## PHYS30201 Mathematical Fundamentals of Quantum Mechanics

Solutions 4

1. Since  $m_s$  can be  $-\frac{3}{2}$ ,  $-\frac{1}{2}$ ,  $\frac{1}{2}$  or  $\frac{3}{2}$ , and  $m_l$  can be -1, 0 or 1, there are 12 possible pairs  $\{m_s, m_l\}$ :

$$\begin{array}{ll} \{-\frac{3}{2},-1\} & \{-\frac{1}{2},-1\} & \{\frac{1}{2},-1\} & \{\frac{3}{2},-1\} \\ & \{-\frac{3}{2},0\} & \{-\frac{1}{2},0\} & \{\frac{1}{2},0\} & \{\frac{3}{2},0\} \\ & & \{-\frac{3}{2},1\} & \{-\frac{1}{2},1\} & \{\frac{1}{2},1\} & \{\frac{3}{2},1\} \end{array}$$

Also we can have for  $\{j, m_j\}$ :

$$\begin{cases} \frac{5}{2}, -\frac{5}{2} \end{cases} \qquad \begin{cases} \frac{5}{2}, -\frac{3}{2} \rbrace \qquad \{ \frac{5}{2}, -\frac{1}{2} \rbrace \qquad \{ \frac{5}{2}, \frac{1}{2} \rbrace \qquad \{ \frac{5}{2}, \frac{3}{2} \rbrace \qquad \{ \frac{5}{2}, \frac{5}{2} \rbrace \\ \\ \{ \frac{3}{2}, -\frac{3}{2} \rbrace \qquad \{ \frac{3}{2}, -\frac{1}{2} \rbrace \qquad \{ \frac{3}{2}, \frac{1}{2} \rbrace \qquad \{ \frac{3}{2}, \frac{3}{2} \rbrace \\ \\ \{ \frac{1}{2}, -\frac{1}{2} \rbrace \qquad \{ \frac{1}{2}, \frac{1}{2} \rbrace \qquad \{ \frac{1}{2}, \frac{1}{2} \rbrace \end{cases}$$

and again, there are 12 in total. Note that the lay-out is such that each column has the same value of  $m_j = m_l + m_s$ , so we can see that the numbers in each table match.

2. First write

$$\begin{split} \hat{\mathbf{J}}^2 &= \left( (\hat{J}_{+}^{(1)} + \hat{J}_{+}^{(2)}) (\hat{J}_{-}^{(1)} + \hat{J}_{-}^{(2)}) + (\hat{J}_{z}^{(1)} + \hat{J}_{z}^{(2)})^2 - \hbar (\hat{J}_{z}^{(1)} + \hat{J}_{z}^{(2)}) \right) \\ &= \left( (\hat{\mathbf{J}}^{(1)})^2 + (\hat{\mathbf{J}}^{(2)})^2 + \hat{J}_{+}^{(1)} \hat{J}_{-}^{(2)} + \hat{J}_{-}^{(1)} \hat{J}_{+}^{(2)} + 2\hat{J}_{z}^{(1)} \hat{J}_{z}^{(2)} \right). \end{split}$$

In the second line the last three terms would more correctly be written in the form  $\hat{J}^{(1)}_{+} \otimes \hat{J}^{(2)}_{-}$  etc; the first two act only in one of the two spaces.) Since our state is constructed from eigenstates of  $(\hat{\mathbf{J}}^{(1)})^2$  and  $(\hat{\mathbf{J}}^{(2)})^2$  with eigenvalues  $2\hbar^2$ , and since both contributions have one state with m = 0 so that the last term vanishes, the only terms which need further work are:

$$\begin{pmatrix} \hat{J}_{+}^{(1)}\hat{J}_{-}^{(2)} + \hat{J}_{-}^{(1)}\hat{J}_{+}^{(2)} \end{pmatrix} \left( |1,0\rangle \otimes |1,-1\rangle - |1,-1\rangle \otimes |1,0\rangle \right) = \hbar^{2} \Big( 0 - 2|1,0\rangle \otimes |1,-1\rangle + 2|1,-1\rangle \otimes |1,0\rangle + 0 \Big).$$

Hence

$$\hat{\mathbf{J}}^2|\alpha\rangle = (2+2-2)\hbar^2 \sqrt{\frac{1}{2}} \Big(|1,0\rangle \otimes |1,-1\rangle - |1,-1\rangle \otimes |1,0\rangle\Big) = 2\hbar^2 |\alpha\rangle.$$

Also  $\hat{J}_z |\alpha\rangle = -\hbar |\alpha\rangle$ , so J = 1, M = -1. The table of Clebsch-Gordan coefficients for this case is given below in to solution to Q4, so we can check this.

3. i),ii) We use the following extract from the PDG tables, with the red-circled columns for (a) and (b) and green-circled rows for (c) and (d), recalling that "-1/2" is shorthand for  $-\sqrt{1/2}$ .



$$\begin{aligned} \text{a)} &|\frac{5}{2}, \frac{3}{2} \rangle = \sqrt{\frac{2}{5}} &|\frac{3}{2}, \frac{3}{2} \rangle \otimes |1, 0\rangle + \sqrt{\frac{3}{5}} &|\frac{3}{2}, \frac{1}{2} \rangle \otimes |1, 1\rangle, \\ \text{b)} &|\frac{1}{2}, -\frac{1}{2} \rangle = \sqrt{\frac{1}{6}} &|\frac{3}{2}, \frac{1}{2} \rangle \otimes |1, -1\rangle - \sqrt{\frac{1}{3}} &|\frac{3}{2}, -\frac{1}{2} \rangle \otimes |1, 0\rangle + \sqrt{\frac{1}{2}} &|\frac{3}{2}, -\frac{3}{2} \rangle \otimes |1, 1\rangle \\ \text{c)} &|\frac{3}{2}, \frac{3}{2} \rangle \otimes |1, 0\rangle = \sqrt{\frac{2}{5}} &|\frac{5}{2}, \frac{3}{2} \rangle + \sqrt{\frac{3}{5}} &|\frac{3}{2}, \frac{3}{2} \rangle, \\ \text{d)} &|\frac{3}{2}, \frac{1}{2} \rangle \otimes |1, -1\rangle = \sqrt{\frac{3}{10}} &|\frac{5}{2}, -\frac{1}{2} \rangle + \sqrt{\frac{8}{15}} &|\frac{3}{2}, -\frac{1}{2} \rangle + \sqrt{\frac{1}{6}} &|\frac{1}{2}, -\frac{1}{2} \rangle. \end{aligned}$$

iii) The results of the initial measurements of the total angular momentum and its z-component mean that the particle is in state (b). A measurement of  $L_z$  gives  $\hbar m_l$ , where we can read off the allowed values of  $m_l$  from the expansion above, and the probabilities are the squares of the Clebsch-Gordan coefficients; hence

$$P(-1) = \frac{1}{6}, \qquad P(0) = \frac{1}{3}, \qquad P(1) = \frac{1}{2}.$$

Once  $m_l$  is known, so is  $m_s$ :  $m_s = -\frac{1}{2} - m_l$ .

iv) The measurements of the z-components of orbital and spin angular momenta destroy our knowledge of the total angular momentum (although its z-component is still $-\frac{1}{2}\hbar$ ). However  $m_l$  and  $m_s$  can be known simultaneously, so the particle is in now the state (d). A subsequent measurement of  $|\mathbf{J}|^2$  gives  $\sqrt{J(J+1)}\hbar$  where the allowed values of J and their probabilities can be read off from the expansion above; hence

$$P(\frac{5}{2}) = \frac{3}{10}, \qquad P(\frac{3}{2}) = \frac{8}{15}, \qquad P(\frac{1}{2}) = \frac{1}{6}.$$

4. We use the following extract from the PDG tables:



The coefficients we want are given by the columns of the central block:

$$\begin{split} |2,0\rangle &= \sqrt{\frac{1}{6}} |1,1\rangle \otimes |1,-1\rangle + \sqrt{\frac{2}{3}} |1,0\rangle \otimes |1,0\rangle + \sqrt{\frac{1}{6}} |1,-1\rangle \otimes |1,1\rangle, \\ |1,0\rangle &= \sqrt{\frac{1}{2}} |1,1\rangle \otimes |1,-1\rangle - \sqrt{\frac{1}{2}} |1,1\rangle \otimes |1,-1\rangle, \\ |0,0\rangle &= \sqrt{\frac{1}{3}} |1,1\rangle \otimes |1,-1\rangle - \sqrt{\frac{1}{3}} |1,0\rangle \otimes |1,0\rangle + \sqrt{\frac{1}{3}} |1,-1\rangle \otimes |1,1\rangle. \end{split}$$

If the particles, which are bosons, are identical and in an s-wave, their spin state must be symmetric. Only the states with S = 2 and S = 0 are allowed. Looking at the other columns of the table confirms that all the S = 1 states are antisymmetric, while all the others are symmetric. It is obvious that the S = 2 states must be symmetric because they include the stretched state  $|1,1\rangle \otimes |1,1\rangle$ . This result generalises: for  $s \otimes s$ , the multiplet with S = 2s is symmetric, and the symmetries alternate as we decrease S. Hence all the even values of S are symmetric for bosons and antisymmetric for fermions.

5. For this question and the next, the following results for Gaussian integrals will be useful:  $\int_{-\infty}^{\infty} e^{-\alpha x^2} dx = \sqrt{\pi/\alpha}, \text{ and } \int_{-\infty}^{\infty} x^{2n} e^{-\alpha x^2} dx = (-1)^n \frac{d^n}{d\alpha^n} \sqrt{\frac{\pi}{\alpha}}.$ 

For  $V(x) = \beta x^4$  and  $\Psi(x) = e^{-\alpha x^2/2}$ , and with  $\tilde{\beta} \equiv (2m\beta/\hbar^2)$ , we have  $E_0 < E_b$ , where

$$E_b(\alpha) = \frac{\int_{-\infty}^{\infty} \Psi^* \hat{H} \Psi \mathrm{d}x}{\int_{-\infty}^{\infty} \Psi^* \Psi \mathrm{d}x} = \frac{\hbar^2}{2m} \left(\frac{\sqrt{\pi\alpha}}{2} + \frac{3\tilde{\beta}\sqrt{\pi}}{4\alpha^{5/2}}\right) \Big/ \sqrt{\frac{\pi}{\alpha}} = \frac{\hbar^2}{2m} \left(\frac{\alpha}{2} + \frac{3\tilde{\beta}}{4\alpha^2}\right),$$

which is minimised at  $\alpha = (3\tilde{\beta})^{1/3}$ , giving  $E_b = (3/8)(6\hbar^4\beta/m^2)^{1/3}$ .

6. The wave function should look something like this, vanishing at x = 0 and tending to zero as  $x \to \infty$ , with no nodes in between:



It is essential that we satisfy the boundary conditions here, so we need to choose a trial wave function which vanishes at the origin. If we do not, the trial wave function cannot be expanded in terms of the true wave functions, and the theorem is not valid. Hence we should choose  $\Psi(x) = xe^{-x^2/(2a^2)}$  with a as a variational parameter. Then we get

$$\frac{\int_0^\infty \Psi^* \hat{H} \Psi \mathrm{d}x}{\int_0^\infty \Psi^* \Psi \mathrm{d}x} = \frac{\hbar^2}{2m} \left( \frac{3a\sqrt{\pi}}{8} + \frac{a^4\tilde{\beta}}{2} \right) \Big/ \frac{a^3\sqrt{\pi}}{4} = \frac{\hbar^2}{2m} \left( \frac{3}{2a^2} + \frac{2\tilde{\beta}a}{\sqrt{\pi}} \right),$$

with  $\tilde{\beta} = 2m\beta/\hbar^2$ . This is minimized for  $a = (3\sqrt{\pi}/2\tilde{\beta})^{1/3}$ , with the minimum energy bound being  $(81\hbar^2\beta^2/4\pi m)^{1/3} = 2.345(\hbar^2\beta^2/2m)^{1/3}$ . [Note: I used the unnormalised function  $\Psi(x)$ because I can't remember the normalisation factors for all the oscillator eigenstates. If I'd had the normalised function  $\phi_1(x)$  to hand, I could have avoided having to divide by the normalisation integral. However, in this case, I would have had to multiply  $\phi_1(x)$  by  $\sqrt{2}$  to account for the fact that here we are integrating from  $0 \to \infty$  only.] From now on, I will denote the energy scale  $(\hbar^2\beta^2/2m)^{1/3}$  by  $\mathcal{E}$ . If we'd chosen the oscillator ground state  $\Psi(x) = e^{-x^2/2a^2}$  instead, we would not have satified the boundary conditions. If fact, we would have been solving a different problem, namely the symmetric well  $V(x) = \beta |x|$ . (Although we integrated only from  $0 \to \infty$ , integrating from  $-\infty \to \infty$  would just double the numerator and denominator, leaving the result is unchanged.) The solution to the semi-infinite well is also that for the first excited state of the symmetric well.

An easy alternative function to try is  $xe^{-x/a}$ , for which we get  $(3/2)(9\hbar^2\beta^2/4m)^{1/3} = 2.476\mathcal{E}$ . Mathematica can cope with  $xe^{-(x/a)^{3/2}}$  which gives almost as good a bound as the Gaussian, 2.347 $\mathcal{E}$ . (I was surprised that it isn't better, because this is closer to the correct asymptotic behaviour as  $x \to \infty$ , but then the Gaussian is already extremely close to the true value.) To do any better, we probably need a two-parameter trial wave function.

From the web notes, we find that the general solution in terms of Airy functions has the form  $C\operatorname{Ai}(z-\mu) + D\operatorname{Bi}(z-\mu)$ , where  $z = x(\hbar^2/(2m\beta))^{-1/3}$  and  $\mu = E/\mathcal{E}$ . The function  $\operatorname{Bi}(z)$  blows up as  $z \to \infty$ , so its coefficient D must be zero. Then we choose  $\mu$  so that the wave function vanishes at z = 0:  $\operatorname{Ai}(-\mu) = 0$ . This can be achieved for  $\mu = 2.338$ , 4.088, 5.521... and the first of these is the solution quoted in the question. The unnormalised ground state wave function is plotted at the start of this solution.

7. This is a three dimensional problem with spherical symmetry, so we can evaluate the volume integrals in polar coordinates, with  $dV = r^2 \sin\theta dr d\theta d\phi$ . To calculate the expectation value of the kinetic term, we need  $\langle \Psi | \hat{\mathbf{p}}^2 | \Psi \rangle = \int \sum_i |\hat{p}_i \Psi|^2 dV = \int |d\Psi/dr|^2 dV$ , where we have used  $\hat{\mathbf{p}}\Psi(\mathbf{r}) = -i\hbar\nabla\Psi(\mathbf{r})$  and  $\nabla\Psi(r) = \hat{\mathbf{r}}\frac{d\Psi(r)}{dr}$ . (We could use the radial part of  $\nabla^2$  instead.) Defining  $\tilde{\beta} = 2m\beta/\hbar^2$  (which has dimensions of inverse length, as has  $\mu$ ), we have

$$E_b(a) = \frac{\int_0^\infty \Psi^* \hat{H} \Psi r^2 \mathrm{d}r}{\int_0^\infty \Psi^* \Psi r^2 \mathrm{d}r} = \frac{\hbar^2}{2m} \left( \frac{a}{4} - \frac{a^2 \tilde{\beta}}{(2+a\mu)^2} \right) \Big/ \frac{a^3}{4} = \frac{\hbar^2}{2m} \left( \frac{1}{a^2} - \frac{4\tilde{\beta}}{a(2+\mu a)^2} \right).$$

In this case, we note that the kinetic energy term  $\sim 1/a^2$  wins out at both very small and very large values of a, and  $E_b(a)$  many not even have a local minimum if the potential is too weak. See the sketches below for various values of  $\beta$ .

The question does not ask us to find the minimum in the general case. Instead it asks how strong the potential has to be for a bound state to be guaranteed. Since the potential vanishes as  $r \to \infty$ , a bound state must have negative energy. This will definitely be the case if there is a value or range of a for which the upper bound on the energy is negative.



The figure above shows the effect of varying  $\beta$  (for  $\mu=1$ ). The critical value is the one for which the minimum of the curve sits exactly at zero: we need simultaneously  $E_b = 0$  and  $dE_b/da = 0$ . This gives  $4\tilde{\beta}a = (2 + a\mu)^2$  and  $2\tilde{\beta}a(2 + 3a\mu) = (2 + a\mu)^3$ , or  $a = 2/\mu$  and  $\tilde{\beta} = 2\mu$ . So provided  $\tilde{\beta}/\mu \geq 2$ , there will be a bound state. In terms of  $\beta$ , we have  $\beta \geq \hbar^2 \mu/m$ .

This analysis does not hold for  $\mu = 0$ , in which case there is always a minimum with  $E_b < 0$  and there is always a bound state. We should not be surprised, since this is a Coulomb potential. In fact, the energy bound is minimised for  $a = 2/\tilde{\beta} = \hbar^2/m\beta$ . For  $\beta = \hbar c\alpha$ , we find  $a = a_0$ , the Bohr radius, and  $E_b = E_{\rm Ry}$ , as expected! This illustrates the fact that if we get lucky and choose the correct functional form for  $\Psi$ , we will reproduce the true ground state. (But of course we won't necessarily know that we have done so.)

8. For a potential with one hard and one soft wall, the WKB approximation says that

$$\int_{a}^{b} k(x') \mathrm{d}x' = \left(n + \frac{3}{4}\right)\pi, \quad \text{where} \quad k(x) = \sqrt{2m(E - V(x))}/\hbar.$$

(The RHS gets  $+\frac{\pi}{2}$  from the hard wall and  $+\frac{\pi}{4}$  from the soft wall.) One turning point is obviously at the hard wall, x = 0. For the linear potential  $V = \beta x$  and energy E, the other is at  $x = E/\beta \equiv b$ , and so we get

$$\int_{a}^{b} k(x') \mathrm{d}x' = \sqrt{\frac{2m\beta}{\hbar^2}} \int_{0}^{b} \sqrt{b - |x|} \, \mathrm{d}x = \sqrt{\frac{2m\beta}{\hbar^2}} \int_{0}^{b} \sqrt{b - x} \, \mathrm{d}x = \frac{2}{3} \sqrt{\frac{2m\beta}{\hbar^2}} b^{3/2} = \frac{2}{3} \left(\frac{2mE^3}{\hbar^2\beta^2}\right)^{1/2}$$

Equating this to  $(n + \frac{3}{4})\pi$  gives  $E = \left(\frac{3}{2}(n + \frac{3}{4})\pi\right)^{2/3} \left(\frac{\hbar^2\beta^2}{2m}\right)^{1/3}$ . The first three states are at 2.320, 4.082, 5.517, in units of  $\left(\frac{\hbar^2\beta^2}{2m}\right)^{1/3}$ . These can be compared with the exact values given above in the solution to Q6. We see that the WKB approximation is surprisingly good even for the lowest states, and rapidly becomes very good indeed.

9. For the harmonic oscillator potential,  $V(x) = \frac{1}{2}m\omega^2 x^2$ . The classical turning points are  $x = \pm \sqrt{2E/m\omega^2} \equiv \pm b$ . For two soft walls the WKB integral is  $(n+\frac{1}{2})\pi$  and so, denoting  $\sqrt{\hbar/m\omega} = x_0$  as usual for the oscillator, we get:

$$\int_{a}^{b} k(x') dx' = (x_0)^{-2} \int_{-b}^{b} \sqrt{b^2 - x^2} dx = \left(\frac{b}{x_0}\right)^2 \frac{1}{2} \left[\theta - \frac{1}{2}\sin 2\theta\right]_{-\pi/2}^{\pi/2} = \frac{2E}{\hbar\omega} \frac{\pi}{2}.$$

where we have used the substitution  $x = b \sin \theta$  to do the integral. Hence we get the exact result for the energy:  $E = (n + \frac{1}{2}) \hbar \omega$ .

In 3D with spherical symmetry, we can use  $\nabla^2 \psi = \frac{1}{r} \frac{\mathrm{d}^2(r\psi)}{\mathrm{d}r^2}$ , and so  $u(r) = r\psi(r)$  satisfies the 1D Schrödinger equation. Since  $\psi(0)$  must be finite, u(0) must vanish. Hence effectively there is one infinite wall (at r = 0) and a harmonic potential for r > 0. The quantisation condition is  $\int_0^b k(x') \mathrm{d}x' = (n + \frac{3}{4})\pi$ . The integral is just half of the one above, namely  $\pi E/(2\hbar\omega)$ , so  $E = (2n + \frac{3}{2})\hbar\omega$ .

The 3D oscillator is equivalent to three 1D oscillators and hence has a zero-point energy of  $\frac{3}{2}\hbar\omega$ . The energy levels of the system are in general  $(n + \frac{3}{2})\hbar\omega$ , but only the even values of n include l = 0 states when expressed in spherical coordinates.

10. We can treat this as an effective one-particle problem with mass  $\mu = m_p/2$ . The potential is  $V(r) = \hbar c \alpha/r$ , and the outer turning point is  $r_c = \hbar c \alpha/E$ ; the inner one can be taken to be the proton radius  $r_p$ . The dominant contribution to the tunnelling probability comes from  $e^{-G}$ , with  $G = 2 \int_{r_p}^{r_c} \kappa(r) dr$ , where  $\kappa(x) = \sqrt{2\mu(V(r) - E)}/\hbar$ . (The tunnelling is inwards, from  $r_c$  to  $r_p$ , but in addition dl = -dr which we take into account by swapping the limits.) Using the substitution  $r = r_c \cos^2 x$ ,

$$\int_{r_p}^{r_c} \kappa(r) \mathrm{d}r = \sqrt{2\mu E} \int_{r_p}^{r_c} \sqrt{r_c/r - 1} \, \mathrm{d}r = \left[\sqrt{r(r_c - r)} - r_c \arccos(\sqrt{r/r_c})\right]_{r_p}^{r_c}$$
$$= \sqrt{2\mu E} \left(-\sqrt{r_p(r_c - r_p)} + r_c \arccos(\sqrt{r_p/r_c})\right).$$

The term in brackets tends to  $r_c \pi/2$  for  $r_p \ll r_c$ . Hence  $G \approx \sqrt{2\mu E} r_c \pi/(\hbar) = (r_c/R_G)^{1/2}$ where  $R_G = \hbar/(\pi^2 m_p c \alpha) = 2.9$  fm. Equivalently we can write  $G \approx (E_G/E)^{1/2}$  where  $E_G = m_p c^2 (\alpha \pi)^2 = 0.493$  MeV. Since  $k_B = 8.617 \times 10^{-5}$  eV K<sup>-1</sup>, temperatures of around  $10^{10}$  K would be needed for fusion to be the most probable outcome of a proton-proton collision.

At the surface of the Sun, the typical thermal energy is of the order of  $k_B T \sim 0.5$  eV and the fusion probability is vanishingly small (~  $10^{-430}$ ). At the centre, the typical energy rises to  $k_B T \sim 860$  eV and the corresponding probability is ~  $10^{-11}$ . This may be tiny, but it is not zero and there are a lot of protons in the core of the Sun. Also, the thermal energies follow a Maxwell–Boltzmann distribution and the fusion probability grows rapidly with energy. For example, for two protons with an energy 10 times higher, the probability rises to  $5 \times 10^{-4}$ .

Of course, the formation of <sup>2</sup>He is not enough to generate energy and start building heavier nuclei. Mostly it just decays back to two protons. But occasionally it will undergo a weak decay, <sup>2</sup>He  $\rightarrow$  d + e<sup>-</sup> +  $\overline{\nu}_e$  which does release energy.