{\frac{3}{16\pi}}\sqrt{2}, \qquad a_{1\,0} = \frac{1}{\sqrt{2}}$$
   $$a_{1\,1}\sqrt{\frac{3}{8\pi}} = \sqrt{\frac{3}{16\pi}}, \qquad a_{1\,1} = \frac{1}{\sqrt{2}}$$

   Note $\sum_{l,m_l} |a_{l\,m_l}|^2 = 1$ which checks the angular part of the wavefunction is indeed normalised. Hence, the angular part is

   $$\sqrt{\frac{3}{16\pi}}\left[\sqrt{2}\cos\theta - \sin\theta e^{i\phi}\right] = \frac{1}{\sqrt{2}}(Y_{1\,0} + Y_{1\,1})$$

   (b) The wavefunction decomposition includes

   $$\begin{array}{llrcl} Y_{1\,0}: & \text{eigenvalue of } L^2 \text{ is} & l(l+1)\hbar^2 & = & 2\hbar^2 \\ & \text{eigenvalue of } L_z \text{ is} & m_l\hbar & = & 0 \\ Y_{1\,1}: & \text{eigenvalue of } L^2 \text{ is} & l(l+1)\hbar^2 & = & 2\hbar^2 \\ & \text{eigenvalue of } L_z \text{ is} & m_l\hbar & = & \hbar \end{array}$$

   Hence, the only possible result of a measurement of L^2 is $2\hbar^2$. The two possible results of a measurement of L_z are 0 or $\hbar$.

   (c) Since $a_{1\,0} = 1/\sqrt{2}$, the probability of measuring $L_z = 0$ is $|a_{1\,0}|^2 = 1/2$.

2. (a) Writing $\psi(\boldsymbol{r})$ as

   $$\psi(\boldsymbol{r}) = R(r)\frac{1}{\sqrt{2}}(Y_{1\,0} + Y_{1\,1})$$

   then the normalisation is checked by calculating

   $$\begin{aligned}\iiint |\psi|^2\, d^3r &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\psi|^2\, r^2\, dr\, \sin\theta\, d\theta\, d\phi \\ &= \int_0^{\infty} |R(r)|^2\, r^2\, dr \int_0^{2\pi}\int_0^{\pi} \frac{1}{2}|Y_{1\,0} + Y_{1\,1}|^2 \sin\theta\, d\theta\, d\phi\end{aligned}$$

Assuming that the spherical harmonics are orthonormal, then the second integral gives

$$\begin{aligned}
\int_0^{2\pi}\int_0^{\pi}\frac{1}{2}|Y_{1\,0}+Y_{1\,1}|^2\sin\theta\,d\theta\,d\phi &= \frac{1}{2}\int_0^{2\pi}\int_0^{\pi}(|Y_{1\,0}|^2+Y_{1\,0}^*Y_{1\,1}+Y_{1\,1}^*Y_{1\,0}+|Y_{1\,1}|^2)\sin\theta\,d\theta\,d\phi \\
&= \frac{1}{2}\left[\int_0^{2\pi}\int_0^{\pi}|Y_{1\,0}|^2\sin\theta\,d\theta\,d\phi+\int_0^{2\pi}\int_0^{\pi}|Y_{1\,1}|^2\sin\theta\,d\theta\,d\phi\right] \\
&= \frac{1}{2}[1+1]=1
\end{aligned}$$

The radial part is

$$\frac{1}{24a_0^3}\int_0^{\infty}\frac{r^2}{a_0^2}e^{-r/a_0}\,r^2\,dr=\frac{1}{24a_0^5}\int_0^{\infty}r^4e^{-r/a_0}\,dr=\frac{1}{24a_0^5}\,(4!a_0^5)=1$$

so the total wavefunction is indeed normalised.

(b) For the mean square radius, the angular part again integrates to unity, so

$$\begin{aligned}
\langle r^2\rangle &= \frac{1}{24a_0^3}\int_0^{\infty}r^2\frac{r^2}{a_0^2}e^{-r/a_0}\,r^2\,dr \\
&= \frac{1}{24a_0^5}\int_0^{\infty}r^6e^{-r/a_0}\,dr=\frac{1}{24a_0^5}\,(6!a_0^7)=30a_0^2
\end{aligned}$$

Hence, the RMS separation is $\sqrt{30}a_0=5.5a_0=2.7\times10^{-10}\,\mathrm{m}$.

(c) Comparing the radial part of the wavefunction

$$R(r)\propto re^{-r/2a_0}$$

with the expectation for an energy eigenstate, then since the eigenstates go as e^{-r/na_0}, then the exponent implies this wavefunction only contains eigenstates with $n=2$. The r factor is a polynomial of degree 1 which is consistent with $n=2$. Also, it clearly goes as r^1 for small r, which implies $l=1$ (which is also consistent with $l<n=2$ and the spherical harmonics considered in part 1). Hence, the radial part is consistent with a single eigenstate, $R_{21}(r)$. Therefore, we conclude

$$\psi=R_{2\,1}\times\frac{1}{\sqrt{2}}(Y_{1\,0}+Y_{1\,1})=\frac{1}{\sqrt{2}}(u_{2\,1\,0}+u_{2\,1\,1})$$

Hence, the only possible energy measurement outcome corresponds to $n=2$, which gives an energy

$$E_n=-\frac{13.6\text{ eV}}{n^2}=-3.4\text{ eV}$$