PHYS2003 - Quantum Physics - 2014/15 Semester 1 Examination
Outline Solutions
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I have tried to mark those parts of questions which are bookwork, i.e. where the solutions have been presented almost identically in the lectures. The remaining questions are intended to be applications of bookwork. Similar, but not identical, questions have either been covered in the lectures or on the problem sheets. There should be no surprises for those students who have fully engaged with the course.

A1 (i) *I ask this to make the students think about dimensions. So often they give solutions to part (ii) which are wrong because of a slip, but the presence of a mistake should be obvious because of dimensions.*

Since the exponent must be dimensionless a has the dimensions of $[L]$. **1 mark**

The integral of $\psi^*\psi$ over all space is 1, and so A^2 has the dimensions of $[L]^{-3}$ and hence A has dimensions of $[L]^{-3/2}$. **1 mark**

(ii) The normalization condition is that

$$A^2 \times 4\pi \times \int_0^\infty dr\, r^2 e^{-2r/a} = 1\,,$$

where the 4π comes from the angular integral. **2 marks**
I imagine that some students will get some aspect of this wrong.

Using the given integral,

$$A^2 \times 4\pi \times 2! \times \left(\frac{a}{2}\right)^3 = 1\,,$$

so that $A^2 \times \pi a^3 = 1$ and

$$A = \frac{1}{\sqrt{\pi a^3}}\,.$$

Correct dimensions! **1 mark**

A2 *Bookwork, in the sense that the students are asked to demonstrate that they understand a concept presented in the lectures.*

The students are simply required to state (in some way) that

$$\int_0^a dx\, \psi_n^*(x)\, \psi_m(x) = \delta_{nm}\,.$$

2 marks if it is clear that the integral is zero if $n \neq m$ and **1 mark** for stating that the integral is 1 if $n = m$.

A3 *Bookwork, in the sense that the students are asked to demonstrate that they understand a concept presented in the lectures.*

Let f be any function in the Hilbert space of square integrable functions. $\hat{Q}$ is Hermitian if

$$\int_{-\infty}^{\infty} d^3x\, (\hat{Q}f(x))^*\, f(x) = \int_{-\infty}^{\infty} d^3x\, f^*(x)\, \hat{Q}f(x)\,,$$

for all functions $f(x)$ in the Hilbert space. **4 marks**

There are many equivalent ways of saying this, most common is to say

$$\int_{-\infty}^{\infty} d^3x\, (\hat{Q}g(x))^*\, f(x) = \int_{-\infty}^{\infty} d^3x\, g^*(x)\, \hat{Q}f(x)\,,$$

for all f and g in the Hilbert space. This is fine.
1 mark will be lost of there is no mention of the Hilbert space and 1 if the $*$ is missing.

A4 (i) By simple matrix multiplication

$$S_x\chi = \frac{\hbar}{2} \times \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = -\frac{\hbar}{2}\chi\,,$$

so that χ is an eigenstate of S_x with eigenvalue $-\hbar/2$. **2 marks**

(ii) We rewrite χ in terms of the eigenstates of S_z:

$$\chi = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} - \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right)\,,$$

where the two terms in the brackets are eigenvectors of S_z with eigenvalues $\pm\hbar/2$. Thus the probability of finding $+\hbar/2$ is $(1/\sqrt{2})^2 = 1/2$. **2 marks**

This is the last topic covered in the course and some fraction of the students will not have mastered this.

A5 The main thing I would like to check is that the students know that

$$\langle V(x) \rangle = \int_{-\infty}^{\infty} dx\, \psi_0^*(x)\, V(x)\, \psi_0(x)\,.$$

2 marks

The remaining **2 marks** are obtained for the evaluation:

$$\begin{aligned} \langle V(x) \rangle &= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \times \frac{1}{2} m\omega^2 \times \int_{-\infty}^{\infty} dx\, x^2 \exp\left[-\frac{m\omega}{\hbar} x^2\right] \\ &= \frac{1}{2} \frac{m^{\frac{3}{2}} \omega^{\frac{5}{2}}}{\sqrt{\pi\hbar}} \times 2 \times \sqrt{\pi} \times 2 \times \frac{1}{2^3} \times \left(\frac{\hbar}{m\omega}\right)^{\frac{3}{2}} \\ &= \frac{\hbar\omega}{4}\,. \end{aligned}$$

2 marks

This is a consequence of the virial theorem for the HO, in which the expectation values of the kinetic and potential energies are equal and the sum is the famous $\hbar\omega/2$.

B1 (i) *This was done explicitly in the lectures but I expect a variety of partial derivations.*

We start with

$$\langle x\rangle = \int_{-\infty}^{\infty} dx\, \Psi^*(x,t)\, x\, \Psi(x,t)\,, \qquad \textbf{1 mark}$$

so that

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \int dx\, x \frac{\partial}{\partial t}\left\{\Psi^*(x,t)\,\Psi(x,t)\right\}, \\ &= \int dx\, x \left\{\frac{\partial \Psi^*(x,t)}{\partial t}\Psi(x,t) + \Psi^*(x,t)\,\frac{\partial \Psi(x,t)}{\partial t}\right\}. \qquad \textbf{1 mark} \end{aligned}$$

Here and below the limits of integration are implicitly taken to be $\pm\infty$.

We now use the Schrödinger equation **2 marks**

$$i\hbar\frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\,\Psi\,,$$

to replace the time derivative by space derivatives (being careful with the signs when taking the complex conjugate)

$$\begin{aligned} \frac{d\langle x\rangle}{dt} &= \int dx\, x \left\{-i\frac{\hbar}{2m}\frac{\partial^2 \Psi^*}{\partial x^2}\Psi - \frac{iV}{\hbar}\Psi^*\Psi + i\frac{\hbar}{2m}\Psi^*\frac{\partial^2 \Psi}{\partial x^2} + \frac{iV}{\hbar}\Psi^*\Psi\right\} \\ &= -i\frac{\hbar}{2m}\int dx\, x \left\{\frac{\partial^2 \Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2 \Psi}{\partial x^2}\right\} \\ &= -i\frac{\hbar}{2m}\int dx\, x \frac{\partial}{\partial x}\left\{\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right\} \qquad \text{(using the given identity)} \\ &= i\frac{\hbar}{2m}\int dx \left\{\frac{\partial \Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial \Psi}{\partial x}\right\} \qquad \text{(using integration by parts)} \\ &= \boxed{-i\frac{\hbar}{m}\int dx\, \Psi^*\frac{\partial \Psi}{\partial x}} \qquad \text{(using integration by parts on first term of previous line)} \end{aligned}$$

We are allowed to use integration by parts because a normalizable wave function vanishes at $x = \pm\infty$.

3 marks for this algebra - 1 mark for first two lines, the middle line and the last two lines.

We have derived an expression for the expectation value of the velocity. Using $p = mv$ we have

$$\langle p\rangle = \int dx\, \Psi^*\left(-i\hbar\frac{\partial}{\partial x}\right)\Psi \equiv \int dx\, \Psi^*\,\hat{P}\,\Psi\,,$$

where

$$\hat{P} = -i\hbar\frac{\partial}{\partial x}$$

is the momentum operator. **3 marks - 2 for understanding and 1 for correct algebra.**

I have used $\hat{P}$ here for the operator but simply p in the question.

(ii) *Bookwork*

For any function $f(x)$ in the Hilbert space

$$xp\,f(x) = -i\hbar x f'(x)\,,$$

where the prime denotes differentiation w.r.t. x. On the other hand

$$px\,f(x) = -i\hbar \frac{\partial}{\partial x}(xf) = -i\hbar f - i\hbar x f'\,.$$

Thus

$$[x,p]f \equiv (xp - px)f = i\hbar f\,.$$

Since this is true for all f, we have $[x,p] = i\hbar$ as an operator statement.

4 marks: 1 for knowing what a commutator is, one for mentioning that this is true for any function in the space and 2 for the algebra.

(iii) The Heisenberg uncertainty principle states that the uncertainties in the position and momentum of a particle must satisfy $\Delta x \Delta p \geq \hbar/2$. **2 marks**

In the course I carefully define what is meant by Δx *and* Δp*, so maybe some of the students will give some more details.*

$\Delta x = 3\times 10^{-5}\,$m and $\Delta p > \hbar/(2\Delta x)$ **1 mark**. $p = h/\lambda$ **1 mark** so that $\Delta p = h/\lambda^2\,\Delta\lambda$ (uncertainties are defined to be positive) **1 mark**.

$$\Delta\lambda = \frac{\lambda^2}{h}\Delta p \geq \frac{\lambda^2}{h}\frac{\hbar}{2\Delta x} = \frac{\lambda^2}{4\pi\Delta x} = \frac{(8\times 10^{-7})^2}{4\pi(3\times 10^{-5})}\text{m} \simeq 1.7\times 10^{-9}\text{m}. \qquad \textbf{1 mark}$$

Thus the uncertainty in the wavelength is at least a few nm.

I expect only a few students to get all of these last 4 marks even though we have done similar exercises in the course.

B2 *Parts (i), (ii) and (iii) are largely bookwork. I do (i) and (ii) in the lectures for the general HO Hamiltonian and study the lowering operator explicitly, telling the students that the raising operator works in a similar way.* i) The key point here is to note that $[x,p] = i\hbar$ **2 marks** so that

$$(x+ip)(x-ip) = x^2 + p^2 - i[x,p] = x^2 + p^2 + \hbar\,.$$

Thus we have $H = x^2 + p^2 = (x+ip)(x-ip) - \hbar$. **2 marks**

ii) The required commutator is

$$[a_-, a_+] = \frac{1}{2\hbar}[x+ip, x-ip] = \frac{i}{2\hbar}(-[x,p] + [p,x]) = \frac{i}{2\hbar}(-2i\hbar) = 1\,.$$

Although I have written the solution in this 1 line form, some students will struggle a little

1 mark for explicitly or implicitly dropping the commutators $[x,x]$ and $[p,p]$, 2 for reorganising the right-hand side in terms of commutators $[x,p]$ and two for completing the calculation correctly.

iii) *We have covered this in the lectures for general m and ω, but I imagine that most students will have to figure out the details, recalling the general ideas.*

From the earlier two parts we have that $H = \hbar(2a_-a_+ - 1)$. Using $H\psi = E\psi$, we have

$$\begin{aligned} H(a_+\psi) &= \hbar\,[2a_-a_+ - 1]\,a_+\psi = \hbar[2a_+a_- + 1]\,a_+\psi, \text{ where we have used the commutator in (ii)} \\ &= \hbar a_+[2a_-a_+ + 1]\psi \\ &= a_+\,[H + 2\hbar]\,\psi = (E + 2\hbar)\,(a_+\psi)\,. \end{aligned}$$

Thus $a_+\psi$ is an eigenfunction of the Hamiltonian with eigenvalue $E + 2\hbar$.

1 mark for each of the 5 equations above (or equivalent if the student proceeds differently, e.g. by rewriting $H = \hbar(2a_+a_- + 1)$ and proceeding as above).

(iv) We have to translate the result in A5.

(a) Kinetic energy = $p^2/2m \;\Rightarrow$ in this question $m = \frac{1}{2}$.

(b) Potential energy = $\frac{1}{2}m\omega^2x^2 = \frac{1}{4}\omega^2x^2 \;\Rightarrow$ in this question $\omega = 2$ and $m\omega = 1$.

Thus from the wave function given in A5 we have

$$\psi_0(x) = \left(\frac{1}{\pi\hbar}\right)^{\frac{1}{4}} \exp\left[-\frac{x^2}{2\hbar}\right].$$

2 marks

Even though this is straightforward, I wanted the students to demonstrate that they see that this question is a particular case of the general Hamiltonian for the HO. The next part is to demonstrate that they understand that a_+ is a raising operator.

$$\psi_1(x) \propto a_+\psi_0(x) \propto (x - ip)\,\psi_0(x) \propto \left(x - \hbar\frac{d}{dx}\right)\exp\left[-\frac{x^2}{2\hbar}\right] = 2x\exp\left[-\frac{x^2}{2\hbar}\right].$$

The stronger students will notice that the $2x$ comes from $x + x$ whereas for the lowering operator we would have had $x - x = 0$ as required for the ground state.

Since we are not required to determine the normalisation constant, it was sufficient to put the $\propto$ symbols in the above equation. Thus the wave function of the first excited state is

$$\psi_1(x) = A_1\,x\exp\left[-\frac{x^2}{2\hbar}\right],$$

where A_1 is a constant.

4 marks: 2 for knowing that they need to evaluate $a_+\psi_0$ and 2 for the correct evaluation.

B3 *Part (i) is bookwork.*

(i) The single-frequency solutions of the Schödinger equation for a free particle are not normalizable and are hence unphysical (e.g. e^{ikx} in one dimension) (**2 marks**). In practice wavefunctions are superpositions of solutions over a range of values of k (and therefore of different energies E). We call such wavefunctions *wavepackets.* **2 marks**

While each component of the wavepacket propagates with its (phase) velocity ω/k, for a wavepacket peaked around a certain k the envelope of the packet propagates with the group velocity, $d\omega/dk$, for a period until it dissipates. **2 marks, the marks for $d\omega/dk$ come in the part(iii).**

(ii) *Even though this question is relatively straightforward, 2nd-year students do find Fourier transforms tricky.* The inverse Fourier transform is

$$\begin{aligned}
\phi(k) &= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dx\, \Psi(x,0)\, e^{-ikx} \qquad \textbf{2 marks} \\
&= \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2a}}\int_{-a}^{a} dx\, e^{-ikx} \\
&= \frac{1}{2\sqrt{\pi a}}\frac{i}{k}\left[e^{-ika}-e^{ika}\right] \\
&= \frac{1}{\sqrt{\pi a}}\frac{\sin ka}{k}. \qquad \textbf{2 marks}
\end{aligned}$$

For a free particle the energy $\omega(k) = \hbar^2 k^2/2m$ (**1 mark**).

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} dk\,\phi(k)\,\exp\left[i\left(kx-\frac{\omega(k)t}{\hbar}\right)\right] = \frac{1}{2\sqrt{\pi a}}\int_{-\infty}^{\infty} dk\,\frac{\sin ka}{k}\,\exp\left[i\left(kx-\frac{\hbar k^2}{2m}t\right)\right].$$

2 marks for the first equation and 1 for correctly rewriting it as in the second.

(iii) In this simple example the wavepacket is peaked around $k = 0$ (**1 mark**) and the group velocity is $\frac{d\omega}{dk}(k=0) = 0$. **2 marks**

For larger a the wavefunction at $t = 0$ is more spread out in x and hence, by the uncertainty principle more narrowly peaked in k-space (this can also be seen mathematically from the form of $\phi(k)$ above, but I do not expect the students to point this out). **1 mark**.

The wavepacket dissipates more slowly of it contains a narrow range of frequencies (or k's) and this will be the case for large a. **2 marks**

B4 *This question is intended to test the understanding of some fundamental aspects of the Hydrogen atom. Part (i) is bookwork.*

(i) It can be shown (indeed it was shown in the lectures) that the three operators H, L^2 and L_z commute, where $\vec{L}$ is the angular momentum and the choice of L_z rather than another component is conventional. Thus we can choose for the basis of energy eigenfunctions ones which are also eigenfunctions of L^2 with eigenvalue $l(l+1)\hbar^2$ and L_z with eigenvalue $m\hbar$. n, the principal quantum number, labels the energy level. **3 marks**

1 mark for understanding about the commutation of the three operators and 2 marks for the explanation of the quantum numbers.

For a given n, $l = 0, 1, \cdots n-1$ and for a given l there are $2l+1$ values of m. **2 marks**

Thus for $n = 2$ there are 1+3=4 states and with the same energy. **1 mark**

(ii) $\langle r\rangle$ is given by $\langle r\rangle = \int d^3r\, r\, \psi^*(\vec{r})\psi(\vec{r})$. **1 mark**

In this case

$$\langle r\rangle = \frac{1}{32\pi a^5}\int d^3r\; r \times r^2 \cos^2\theta\, e^{-r/a}\,. \qquad \textbf{1 mark}$$

Now the ϕ integration simply gives 2π (**1 mark**) and the θ integration gives

$$\int_{-1}^{1} dc\; c^2 = \frac{2}{3}\,. \qquad \textbf{2 marks}$$

Finally, using the given integral, the integration over r is

$$\int_0^\infty dr\; r^5\, e^{-r/a} = 120\, a^6\,. \qquad \textbf{2 marks}$$

Putting everything together we have

$$\langle r\rangle = \frac{1}{32\pi a^5} \times 2\pi \times \frac{2}{3} \times 120\, a^6 = 5a\,. \qquad \textbf{1 mark}$$

Some students find the use of spherical polar coordinates to be difficult, even though they first meet them in Year 1. I expect a variety of answers and a spread of marks. As always, I will have to mark the answers carefully, giving credit for partial understanding.

(iii) The energy of the emitted photon is $-13.6(1/9-1)$ eV=12.09 eV. **2 marks**

In terms of the wavelength λ, the energy of a photon is $h\nu = hc/\lambda$. **2 marks**

The students have been told that 1 eV=1.602×10^{-19} J and from the table of constants they have $h = 6.626\times10^{-34}$ J s and $c = 2.998\times10^{8}\ \mathrm{m\,s^{-1}}$. This gives

$$\lambda = 1.03\times10^{-7}\,\mathrm{m}\,. \qquad \textbf{2 marks}$$

The students generally find such questions, i.e. part (iii), straightforward.