Solutions to Tutorial Sheet 1: Mainly revision

1. *Given the expansion of an arbitrary wavefunction or state vector as a linear superposition of eigenstates of the operator* $\hat{A}$

$$\Psi(\underline{r},t) = \sum_i c_i(t) u_i(\underline{r}) \quad \text{or} \quad |\Psi,t\rangle = \sum_i c_i(t)\,|u_i\rangle$$

use the orthonormality properties of the eigenstates to prove that

$$c_i(t) = \int u_i^*(\underline{r})\Psi(\underline{r},t)\,\mathrm{d}^3r \quad \text{or} \quad c_i(t) = \langle u_i|\Psi,t\rangle$$

Work through the proof in both wavefunction and Dirac notations.

Firstly in wavefunction notation the expansion is:

$$\Psi(\underline{r},t) = \sum_i c_i(t) u_i(\underline{r})$$

Multiply both sides by $u_j^*(\underline{r})$ and integrate over all space:

$$\int u_j^*(\underline{r})\Psi(\underline{r},t)\;\mathrm{d}^3r = \sum_i\; c_i(t)\int\; u_j^*(\underline{r})\,u_i(\underline{r})\;\mathrm{d}^3r = \sum_i\; c_i(t)\,\delta_{ji} = c_j(t)$$

where we have used the orthonormality property of the eigenfunctions:

$$\int u_j^*(\underline{r})u_i(\underline{r})\;\mathrm{d}^3r = \delta_{ji}$$

and the so-called *sifting property* of the Kronecker delta:

$$\sum_i\; c_i(t)\,\delta_{ji} = c_j(t)$$

Relabelling the free index $j \to i$ gives the desired result:

$$c_i(t) = \int u_i^*(\underline{r})\Psi(\underline{r},t)\,\mathrm{d}^3r$$

In Dirac notation we start from the expansion:

$$|\Psi,t\rangle = \sum_i c_i(t)\,|u_i\rangle$$

and take the *scalar product* of both sides with the bra vector $\langle u_j|$ to give

$$\langle u_j|\Psi,t\rangle = \sum_i\; c_i(t)\,\langle u_j|u_i\rangle = \sum_i\; c_i(t)\,\delta_{ji} = c_j(t)$$

using the orthonormality property $\langle u_j|u_i\rangle = \delta_{ji}$ as before.

The state $|\Psi, t\rangle$ is said to be normalised if $\langle\Psi, t|\Psi, t\rangle = 1$. Show that this implies that

$$\sum_i |c_i(t)|^2 = 1$$

Hint: use the expansion $|\Psi, t\rangle = \sum_i c_i(t)|u_i\rangle$ and the corresponding conjugate expansion $\langle\Psi, t| = \sum_j c_j^*(t)\langle u_j|$.

Substituting for $\langle\Psi, t|$ and $|\Psi, t\rangle$ in $\langle\Psi, t|\Psi, t\rangle$ we find

$$\langle\Psi, t|\Psi, t\rangle = \sum_j \sum_i c_j^*(t)c_i(t)\langle u_j|u_i\rangle = \sum_j \sum_i c_j^*(t)c_i(t)\delta_{ji} = \sum_i |c_i(t)|^2$$

where we have used the orthonormality of the eigenbasis $\langle u_j|u_i\rangle = \delta_{ji}$ and the sifting property of the Kronecker delta. Thus we have the result quoted in Lecture 1:

$$\sum_i |c_i(t)|^2 = 1$$

If the expectation value $\langle\hat{A}\rangle_t = \langle\Psi, t|\hat{A}|\Psi, t\rangle$, show by making use of the same expansions that

$$\langle\hat{A}\rangle_t = \sum_i |\langle u_i|\Psi, t\rangle|^2 \, A_i$$

and give the physical interpretation of this result.

The suggested expansion of the state vector is, in Dirac notation,

$$|\Psi, t\rangle = \sum_i \; c_i(t)|u_i\rangle \quad \text{where} \quad c_i(t) = \langle u_i|\Psi, t\rangle$$

and, correspondingly,

$$\langle\Psi, t| = \sum_j \; c_j^*(t)\langle u_j|$$

Substituting for $|\Psi, t\rangle$ and $\langle\Psi, t|$ in the expression for the expectation value gives

$$\langle\hat{A}\rangle_t = \sum_j \sum_i \; c_j^*(t)c_i(t)\langle u_j|\hat{A}|u_i\rangle = \sum_j \sum_i \; c_j^*(t)c_i(t)A_i\langle u_j|u_i\rangle$$

where we have used the eigenvalue equation for $\hat{A}$:

$$\hat{A}|u_i\rangle = A_i|u_i\rangle$$

We again use the orthonormality of the eigenbasis $\langle u_j|u_i\rangle = \delta_{ji}$ to write

$$\langle\hat{A}\rangle_t = \sum_j \sum_i \; c_j^*(t)c_i(t)A_i\delta_{ji} = \sum_i \; |c_i(t)|^2 A_i = \sum_i \; |\langle u_i|\Psi, t\rangle|^2 \, A_i$$

which is the desired result. As discussed in lectures, the interpretation is that $|c_i(t)|^2$ is the probability of getting the result A_i in a measurement of the observable $\mathcal{A}$, and the mean value of a set of repeated measurements of $\mathcal{A}$ is just a sum over the possible values weighted by the probabilities of obtaining them.

2. *The observables $\mathcal{A}$ and $\mathcal{B}$ are represented by operators $\hat{A}$ and $\hat{B}$ with eigenvalues $\{A_i\}$, $\{B_i\}$ and eigenstates $\{|u_i\rangle\}$, $\{|v_i\rangle\}$ respectively, such that*

$$\begin{aligned}|v_1\rangle &= \{\sqrt{3}\,|u_1\rangle + |u_2\rangle\}/2\\ |v_2\rangle &= \{|u_1\rangle - \sqrt{3}\,|u_2\rangle\}/2\\ |v_n\rangle &= |u_n\rangle, \quad n \geq 3.\end{aligned}$$

Show that if $\{|u_i\rangle\}$ is an orthonormal basis then so is $\{|v_i\rangle\}$.

This problem is designed to test your understanding of measurement and wavefunction collapse.

Orthonormality of the two bases means that

$$\langle u_i|u_j\rangle = \delta_{ij} \quad \text{and} \quad \langle v_i|v_j\rangle = \delta_{ij}$$

Given the expressions for $|v_1\rangle$ and $|v_2\rangle$ in terms of $|u_1\rangle$ and $|u_2\rangle$ we see that

$$\begin{aligned}\langle v_1|v_1\rangle &= \frac{1}{4}\left(\sqrt{3}\langle u_1| + \langle u_2|\right)\left(\sqrt{3}|u_1\rangle + |u_2\rangle\right)\\ &= \frac{1}{4}\left(3\langle u_1|u_1\rangle + \sqrt{3}\langle u_1|u_2\rangle + \sqrt{3}\langle u_2|u_i\rangle + \langle u_2|u_2\rangle\right) = \frac{1}{4}(3+0+0+1) = 1\end{aligned}$$

as it should. Similarly,

$$\begin{aligned}\langle v_1|v_2\rangle &= \frac{1}{4}\left(\sqrt{3}\langle u_1| + \langle u_2|\right)\left(|u_1\rangle - \sqrt{3}|u_2\rangle\right)\\ &= \frac{1}{4}\left(\sqrt{3}\langle u_1|u_1\rangle - 3\langle u_1|u_2\rangle + \langle u_2|u_i\rangle - \sqrt{3}\langle u_2|u_2\rangle\right) = \frac{1}{4}\left(\sqrt{3} - 0 + 0 - \sqrt{3}\right) = 0\end{aligned}$$

By the same methods you can show that $\langle v_2|v_2\rangle = 1$ and $\langle v_2|v_1\rangle = 0$ so that the relations between $|v_1\rangle$, $|v_2\rangle$ and $|u_1\rangle$, $|u_2\rangle$ are consistent with both bases being orthonormal (for $n \geq 3$ it is trivial).

A certain system is subjected to three successive measurements:

(1) a measurement of $\mathcal{A}$ followed by

(2) a measurement of $\mathcal{B}$ followed by

(3) another measurement of $\mathcal{A}$

Show that if measurement (1) yields any of the values $A_3, A_4, \ldots$ then (3) gives the same result but that if (1) yields the value A_1 there is a probability of $\frac{5}{8}$ that (3) will yield A_1 and a probability of $\frac{3}{8}$ that it will yield A_2. What may be said about the compatibility of $\mathcal{A}$ and $\mathcal{B}$?

If measurement (1) yields any of the eigenvalues $A_3, A_4, \ldots$ then the state of the system immediately afterwards is the corresponding eigenstate $|u_3\rangle, |u_4\rangle, \ldots$ of the operator $\hat{A}$. But $|u_3\rangle = |v_3\rangle$ etc. and so measurement (2) is made with the system in an eigenstate of $\hat{B}$, guaranteeing the outcome of (2) and *leaving the state of the system unchanged*, since for $n \geq 3$, $|u_n\rangle = |v_n\rangle$. Thus measurement (3) is *certain* to yield the same result as (1).

If measurement (1) yields the result A_1, however, the system is forced into the state $|u_1\rangle$ so that measurement (2), of the observable $\mathcal{B}$, is made with the system in the state $|u_1\rangle$. Inverting the given equations shows that

$$\begin{aligned}
|u_1\rangle &= \left\{\sqrt{3}|v_1\rangle + |v_2\rangle\right\}/2 \\
|u_2\rangle &= \left\{|v_1\rangle - \sqrt{3}|v_2\rangle\right\}/2
\end{aligned}$$

The first of these is just the expansion of $|u_1\rangle$ in the eigenbasis of $\hat{B}$ and the coefficients are the probability amplitudes from which we can compute the probabilities of getting the various possible values of $\mathcal{B}$:

$$\begin{aligned}
\text{prob of } B_1 &= \left|\frac{\sqrt{3}}{2}\right|^2 = \frac{3}{4} \\
\text{prob of } B_2 &= \left|\frac{1}{2}\right|^2 = \frac{1}{4}
\end{aligned}$$

Suppose that we get the result B_1. The wavefunction has collapsed onto the corresponding eigenstate of $\hat{B}$, that is $|v_1\rangle$. But we know that

$$|v_1\rangle = \{\sqrt{3}\,|u_1\rangle + |u_2\rangle\}/2$$

which is the expansion of $|v_1\rangle$ in the eigenbasis of $\hat{A}$, enabling us to compute the probabilities of getting the various possible values of $\mathcal{A}$:

$$\begin{aligned}
\text{prob of } A_1 &= \left|\frac{\sqrt{3}}{2}\right|^2 = \frac{3}{4} \\
\text{prob of } A_2 &= \left|\frac{1}{2}\right|^2 = \frac{1}{4}
\end{aligned}$$

On the other hand, if we get the result B_2 from measurement (2), the system is left in the state $|v_2\rangle$ and

$$|v_2\rangle = \{|u_1\rangle - \sqrt{3}\,|u_2\rangle\}/2$$

so that in this case when we make measurement (3)

$$\begin{aligned}
\text{prob of } A_1 &= \left|\frac{1}{2}\right|^2 = \frac{1}{4} \\
\text{prob of } A_2 &= \left|\frac{\sqrt{3}}{2}\right|^2 = \frac{3}{4}
\end{aligned}$$

Thus the probability of getting the result A_1 in measurement (3), *irrespective of the outcome of measurement (2)*, is given by

(prob that (2) gives B_1) $\times$ (prob that (3) gives A_1 given outcome B_1 in (2))

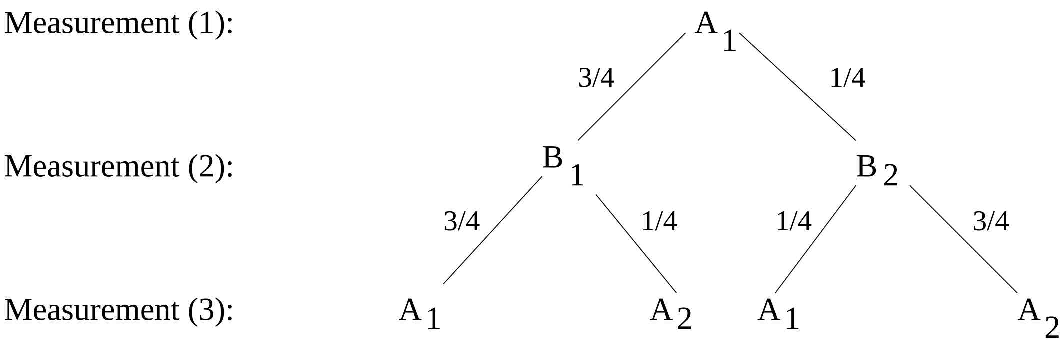
$+$

(prob that (2) gives B_2) $\times$ (prob that (3) gives A_1 given outcome B_2 in (2))

$$= \frac{3}{4} \times \frac{3}{4} + \frac{1}{4} \times \frac{1}{4} = \frac{5}{8}$$

Since (3) can only give A_1 or A_2, the probability of getting A_2 is 3/8.

We can represent the situation by a probability tree:



$\hat{A}$ and $\hat{B}$ are not compatable operators, even though many of their eigenstates are the same.

3. *The normalised energy eigenfunction of the ground state of the hydrogen atom ($Z = 1$) is*

$$u_{100}(\underline{r}) = R_{10}(r)Y_{00}(\theta, \phi) = C\ \exp(-r/a_0)$$

where a_0 is the Bohr radius and C is a normalisation constant. For this state

(a) *Calculate the normalisation constant, C, by noting the useful integral*

$$\int_0^\infty \exp(-br)\, r^n\, \mathrm{d}r = n!/b^{n+1}, \quad n > -1$$

Alternatively, you can use the computer algebra program Maple if you know how to!

The normalisation condition is as usual

$$\int u^*_{100}(\underline{r})u_{100}(\underline{r})\ \mathrm{d}^3r = 1$$

which in spherical polar coordinates gives

$$\int_{\phi=0}^{2\pi}\int_{\theta=0}^{\pi}\int_{r=0}^{\infty} |C|^2 \exp(-2r/a_0)r^2 \sin\theta \mathrm{d}r\mathrm{d}\theta\mathrm{d}\phi \ = \ 1$$

The ϕ integration gives 2π, whilst the θ integration gives 2 so that

$$4\pi|C|^2 \int_0^\infty \exp(-2r/a_0)r^2\ \mathrm{d}r = 1$$

We use the given integration formula and we find that

$$\int \exp(-2r/a_0)r^2\ \mathrm{d}r = 2!\left(\frac{a_0}{2}\right)^3 = \frac{a_0^3}{4}$$

Making the usual convention that the normalisation constant C is real and positive gives

$$C = \frac{1}{\sqrt{\pi a_0^3}}\ ; \quad u_{100}(\underline{r}) = (\pi a_0^3)^{-1/2} \exp(-r/a_0)$$

Maple can be used to evaluate the required integral (and related integrals which occur in the subsequent parts of the question).

```
> assume(a>0);
> int(exp(-2*r/a)*r*r,r=0..infinity);
```

(b) *Determine the radial distribution function, $D_{10}(r) \equiv r^2|R_{10}(r)|^2$, and sketch its behaviour; determine the most probable value of the radial coordinate, r, and the probability that the electron is within a sphere of radius a_0; recall that $Y_{00}(\theta, \phi) = 1/\sqrt{4\pi}$; again, you can use Maple to help you if you know how;*

Recall that

$$u_{n\ell m}(\underline{r}) = R_{n\ell}(r)\, Y_{\ell m}(\theta, \phi)$$

so that

$$u_{100}(\underline{r}) = R_{10}(r)\, Y_{00}(\theta, \phi) = \frac{1}{\sqrt{4\pi}} R_{10}(r)$$

Using the result for $u_{100}(\underline{r})$ from the previous part of the question,

$$D_{10}(r) \equiv r^2|R_{10}(r)|^2 = \frac{4r^2}{a_0^3} \exp(-2r/a_0)$$

To plot the radial distribution using Maple, use the following Maple command:

```
> plot(4*r*r*exp(-2*r),r=0..3);
```

This will produce a graph with a_0 scaled to 1.

$D_{10}(r)\,\mathrm{d}r$ is the probability of finding the electron between r and $r + \mathrm{d}r$, so that the most probable value of r corresponds to the maximum of the distribution, which may be found by differentiation with respect to r;

$$\frac{dD_{10}}{dr} = \frac{8r}{a_0^3} \exp(-2r/a_0) - \frac{8r^2}{a_0^4} \exp(-2r/a_0) = \frac{8r}{a_0^4}(a_0 - r) \exp(-2r/a_0)$$

Thus the derivative vanishes at the origin and at $r = a_0$, the latter corresponding to the maximum of D_{10}.

The following piece of Maple finds the points at which the derivative vanishes:

```
> assume(a>0);
> d:=4*r*r*exp(-2*r/a)/a**3;
> dprime:=diff(d,r);
> solve({dprime=0},{r});
```

The probability that the electron is within a sphere of radius a_0 is given by integrating the radial probability distribution from $r = 0$ to $r = a_0$:

$$\int_0^{a_0} D_{10}(r)\,\mathrm{d}r = \frac{4}{a_0^3} \int_0^{a_0} r^2 \exp(-2r/a_0)\,\mathrm{d}r$$

Unfortunately, the given integral doesn't help because here the upper limit is a_0 and not ∞. However, integrating by parts or using Maple yields the result

$$\text{probability } = 1 - 5e^{-2} = 0.32$$

The Maple is

```
> d:=4*r*r*exp(-2*r/a)/a**3;
> prob:=int(d,r=0..a);
> evalf(prob);
```

(c) *Calculate the expectation value of r;*

$$\langle r\rangle = \int u_{100}^*(\underline{r}) r\, u_{100}(\underline{r})\ \mathrm{d}^3r = \frac{4\pi}{\pi a_0^3}\int_0^\infty r^3 \exp(-2r/a_0)\ \mathrm{d}r$$

Using the given integral, or Maple,

$$\langle r\rangle = \frac{4}{a_0^3}\ 3!\left(\frac{a_0}{2}\right)^4 = \frac{3}{2}a_0$$

So, the mean value of r is 50% larger than the most probable value. This is due to the long "tail" of the wavefunction.

(d) *Calculate the expectation value of the potential energy, $V(r)$;*

$$\begin{aligned}
\langle V(r)\rangle &= -\frac{e^2}{4\pi\epsilon_0}\int u_{100}^*(\underline{r})\ \frac{1}{r}\ u_{100}(\underline{r})\ \mathrm{d}^3r \\
&= -\frac{e^2}{4\pi\epsilon_0}\ 4\pi\ \frac{1}{\pi a_0^3}\int_0^\infty r\exp(-2r/a_0)\ \mathrm{d}r \\
&= -\frac{e^2}{4\pi\epsilon_0}\ \frac{4}{a_0^3}\left(\frac{a_0}{2}\right)^2 \quad \text{from the given integral} \\
&= -\frac{e^2}{4\pi\epsilon_0 a_0}
\end{aligned}$$

(e) *Calculate the uncertainty, Δr, in r.*

The uncertainty is defined by

$$\Delta r \equiv \sqrt{\langle r^2\rangle - \langle r\rangle^2}$$

so we need to compute $\langle r^2\rangle$:

$$\begin{aligned}
\langle r^2\rangle &= \int u_{100}^*(\underline{r})\ r^2\ u_{100}(\underline{r})\ \mathrm{d}^3r \\
&= 4\pi\frac{1}{\pi a_0^3}\int_0^\infty r^4\exp(-2r/a_0)\ \mathrm{d}r \\
&= \frac{4}{a_0^3}\ 4!\left(\frac{a_0}{2}\right)^5 \\
&= 3a_0^2
\end{aligned}$$

Thus

$$\Delta r = \sqrt{3a_0^2 - (1.5a_0)^2} = \frac{\sqrt{3}}{2} \approx 0.87a_0$$

4. *At $t = 0$, a particle has a wavefunction $\psi(x, y, z) = A\, z\, \exp[-b(x^2 + y^2 + z^2)]$, where A and b are constants.*

(a) *Show that this wavefunction is an eigenfunction of $\hat{L}^2$ and of $\hat{L}_z$ and find the corresponding eigenvalues.* Hint: *express ψ in spherical polars and use the spherical polar expressions for $\hat{L}^2$ and $\hat{L}_z$.*

$$\begin{aligned}\hat{L}^2 &= -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right] \\ \hat{L}_z &= -i\hbar\frac{\partial}{\partial\phi}\end{aligned}$$

First note that $x^2 + y^2 + z^2 = r^2$ and $z = r\cos\theta$, so that

$$u(r, \theta, \phi) = Ar\cos\theta\ \exp(-br^2)$$

In spherical polars,

$$\hat{L}^2 = -\hbar^2 \left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

Since u is actually independent of ϕ, we can ignore the second term when we apply $\hat{L}^2$ to the wavefunction u and note that

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\cos\theta\right) = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(-\sin^2\theta\right) = -2\cos\theta$$

Thus

$$\hat{L}^2\ u(r, \theta, \phi) = 2\hbar^2 Ar\cos\theta\exp(-br^2) = 2\hbar^2 u(r, \theta, \phi)$$

so that $u(r, \theta, \phi)$ is an eigenfunction of $\hat{L}^2$ with eigenvalue $2\hbar^2$. Writing $2\hbar^2 = \ell(\ell+1)\hbar^2$, we see that the orbital angular momentum quantum number $\ell = 1$.

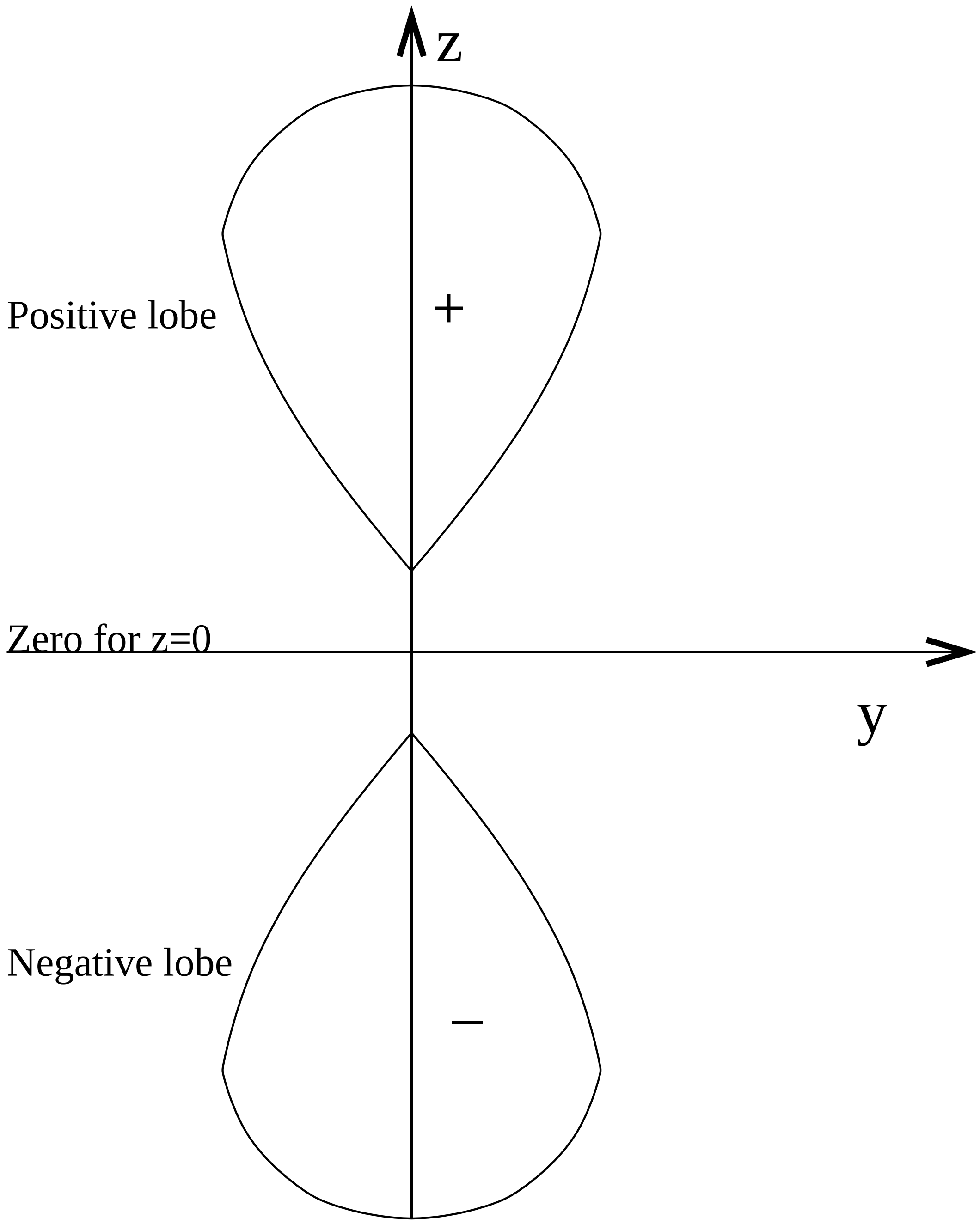
We have already noted that $u(r, \theta, \phi)$ is independent of ϕ which tells us immediately that it is an eigenfunction of $\hat{L}_z$ belonging to eigenvalue $m = 0$. Explicitly, we note that in spherical polar coordinates,

$$\hat{L}_z = -i\hbar\frac{\partial}{\partial\phi}$$

so that $\hat{L}_z u(r, \theta, \phi) = 0$. A short cut to the answer is to note that $u(r, \theta, \phi) \propto Y_{10}(\theta, \phi)$ and hence $\ell = 1$ and $m = 0$.

(b) *Sketch the wavefunction, e.g. with a contour plot in the x=0 plane.*

The function is zero at the origin. It has positive and negative lobes pointing aong the z-axis, decaying away to zero far from the origin. In fact, it looks a bit like a hydrogenic p-orbital ($l = 1$), though it isn't quite the same.



(c) *Can you identify the Hamiltonian for which this is an energy eigenstate ?*

The given function is an eigenfunction of the 3-dimensional isotropic simple harmonic oscillator with b related to the mass m and angular frequency ω through $b = m\omega/2\hbar$. It is the state with $n_x = n_y = 0$ and $n_z = 1$.

note: the 2007 version asked you to identify a physical system - this is rather challenging, an "atom trap" can capture single particles, which won a 1997 Nobel Prize for Chu, Cohen-Tannoudji and Phillips, and another in 2001 for Wieman, Ketterle and Cornell who trapped millons of Rubidium atoms in the same quantum state, forming a Bose Condensate. Optical tweezers are a method by which a particle can be trapped in a laser cavity. If you don't know about this stuff, look it up.

More esoterically (see 2007 exam), a neutrino trapped in the gravitational field of a constant density planet is a possibility!