

## Introduction to Quantum Mechanics MT 2009

### Problems 1 (weeks 5-6 of MT)

**1.1** What physical phenomenon requires us to work with probability amplitudes rather than just with probabilities, as in other fields of endeavour?

**1.2** What properties cause complete sets of amplitudes to constitute the elements of a vector space?

**1.3**  $V'$  is the adjoint space of the vector space  $V$ . For a mathematician, what objects comprise  $V'$ ?

**1.4** In quantum mechanics, what objects are the members of the vector space  $V$ ? Give an example for the case of quantum mechanics of a member of the adjoint space  $V'$  and explain how members of  $V'$  enable us to predict the outcomes of experiments.

**1.5** Given that  $|\psi\rangle = e^{i\pi/5}|a\rangle + e^{i\pi/4}|b\rangle$ , express  $\langle\psi|$  as a linear combination of  $\langle a|$  and  $\langle b|$ .

**1.6** What properties characterise the bra  $\langle a|$  that is associated with the ket  $|a\rangle$ ?

**1.7** An electron can be in one of two potential wells that are so close that it can “tunnel” from one to the other (see §5.2 for a description of quantum-mechanical tunnelling). Its state vector can be written

$$|\psi\rangle = a|A\rangle + b|B\rangle, \quad (1.1)$$

where  $|A\rangle$  is the state of being in the first well and  $|B\rangle$  is the state of being in the second well and all kets are correctly normalised. What is the probability of finding the particle in the first well given that: (a)  $a = i/2$ ; (b)  $b = e^{i\pi}$ ; (c)  $b = \frac{1}{3} + i/\sqrt{2}$ ?

**1.8** An electron can “tunnel” between potential wells that form a chain, so its state vector can be written

$$|\psi\rangle = \sum_{-\infty}^{\infty} a_n |n\rangle, \quad (1.2a)$$

where  $|n\rangle$  is the state of being in the  $n^{\text{th}}$  well, where  $n$  increases from left to right. Let

$$a_n = \frac{1}{\sqrt{2}} \left( \frac{-i}{3} \right)^{|n|/2} e^{in\pi}. \quad (1.2b)$$

a. What is the probability of finding the electron in the  $n^{\text{th}}$  well?

b. What is the probability of finding the electron in well 0 or anywhere to the right of it?

**1.9** How is a wave-function  $\psi(x)$  written in Dirac’s notation? What’s the physical significance of the complex number  $\psi(x)$  for given  $x$ ?

**1.10** Let  $Q$  be an operator. Under what circumstances is the complex number  $\langle a|Q|b\rangle$  equal to the complex number  $(\langle b|Q|a\rangle)^*$  for any states  $|a\rangle$  and  $|b\rangle$ ?

**1.11** Let  $Q$  be the operator of an observable and let  $|\psi\rangle$  be the state of our system.

a. What are the physical interpretations of  $\langle\psi|Q|\psi\rangle$  and  $|\langle q_n|\psi\rangle|^2$ , where  $|q_n\rangle$  is the  $n^{\text{th}}$  eigenket of the observable  $Q$  and  $q_n$  is the corresponding eigenvalue?

b. What is the operator  $\sum_n |q_n\rangle\langle q_n|$ , where the sum is over all eigenkets of  $Q$ ? What is the operator  $\sum_n q_n |q_n\rangle\langle q_n|$ ?

c. If  $u_n(x)$  is the wavefunction of the state  $|q_n\rangle$ , write down an integral that evaluates to  $\langle q_n|\psi\rangle$ .

**1.12** What does it mean to say that two operators commute? What is the significance of two observables having mutually commuting operators?

Given that the commutator  $[P, Q] \neq 0$  for some observables  $P$  and  $Q$ , does it follow that for all  $|\psi\rangle \neq 0$  we have  $[P, Q]|\psi\rangle \neq 0$ ?

**1.13** Let  $\psi(x, t)$  be the correctly normalised wavefunction of a particle of mass  $m$  and potential energy  $V(x)$ . Write down expressions for the expectation values of (a)  $x$ ; (b)  $x^2$ ; (c) the momentum  $p_x$ ; (d)  $p_x^2$ ; (e) the energy.

What is the probability that the particle will be found in the interval  $(x_1, x_2)$ ?

**1.14** A system has a time-independent Hamiltonian that has spectrum  $\{E_n\}$ . Prove that the probability  $P_k$  that a measurement of energy will yield the value  $E_k$  is time-independent. Hint: you can do this either from Ehrenfest's theorem, or by differentiating  $\langle E_k | \psi \rangle$  w.r.t.  $t$  and using the TDSE.

**1.15** A particle moves in the potential  $V(\mathbf{x})$  and is known to have energy  $E_n$ . (a) Can it have well defined momentum for some particular  $V(\mathbf{x})$ ? (b) Can the particle simultaneously have well-defined energy and position?

**1.16** The states  $\{|1\rangle, |2\rangle\}$  form a complete orthonormal set of states for a two-state system. With respect to these basis states the operator  $\sigma_y$  has matrix

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (1.3)$$

Could  $\sigma$  be an observable? What are its eigenvalues and eigenvectors in the  $\{|1\rangle, |2\rangle\}$  basis? Determine the result of operating with  $\sigma_y$  on the state

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle). \quad (1.4)$$

**1.17** Prove for any four operators  $A, B, C, D$  that

$$[ABC, D] = AB[C, D] + A[B, D]C + [A, D]BC. \quad (1.5)$$

Explain the similarity with the rule for differentiating a product.

**1.18** Show that a classical harmonic oscillator satisfies the virial equation  $2\langle \text{KE} \rangle = \alpha \langle \text{PE} \rangle$  and determine the relevant value of  $\alpha$ .

**1.19** A classical fluid of density  $\rho(\mathbf{x})$  flows with velocity  $\mathbf{v}(\mathbf{x})$ . By differentiating with respect to time the mass  $m \equiv \int_V d^3\mathbf{x} \rho$  contained in an arbitrary volume  $V$ , show that conservation of mass requires that

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0. \quad (1.6)$$

Hint: the flux of matter at any point is  $\rho \mathbf{v}$  and the integral of this flux over the boundary of  $V$  must equal the rate of accumulation of mass within  $V$ .

$\mathbf{J}$  is defined to be

$$\mathbf{J}(\mathbf{x}) \equiv \frac{i\hbar}{2m} (\psi \nabla \psi^* - \psi^* \nabla \psi), \quad (1.7)$$

where  $\psi(\mathbf{x})$  is the wavefunction of a spinless particle of mass  $m$ . Working from the TDSE, show that

$$\frac{\partial |\psi|^2}{\partial t} + \nabla \cdot \mathbf{J} = 0. \quad (1.8)$$

Give a physical interpretation of this result.

Show that when we write the wavefunction in amplitude-modulus form,  $\psi = |\psi|e^{i\theta}$ ,

$$\mathbf{J} = |\psi|^2 \frac{\hbar \nabla \theta}{m}. \quad (1.9)$$

Interpret this result physically. Given that  $\psi = Ae^{i(kz - \omega t)} + Be^{-i(kz + \omega t)}$ , where  $A$  and  $B$  are constants, show that

$$\mathbf{J} = v(|A|^2 - |B|^2) \hat{\mathbf{z}}, \quad (1.10)$$

where  $v = \hbar k/m$ . Interpret the result physically.

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### Problems 2 (Weeks 7–8)

**2.1** Write down the time-independent (TISE) and the time-dependent (TDSE) Schrödinger equations. Is it necessary for the wavefunction of a system to satisfy the TDSE? Under what circumstances does the wavefunction of a system satisfy the TISE?

**2.2** Why is the TDSE first-order in time, rather than second-order like Newton's equations of motion?

**2.3** A particle is confined in a potential well such that its allowed energies are  $E_n = n^2\mathcal{E}$ , where  $n = 1, 2, \dots$  is an integer and  $\mathcal{E}$  a positive constant. The corresponding energy eigenstates are  $|1\rangle, |2\rangle, \dots, |n\rangle, \dots$ . At  $t = 0$  the particle is in the state

$$|\psi(0)\rangle = 0.2|1\rangle + 0.3|2\rangle + 0.4|3\rangle + 0.843|4\rangle. \quad (2.1)$$

- a. What is the probability, if the energy is measured at  $t = 0$  of finding a number smaller than  $6\mathcal{E}$ ?
- b. What is the mean value and what is the rms deviation of the energy of the particle in the state  $|\psi(0)\rangle$ ?
- c. Calculate the state vector  $|\psi\rangle$  at time  $t$ . Do the results found in (a) and (b) for time  $t$  remain valid for arbitrary time  $t$ ?
- d. When the energy is measured it turns out to be  $16\mathcal{E}$ . After the measurement, what is the state of the system? What result is obtained if the energy is measured again?

**2.4** Let  $\psi(x)$  be a properly normalised wavefunction and  $Q$  an operator on wavefunctions. Let  $\{q_r\}$  be the spectrum of  $Q$  and  $\{u_r(x)\}$  be the corresponding correctly normalised eigenfunctions. Write down an expression for the probability that a measurement of  $Q$  will yield the value  $q_r$ . Show that  $\sum_r P(q_r|\psi) = 1$ . Show further that the expectation of  $Q$  is  $\langle Q \rangle \equiv \int_{-\infty}^{\infty} \psi^* Q \psi dx$ .<sup>1</sup>

**2.5** Find the energy of neutron, electron and electromagnetic waves of wavelength 0.1 nm.

**2.6** Neutrons are emitted from an atomic pile with a Maxwellian distribution of velocities for temperature 400 K. Find the most probable de Broglie wavelength in the beam.

**2.7** A beam of neutrons with energy  $E$  runs horizontally into a crystal. The crystal transmits half the neutrons and deflects the other half vertically upwards. After climbing to height  $H$  these neutrons are deflected through  $90^\circ$  onto a horizontal path parallel to the originally transmitted beam. The two horizontal beams now move a distance  $L$  down the laboratory, one distance  $H$  above the other. After going distance  $L$ , the lower beam is deflected vertically upwards and is finally deflected into the path of the upper beam such that the two beams are co-spatial as they enter the detector. Given that particles in both the lower and upper beams are in states of well-defined momentum, show that the wavenumbers  $k, k'$  of the lower and upper beams are related by

$$k' \simeq k \left( 1 - \frac{m_n g H}{2E} \right). \quad (2.2)$$

In an actual experiment (R. Colella et al., 1975, Phys. Rev. Let., 34, 1472)  $E = 0.042$  eV and  $LH \sim 10^{-3} \text{ m}^2$  (the actual geometry was slightly different). Determine the phase difference between the two beams at the detector. Sketch the intensity in the detector as a function of  $H$ .

**2.8** A three-state system has a complete orthonormal set of states  $|1\rangle, |2\rangle, |3\rangle$ . With respect to this basis the operators  $H$  and  $B$  have matrices

$$H = \hbar\omega \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix} \quad B = b \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad (2.3)$$

where  $\omega$  and  $b$  are real constants.

- a. Are  $H$  and  $B$  Hermitian?
- b. Write down the eigenvalues of  $H$  and find the eigenvalues of  $B$ . Solve for the eigenvectors of both  $H$  and  $B$ . Explain why neither matrix uniquely specifies its eigenvectors.
- c. Show that  $H$  and  $B$  commute. Give a basis of eigenvectors common to  $H$  and  $B$ .

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<sup>1</sup> In the most elegant formulation of quantum mechanics, this last result is the basic postulate of the theory, and one derives other rules for the physical interpretation of the  $q_n, a_n$  etc. from it – see J. von Neumann, *Mathematical Foundations of Quantum Mechanics*.

**2.9** Given that  $A$  and  $B$  are Hermitian operators, show that  $i[A, B]$  is a Hermitian operator.

**2.10** Given a ordinary function  $f(x)$  and an operator  $R$ , the operator  $f(R)$  is defined to be

$$f(R) = \sum_i f(r_i) |r_i\rangle \langle r_i|, \quad (2.4)$$

where  $r_i$  are the eigenvalues of  $R$  and  $|r_i\rangle$  are the associated eigenkets. Show that when  $f(x) = x^2$  this definition implies that  $f(R) = RR$ , that is, that operating with  $f(R)$  is equivalent to applying the operator  $R$  twice. What bearing does this result have in the meaning of  $e^{R}$ ?

**2.11** Show that if there is a complete set of mutual eigenkets of the Hermitian operators  $A$  and  $B$ , then  $[A, B] = 0$ . Explain the physical significance of this result.

**2.12** Given that for any two operators  $(AB)^\dagger = B^\dagger A^\dagger$ , show that

$$(ABCD)^\dagger = D^\dagger C^\dagger B^\dagger A^\dagger. \quad (2.5)$$



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### Problems 4 (Weeks 1–2)

**4.1** A particle is confined by the potential well

$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ \infty & \text{otherwise.} \end{cases} \quad (4.1)$$

Explain (a) why we can assume that there is a complete set of stationary states with well-defined parity and (b) why to find the stationary states we solve the TISE subject to the boundary condition  $\psi(\pm a) = 0$ .

Determine the particle's energy spectrum and give the wavefunctions of the first two stationary states.

**4.2** At  $t = 0$  the particle of Problem 4.1 has the wavefunction

$$\psi(x) = \begin{cases} 1/\sqrt{2a} & \text{for } |x| < a \\ 0 & \text{otherwise.} \end{cases} \quad (4.2)$$

Find the probabilities that a measurement of its energy will yield: (a)  $9\hbar^2\pi^2/(8ma^2)$ ; (b)  $16\hbar^2\pi^2/(8ma^2)$ .

**4.3** Find the probability distribution of measuring momentum  $p$  for the particle described in Problem 4.2. Sketch and comment on your distribution. Hint: express  $\langle p|x\rangle$  in the position representation.

**4.4** Particles move in the potential

$$V(x) = \begin{cases} 0 & \text{for } x < 0 \\ V_0 & \text{for } x > 0. \end{cases} \quad (4.3)$$

Particles of mass  $m$  and energy  $E > V_0$  are incident from  $x = -\infty$ . Show that the probability that a particle is reflected is

$$\left(\frac{k-K}{k+K}\right)^2, \quad (4.4)$$

where  $k \equiv \sqrt{2mE}/\hbar$  and  $K \equiv \sqrt{2m(E-V_0)}/\hbar$ . Show directly from the TISE that the probability of transmission is

$$\frac{4kK}{(k+K)^2} \quad (4.5)$$

and check that the flux of particles moving away from the origin is equal to the incident particle flux.

**4.5** Show that the energies of bound, odd-parity stationary states of the square potential well

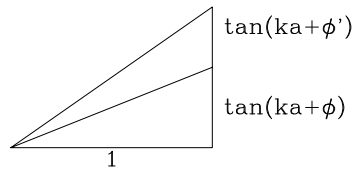
$$V(x) = \begin{cases} 0 & \text{for } |x| < a \\ V_0 > 0 & \text{otherwise,} \end{cases} \quad (4.6)$$

are governed by

$$\cot(ka) = -\sqrt{\frac{W^2}{(ka)^2} - 1} \quad \text{where} \quad W \equiv \sqrt{\frac{2mV_0a^2}{\hbar^2}} \quad \text{and} \quad k^2 = 2mE/\hbar^2. \quad (4.7)$$

Show that for a bound odd-parity state to exist, we require  $W > \pi/2$ .

**4.6** Give an example of a potential in which there is a complete set of bound stationary states of well-defined parity, and an alternative complete set of bound stationary states that are not eigenkets of the parity operator. Hint: modify the potential discussed apropos NH<sub>3</sub>.



**Figure 4.0** A triangle for Problem 5.9

**4.7** A free particle of energy  $E$  approaches a square, one-dimensional potential well of depth  $V_0$  and width  $2a$ . Show that the probability of being reflected by the well vanishes when  $Ka = n\pi/2$ , where  $n$  is an integer and  $K = (2m(E + V_0)/\hbar^2)^{1/2}$ . Explain this phenomenon in physical terms.

**4.8** Show that the phase shifts  $\phi$  (for the even-parity stationary state) and  $\phi'$  (for the odd-parity state) that are associated with scattering by a classically allowed region of potential  $V_0$  and width  $2a$ , satisfy

$$\tan(ka + \phi) = -(k/K) \cot(Ka) \quad \text{and} \quad \tan(ka + \phi') = (k/K) \tan(Ka),$$

where  $k$  and  $K$  are, respectively, the wavenumbers at infinity and in the scattering potential. Show that

$$P_{\text{refl}} = \cos^2(\phi' - \phi) = \frac{(K/k - k/K)^2 \sin^2(2Ka)}{(K/k + k/K)^2 \sin^2(2Ka) + 4 \cos^2(2Ka)}. \quad (4.8)$$

Hint: apply the cosine rule for an angle in a triangle in terms of the lengths of the triangle's sides to the top triangle in Figure 4.0.

**4.9** A particle of energy  $E$  approaches from  $x < 0$  a barrier in which the potential energy is  $V(x) = V_0 \delta(x)$ . Show that the probability of its passing the barrier is

$$P_{\text{tun}} = \frac{1}{1 + (K/2k)^2} \quad \text{where} \quad k = \sqrt{\frac{2mE}{\hbar^2}}, \quad K = \frac{2mV_0}{\hbar^2}. \quad (4.9)$$

**4.10** A system AB consists of two non-interacting parts A and B. The dynamical state of A is described by  $|a\rangle$ , and that of B by  $|b\rangle$ , so  $|a\rangle$  satisfies the TDSE for A and similarly for  $|b\rangle$ . What is the ket describing the dynamical state of AB? In terms of the Hamiltonians  $H_A$  and  $H_B$  of the subsystems, write down the TDSE for the evolution of this ket and show that it is automatically satisfied. Do  $H_A$  and  $H_B$  commute? How is the TDSE changed when the subsystems are coupled by a small dynamical interaction  $H_{\text{int}}$ ? If A and B are harmonic oscillators, write down  $H_A$ ,  $H_B$ . The oscillating particles are connected by a weak spring. Write down the appropriate form of the interaction Hamiltonian  $H_{\text{int}}$ . Does  $H_A$  commute with  $H_{\text{int}}$ ? Explain the physical significance of your answer.

**4.11** Explain what is implied by the statement that “the physical state of system A is correlated with the state of system B.” Illustrate your answer by considering the momenta of cars on (i) the M25 at rush-hour, and (ii) the road over the Nullarbor Plain in southern Australia in the dead of night.

Explain why the states of A and B must be uncorrelated if it is possible to write the state of AB as a ket  $|\text{AB}; \psi\rangle = |\text{A}; \psi_1\rangle |\text{B}; \psi_2\rangle$  that is a product of states of A and B. Given a complete set of states for A,  $\{|\text{A}; i\rangle\}$  and a corresponding complete set of states for B,  $\{|\text{B}; i\rangle\}$ , write down an expression for a state of AB in which B is possibly correlated with A.

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### Problems 5 (week 3)

**5.1** Show that  $L_i$  commutes with  $\mathbf{x} \cdot \mathbf{p}$  and thus also with scalar functions of  $\mathbf{x}$  and  $\mathbf{p}$ .

**5.2** In the rotation spectrum of  $^{12}\text{C}^{16}\text{O}$  the line arising from the transition  $l = 4 \rightarrow 3$  is at 461.04077 GHz, while that arising from  $l = 36 \rightarrow 35$  is at 4115.6055 GHz. Show from these data that in a non-rotating CO molecule the intra-nuclear distance is  $s \simeq 0.113$  nm, and that the electrons provide a spring between the nuclei that has force constant  $\sim 1904$  N m $^{-1}$ . Hence show that the vibrational frequency of CO should lie near  $6.47 \times 10^{13}$  Hz (measured value is  $6.43 \times 10^{13}$  Hz). Hint: show from classical mechanics that the distance of O from the centre of mass is  $\frac{3}{7}s$  and that the molecule's moment of inertia is  $\frac{48}{7}m_{\text{p}}s^2$ . Recall also the classical relation  $L = I\omega$ .

**5.3** The angular part of a system's wavefunction is

$$\langle \theta, \phi | \psi \rangle \propto (\sqrt{2} \cos \theta + \sin \theta e^{-i\phi} - \sin \theta e^{i\phi}).$$

What are the possible results of measurement of (a)  $L^2$ , and (b)  $L_z$ , and their probabilities? What is the expectation value of  $L_z$ ?

**5.4** A system's wavefunction is proportional to  $\sin^2 \theta e^{2i\phi}$ . What are the possible results of measurements of (a)  $L_z$  and (b)  $L^2$ ?

**5.5** A system's wavefunction is proportional to  $\sin^2 \theta$ . What are the possible results of measurements of (a)  $L_z$  and (b)  $L^2$ ? Give the probabilities of each possible outcome.

**5.6** Let  $\mathbf{n}$  be any unit vector and  $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$  be the vector whose components are the Pauli matrices. Why is it physically necessary that  $\mathbf{n} \cdot \boldsymbol{\sigma}$  satisfy  $(\mathbf{n} \cdot \boldsymbol{\sigma})^2 = I$ , where  $I$  is the  $2 \times 2$  identity matrix? Let  $\mathbf{m}$  be a unit vector such that  $\mathbf{m} \cdot \mathbf{n} = 0$ . Why do we require that the commutator  $[\mathbf{m} \cdot \boldsymbol{\sigma}, \mathbf{n} \cdot \boldsymbol{\sigma}] = 2i(\mathbf{m} \times \mathbf{n}) \cdot \boldsymbol{\sigma}$ ? Prove that these relations follow from the algebraic properties of the Pauli matrices. You should be able to show that  $[\mathbf{m} \cdot \boldsymbol{\sigma}, \mathbf{n} \cdot \boldsymbol{\sigma}] = 2i(\mathbf{m} \times \mathbf{n}) \cdot \boldsymbol{\sigma}$  for any two vectors  $\mathbf{n}$  and  $\mathbf{m}$ .

**5.7** Let  $\mathbf{n}$  be the unit vector in the direction with polar coordinates  $(\theta, \phi)$ . Write down the matrix  $\mathbf{n} \cdot \boldsymbol{\sigma}$  and find its eigenvectors. Hence show that the state of a spin-half particle in which a measurement of the component of spin along  $\mathbf{n}$  is certain to yield  $\frac{1}{2}\hbar$  is

$$|+, \mathbf{n}\rangle = \sin(\theta/2) e^{i\phi/2} |-\rangle + \cos(\theta/2) e^{-i\phi/2} |+\rangle, \quad (5.1)$$

where  $|\pm\rangle$  are the states in which  $\pm\frac{1}{2}$  is obtained when  $s_z$  is measured. Obtain the corresponding expression for  $|-, \mathbf{n}\rangle$ . Explain physically why the amplitudes in (5.1) have modulus  $2^{-1/2}$  when  $\theta = \pi/2$  and why one of the amplitudes vanishes when  $\theta = \pi$ .

**5.8** Write down the  $3 \times 3$  matrix that represents  $S_x$  for a spin-one system in the basis in which  $S_z$  is diagonal (i.e., the basis states are  $|0\rangle$  and  $|\pm\rangle$  with  $S_z|+\rangle = |+\rangle$ , etc.)

A beam of spin-one particles emerges from an oven and enters a Stern–Gerlach filter that passes only particles with  $J_z = \hbar$ . On exiting this filter, the beam enters a second filter that passes only particles with  $J_x = \hbar$ , and then finally it encounters a filter that passes only particles with  $J_z = -\hbar$ . What fraction of the particles stagger right through?

**5.9** A box containing two spin-one gyros A and B is found to have angular-momentum quantum numbers  $j = 2$ ,  $m = 1$ . Determine the probabilities that when  $J_z$  is measured for gyro A, the values  $m = \pm 1$  and 0 will be obtained.

What is the value of the Clebsch–Gordan coefficient  $C(2, 1; 1, 1, 1, 0)$ ?

**5.10** The angular momentum of a hydrogen atom in its ground state is entirely due to the spins of the electron and proton. The atom is in the state  $|1, 0\rangle$  in which it has one unit of angular momentum but none of it is parallel to the  $z$ -axis. Express this state as a linear combination of products of the spin states  $|\pm, e\rangle$  and  $|\pm, p\rangle$  of the proton and electron. Show that the states  $|x\pm, e\rangle$  in which the electron has well-defined spin along the  $x$ -axis are

$$|x\pm, e\rangle = \frac{1}{\sqrt{2}} (|+, e\rangle \pm |-, e\rangle). \quad (5.2)$$

By writing

$$|1, 0\rangle = |x+, e\rangle \langle x+, e|1, 0\rangle + |x-, e\rangle \langle x-, e|1, 0\rangle, \quad (5.3)$$

express  $|1, 0\rangle$  as a linear combination of the products  $|x\pm, e\rangle |x\pm, p\rangle$ . Explain the physical significance of your result.

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### Problems 6 (weeks 4–5)

**6.1** Some things about hydrogen's gross structure that it's important to know (ignore spin throughout):

- a) What quantum numbers characterise stationary states of hydrogen?
- b) What combinations of values of these numbers are permitted?
- c) Give the formula for the energy of a stationary state in terms of the Rydberg  $\mathcal{R}$ . What is the value of  $\mathcal{R}$  in eV?
- d) How many stationary states are there in the first excited level and in the second excited level?
- e) What is the wavefunction of the ground state?
- f) Write down an expression for the mass of the reduced particle.
- g) We can apply hydrogenic formulae to any two charged particles that are electrostatically bound. How does the ground-state energy then scale with (i) the mass of the reduced particle, and (ii) the charge  $Ze$  on the nucleus? (iii) How does the radial scale of the system scale with  $Z$ ?

**6.2** In the Bohr atom, electrons move on classical circular orbits that have angular momenta  $l\hbar$ , where  $l = 1, 2, \dots$ . Show that the radius of the first Bohr orbit is  $a_0$  and that the model predicts the correct energy spectrum. In fact the ground state of hydrogen has zero angular momentum. Why did Bohr get correct answers from an incorrect hypothesis?

**6.3** Show that the speed of a classical electron in the lowest Bohr orbit (Problem 6.2) is  $v = \alpha c$ , where  $\alpha = e^2/4\pi\epsilon_0\hbar c$  is the fine-structure constant. What is the corresponding speed for a hydrogen-like Fe ion (atomic number  $Z = 26$ )?

**6.4** Show that Bohr's hypothesis (that a particle's angular momentum must be an integer multiple of  $\hbar$ ), when applied to the three-dimensional harmonic oscillator, predicts energy levels  $E = l\hbar\omega$  with  $l = 1, 2, \dots$ . Is there an experiment that would falsify this prediction?

**6.5** Show that the electric field experienced by an electron in the ground state of hydrogen is of order  $5 \times 10^{11} \text{ V m}^{-1}$ . Can comparable macroscopic fields be generated in the laboratory?

**6.6** Positronium consists of an electron and a positron (both spin-half and of equal mass) in orbit around one another. What are its energy levels? By what factor is a positronium atom bigger than a hydrogen atom?

**6.7** The emission spectrum of the  $\text{He}^+$  ion contains the Pickering series of spectral lines that is analogous to the Lyman, Balmer and Paschen series in the spectrum of hydrogen.

Balmer $i = 1, 2, \dots$	0.456806	0.616682	0.690685	0.730884
Pickering $i = 2, 4, \dots$	0.456987	0.616933	0.690967	0.731183

The table gives the frequencies (in  $10^{15} \text{ Hz}$ ) of the first four lines of the Balmer series and the first four even-numbered lines of the Pickering series. The frequencies of these lines in the Pickering series are almost coincident with the frequencies of lines of the Balmer series. Explain this finding. Provide a quantitative explanation of the small offset between these nearly coincident lines in terms of the reduced mass of the electron in the two systems. (In 1896 E.C. Pickering identified the odd-numbered lines in his series in the spectrum of the star  $\zeta$  Puppis. Helium had yet to be discovered and he believed that the lines were being produced by hydrogen. Naturally he confused the even-numbered lines of his series with ordinary Balmer lines.)

**6.8** Show that for hydrogen the matrix element  $\langle 2, 0, 0 | z | 2, 1, 0 \rangle = -3a_0$ . On account of the non-zero value of this matrix element, when an electric field is applied to a hydrogen atom in its first excited state, the atom's energy is linear in the field strength (§9.1.2).

## Introduction to Quantum Mechanics HT 2010

### Problems 7 (Easter vacation)

**7.1\*** By expressing the annihilation operator  $A$  of the harmonic oscillator in the momentum representation, obtain  $\langle p|0\rangle$ . Check that your expression agrees with that obtained from the Fourier transform of

$$\langle x|0\rangle = \frac{1}{(2\pi\ell^2)^{1/4}} e^{-x^2/4\ell^2}, \quad \text{where } \ell \equiv \sqrt{\frac{\hbar}{2m\omega}}. \quad (7.1)$$

**7.2** Show that for any two  $N \times N$  matrices  $A, B$ ,  $\text{trace}([A, B]) = 0$ . Comment on this result in the light of the results of Problem 3.7 and the canonical commutation relation  $[x, p] = i\hbar$ .

**7.3\*** A **Fermi oscillator** has Hamiltonian  $H = f^\dagger f$ , where  $f$  is an operator that satisfies

$$f^2 = 0 \quad ; \quad f f^\dagger + f^\dagger f = 1. \quad (7.2)$$

Show that  $H^2 = H$ , and thus find the eigenvalues of  $H$ . If the ket  $|0\rangle$  satisfies  $H|0\rangle = 0$  with  $\langle 0|0\rangle = 1$ , what are the kets (a)  $|a\rangle \equiv f|0\rangle$ , and (b)  $|b\rangle \equiv f^\dagger|0\rangle$ ?

In quantum field theory the vacuum is pictured as an assembly of oscillators, one for each possible value of the momentum of each particle type. A boson is an excitation of a harmonic oscillator, while a fermion is an excitation of a Fermi oscillator. Explain the connection between the spectrum of  $f^\dagger f$  and the Pauli principle.

**7.4** In the time interval  $(t + \delta t, t)$  the Hamiltonian  $H$  of some system varies in such a way that  $|H|\psi\rangle|$  remains finite. Show that under these circumstances  $|\psi\rangle$  is a continuous function of time.

A harmonic oscillator with frequency  $\omega$  is in its ground state when the stiffness of the spring is instantaneously reduced by a factor  $f^4 < 1$ , so its natural frequency becomes  $f^2\omega$ . What is the probability that the oscillator is subsequently found to have energy  $\frac{3}{2}\hbar f^2\omega$ ? Discuss the classical analogue of this problem.

**7.5\***  $P$  is the probability that at the end of the experiment described in Problem 7.4, the oscillator is in its second excited state. Show that when  $f = \frac{1}{2}$ ,  $P = 0.144$  as follows. First show that the annihilation operator of the original oscillator

$$A = \frac{1}{2} \{ (f^{-1} + f)A' + (f^{-1} - f)A'^\dagger \}, \quad (7.3)$$

where  $A'$  and  $A'^\dagger$  are the annihilation and creation operators of the final oscillator. Then writing the ground-state ket of the original oscillator as a sum  $|0\rangle = \sum_n c_n |n'\rangle$  over the energy eigenkets of the final oscillator, impose the condition  $A|0\rangle = 0$ . Finally use the normalisation of  $|0\rangle$  and the orthogonality of the  $|n'\rangle$ . What value do you get for the probability of the oscillator remaining in the ground state?

Show that at the end of the experiment the expectation value of the energy is  $0.2656\hbar\omega$ . Explain physically why this is less than the original ground-state energy  $\frac{1}{2}\hbar\omega$ .

This example contains the physics behind the inflationary origin of the Universe: gravity explosively enlarges the vacuum, which is an infinite collection of harmonic oscillators (Problem 7.3). Excitations of these oscillators correspond to elementary particles. Before inflation the vacuum is unexcited so every oscillator is in its ground state. At the end of inflation, there is non-negligible probability of many oscillators being excited and each excitation implies the existence of a newly created particle.

**7.6\*** Let  $B = cA + sA^\dagger$ , where  $c \equiv \cosh \theta$ ,  $s \equiv \sinh \theta$  with  $\theta$  a real constant and  $A, A^\dagger$  are the usual ladder operators. Show that  $[B, B^\dagger] = 1$ .

Consider the Hamiltonian

$$H = \epsilon A^\dagger A + \frac{1}{2}\lambda(A^\dagger A^\dagger + AA), \quad (7.4)$$

where  $\epsilon$  and  $\lambda$  are real and such that  $\epsilon > \lambda > 0$ . Show that when

$$\epsilon c - \lambda s = E c \quad ; \quad \lambda c - \epsilon s = E s \quad (7.5)$$

with  $E$  a constant,  $[B, H] = EB$ . Hence determine the spectrum of  $H$  in terms of  $\epsilon$  and  $\lambda$ .

**7.7** Verify that  $[\mathbf{J}, \mathbf{x} \cdot \mathbf{x}] = 0$  and  $[\mathbf{J}, \mathbf{x} \cdot \mathbf{p}] = 0$  by using the commutation relations  $[x_i, J_j] = i \sum_k \epsilon_{ijk} x_k$  and  $[p_i, J_j] = i \sum_k \epsilon_{ijk} p_k$ .

**7.8\*** The matrix for rotating an ordinary vector by  $\phi$  around the  $z$  axis is

$$\mathbf{R}(\phi) \equiv \begin{pmatrix} \cos \phi & -\sin \phi & 0 \\ \sin \phi & \cos \phi & 0 \\ 0 & 0 & 1 \end{pmatrix} \quad (7.6)$$

From  $\mathbf{R}$  calculate the matrix  $\mathcal{J}_z$  that appears in  $\mathbf{R}(\phi) = \exp(-i\mathcal{J}_z\phi)$ . Introduce new coordinates  $u_1 \equiv (x - iy)/\sqrt{2}$ ,  $u_2 = z$  and  $u_3 \equiv (x + iy)/\sqrt{2}$ . Write down the matrix  $\mathbf{M}$  that appears in  $\mathbf{u} = \mathbf{M} \cdot \mathbf{x}$  [where  $\mathbf{x} \equiv (x, y, z)$ ] and show that it is unitary. Then show that

$$\mathcal{J}'_z \equiv \mathbf{M} \cdot \mathcal{J}_z \cdot \mathbf{M}^\dagger. \quad (7.7)$$

is identical with  $S_z$  in the set of spin-one Pauli analogues

$$S_x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}. \quad (7.8)$$

Write down the matrix  $\mathcal{J}_x$  whose exponential generates rotations around the  $x$  axis, calculate  $\mathcal{J}'_x$  by analogy with equation (7.7) and check that your result agrees with  $S_x$  in the set (7.8). Explain as fully as you can the meaning of these calculations.

**7.9** Determine the commutator  $[\mathcal{J}'_x, \mathcal{J}'_z]$  of the generators used in Problem 7.8. Show that it is equal to  $-i\mathcal{J}'_y$ , where  $\mathcal{J}'_y$  is identical with  $S_y$  in the set (7.8).

**7.10\*** In this problem you derive the wavefunction

$$\langle \mathbf{x} | \mathbf{p} \rangle = e^{i\mathbf{p} \cdot \mathbf{x} / \hbar} \quad (7.9)$$

of a state of well defined momentum from the properties of the translation operator  $U(\mathbf{a})$ . The state  $|\mathbf{k}\rangle$  is one of well-defined momentum  $\hbar\mathbf{k}$ . How would you characterise the state  $|\mathbf{k}'\rangle \equiv U(\mathbf{a})|\mathbf{k}\rangle$ ? Show that the wavefunctions of these states are related by  $u_{\mathbf{k}'}(\mathbf{x}) = e^{-i\mathbf{a} \cdot \mathbf{k}} u_{\mathbf{k}}(\mathbf{x})$  and  $u_{\mathbf{k}'}(\mathbf{x}) = u_{\mathbf{k}}(\mathbf{x} - \mathbf{a})$ . Hence obtain equation (7.9).

**7.11** An electron moves along an infinite chain of potential wells. For sufficiently low energies we can assume that the set  $\{|n\rangle\}$  is complete, where  $|n\rangle$  is the state of definitely being in the  $n^{\text{th}}$  well. By analogy with our analysis of the  $\text{NH}_3$  molecule we assume that for all  $n$  the only non-vanishing matrix elements of the Hamiltonian are  $\mathcal{E} \equiv \langle n | H | n \rangle$  and  $A \equiv \langle n \pm 1 | H | n \rangle$ . Give physical interpretations of the numbers  $A$  and  $\mathcal{E}$ .

Explain why we can write

$$H = \sum_{n=-\infty}^{\infty} \mathcal{E} |n\rangle \langle n| + A (|n\rangle \langle n+1| + |n+1\rangle \langle n|). \quad (7.10)$$

Writing an energy eigenket  $|E\rangle = \sum_n a_n |n\rangle$  show that

$$a_m (E - \mathcal{E}) - A (a_{m+1} + a_{m-1}) = 0. \quad (7.11)$$

Obtain solutions of these equations in which  $a_m \propto e^{ikm}$  and thus find the corresponding energies  $E_k$ . Why is there an upper limit on the values of  $k$  that need be considered?

Initially the electron is in the state

$$|\psi\rangle = \frac{1}{\sqrt{2}} (|E_k\rangle + |E_{k+\Delta}\rangle), \quad (7.12)$$

where  $0 < k \ll 1$  and  $0 < \Delta \ll k$ . Describe the electron's subsequent motion in as much detail as you can.

**7.12**  $^{238}\text{U}$  decays by  $\alpha$  emission with a mean lifetime of 6.4 Gyr. Take the nucleus to have a diameter  $\sim 10^{-14}$  m and suppose that the  $\alpha$  particle has been bouncing around within it at speed  $\sim c/3$ . Modelling the potential barrier that confines the  $\alpha$  particle to be a square one of height  $V_0$  and width  $2a$ , give an order-of-magnitude estimate of  $W = (2mV_0a^2/\hbar^2)^{1/2}$ . Given that the energy released by the decay is  $\sim 4$  MeV and the atomic number of uranium is  $Z = 92$ , estimate the width of the barrier through which the  $\alpha$  particle has to tunnel. Hence give a very rough estimate of the barrier's typical height. Outline numerical work that would lead to an improved estimate of the structure of the barrier.

**7.13\*** Particles of mass  $m$  and momentum  $\hbar k$  at  $x < -a$  move in the potential

$$V(x) = V_0 \begin{cases} 0 & \text{for } x < -a \\ \frac{1}{2}[1 + \sin(\pi x/2a)] & \text{for } |x| < a \\ 1 & \text{for } x > a, \end{cases} \quad (7.13)$$

where  $V_0 < \hbar^2 k^2/2m$ . Numerically reproduce the reflection probabilities plotted Figure 5.20 as follows. Let  $\psi_i \equiv \psi(x_j)$  be the value of the wavefunction at  $x_j = j\Delta$ , where  $\Delta$  is a small increment in the  $x$  coordinate. From the TISE show that

$$\psi_j \simeq (2 - \Delta^2 k^2)\psi_{j+1} - \psi_{j+2}, \quad (7.14)$$

where  $k \equiv \sqrt{2m(E - V)}/\hbar$ . Determine  $\psi_j$  at the two grid points with the largest values of  $x$  from a suitable boundary condition, and use the recurrence relation (7.14) to determine  $\psi_j$  at all other grid points. By matching the values of  $\psi$  at the points with the smallest values of  $x$  to a sum of sinusoidal waves, determine the probabilities required for the figure. Be sure to check the accuracy of your code when  $V_0 = 0$ , and in the general case explicitly check that your results are consistent with equal fluxes of particles towards and away from the origin.

Equation (11.40) gives an analytical approximation for  $\psi$  in the case that there is negligible reflection. Compute this approximate form of  $\psi$  and compare it with your numerical results for larger values of  $a$ .

**7.14\*** We have that

$$L_+ \equiv L_x + iL_y = e^{i\phi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \phi} \right). \quad (7.15)$$

From the Hermitian nature of  $L_z = -i\partial/\partial\phi$  we infer that derivative operators are anti-Hermitian. So using the rule  $(AB)^\dagger = B^\dagger A^\dagger$  on equation (7.15), we infer that

$$L_- \equiv L_+^\dagger = \left( -\frac{\partial}{\partial \theta} + i \frac{\partial}{\partial \phi} \cot \theta \right) e^{-i\phi}.$$

This argument and the result it leads to is wrong. Obtain the correct result by integrating by parts  $\int d\theta \sin \theta \int d\phi (f^* L_+ g)$ , where  $f$  and  $g$  are arbitrary functions of  $\theta$  and  $\phi$ . What is the fallacy in the given argument?

**7.15\*** By writing  $\hbar^2 L^2 = (\mathbf{x} \times \mathbf{p}) \cdot (\mathbf{x} \times \mathbf{p}) = \sum_{ijklm} \epsilon_{ijk} x_j p_k \epsilon_{ilm} x_l p_m$  show that

$$p^2 = \frac{\hbar^2 L^2}{r^2} + \frac{1}{r^2} \{(\mathbf{r} \cdot \mathbf{p})^2 - i\hbar \mathbf{r} \cdot \mathbf{p}\}. \quad (7.16)$$

By showing that  $\mathbf{p} \cdot \hat{\mathbf{r}} - \hat{\mathbf{r}} \cdot \mathbf{p} = -2i\hbar/r$ , obtain  $\mathbf{r} \cdot \mathbf{p} = rp_r + i\hbar$ . Hence obtain

$$p^2 = p_r^2 + \frac{\hbar^2 L^2}{r^2}. \quad (7.17)$$

Give a physical interpretation of one over  $2m$  times this equation.

**7.16** A system that has total orbital angular momentum  $\sqrt{6\hbar}$  is rotated through an angle  $\phi$  around the  $z$  axis. Write down the  $5 \times 5$  matrix that updates the amplitudes  $a_m$  that  $L_z$  will take the value  $m$ .

**7.17** Write down the expression for the commutator  $[\sigma_i, \sigma_j]$  of two Pauli matrices. Show that the anticommutator of two Pauli matrices is

$$\{\sigma_i, \sigma_j\} = 2\delta_{ij}. \quad (7.18)$$

**7.18** Tritium,  ${}^3\text{H}$ , is highly radioactive and decays with a half-life of 12.3 years to  ${}^3\text{He}$  by the emission of an electron from its nucleus. The electron departs with 16 keV of kinetic energy. Explain why its departure can be treated as sudden in the sense that the electron of the original tritium atom barely moves while the ejected electron leaves.

Calculate the probability that the newly-formed  ${}^3\text{He}$  atom is in an excited state. Hint: evaluate  $\langle 1, 0, 0; Z = 2 | 1, 0, 0; Z = 1 \rangle$ .

**7.19\*** A spherical potential well is defined by

$$V(r) = \begin{cases} 0 & \text{for } r < a \\ V_0 & \text{otherwise,} \end{cases} \quad (7.19)$$

where  $V_0 > 0$ . Consider a stationary state with angular-momentum quantum number  $l$ . By writing the wavefunction  $\psi(\mathbf{x}) = R(r)Y_l^m(\theta, \phi)$  and using  $p^2 = p_r^2 + \hbar^2 L^2/r^2$ , show that the state's radial wavefunction  $R(r)$  must satisfy

$$-\frac{\hbar^2}{2m} \left( \frac{d}{dr} + \frac{1}{r} \right)^2 R + \frac{l(l+1)\hbar^2}{2mr^2} R + V(r)R = ER. \quad (7.20)$$

Show that in terms of  $S(r) \equiv rR(r)$ , this can be reduced to

$$\frac{d^2 S}{dr^2} - l(l+1) \frac{S}{r^2} + \frac{2m}{\hbar^2} (E - V)S = 0. \quad (7.21)$$

Assume that  $V_0 > E > 0$ . For the case  $l = 0$  write down solutions to this equation valid at (a)  $r < a$  and (b)  $r > a$ . Ensure that  $R$  does not diverge at the origin. What conditions must  $S$  satisfy at  $r = a$ ? Show that these conditions can be simultaneously satisfied if and only if a solution can be found to  $k \cot ka = -K$ , where  $\hbar^2 k^2 = 2mE$  and  $\hbar^2 K^2 = 2m(V_0 - E)$ . Show graphically that the equation can only be solved when  $\sqrt{2mV_0}a/\hbar > \pi/2$ . Compare this result with that obtained for the corresponding one-dimensional potential well.

The deuteron is a bound state of a proton and a neutron with zero angular momentum. Assume that the strong force that binds them produces a sharp potential step of height  $V_0$  at interparticle distance  $a = 2 \times 10^{-15}$  m. Determine in MeV the minimum value of  $V_0$  for the deuteron to exist. Hint: remember to consider the dynamics of the *reduced* particle.

**7.20\*** Given that the ladder operators for hydrogen satisfy

$$A_l^\dagger A_l = \frac{a_0^2 \mu}{\hbar^2} H_l + \frac{Z^2}{2(l+1)^2} \quad \text{and} \quad [A_l, A_l^\dagger] = \frac{a_0^2 \mu}{\hbar^2} (H_{l+1} - H_l), \quad (7.22)$$

where  $H_l$  is the Hamiltonian for angular-momentum quantum number  $l$ , show that

$$A_{l-1} A_{l-1}^\dagger = \frac{a_0^2 \mu}{\hbar^2} H_l + \frac{Z^2}{2l^2}. \quad (7.23)$$

Hence show that

$$A_{l-1}^\dagger |E, l\rangle = \frac{Z}{\sqrt{2}} \left( \frac{1}{l^2} - \frac{1}{n^2} \right)^{1/2} |E, l-1\rangle, \quad (7.24)$$

where  $n$  is the principal quantum number. Explain the physical meaning of this equation and its use in setting up the theory of the hydrogen atom.

**7.21\*** From equation (8.42) show that  $l' + \frac{1}{2} = \sqrt{(l + \frac{1}{2})^2 - \beta}$  and that the increment  $\Delta$  in  $l'$  when  $l$  is increased by one satisfies  $\Delta^2 + \Delta(2l' + 1) = 2(l + 1)$ . By considering the amount by which the solution of this equation changes when  $l'$  changes from  $l$  as a result of  $\beta$  increasing from zero to a small number, show that

$$\Delta = 1 + \frac{2\beta}{4l^2 - 1} + \text{O}(\beta^2). \quad (7.25)$$

Explain the physical significance of this result.

**7.22** Show that Ehrenfest's theorem yields equation (8.66) with  $\mathbf{B} = 0$  as the classical equation of motion of the vector  $\mathbf{S}$  that is implied by the spin-orbit Hamiltonian (8.67).