Further Quantum Mechanics: Problem Set 1.

Hilary Term, weeks 6 – 8

Problems 2-8 are taken from the book by Binney and Skinner. † denotes relatively advanced material.

Qu 1.† A particle with mass m, charge q and momentum $\hat{\mathbf{p}}$ moves in a magnetic field described by the vector potential $\mathbf{A}$. The Hamiltonian is

$$H = \frac{1}{2m}(\hat{\mathbf{p}} - q\mathbf{A})^2 \,.$$

The wavefunction $\psi(\mathbf{r}, t)$ satisfies the time-dependent Schrödinger equation with this Hamiltonian, and the probability density $\rho \equiv |\psi(\mathbf{r}, t)|^2$ obeys the continuity equation

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{j} \,.$$

Show from the time-dependent Schrödinger equation that

$$\mathbf{j} = \frac{\hbar}{2im}\{\psi^* \nabla\psi - \psi\nabla\psi^*\} - \frac{q}{m}|\psi|^2\mathbf{A} \,.$$

The particle moves in the x-y plane with a uniform magnetic field in the z-direction, represented by

$$\mathbf{A} = \frac{B}{2}(-y, x, 0).$$

Show that the function

$$\varphi(x, y) = \exp(-[x^2 + y^2]/4\ell_{\rm B}^2)$$

is an eigenfunction for a suitably chosen value for $\ell_{\rm B}$. Find this value of $\ell_{\rm B}$ and the energy. Evaluate $\mathbf{j}$ for this state. Discuss the physical significance of your results.

Qu 2. The Hamiltonian of a two-state system can be written

$$H = \begin{pmatrix} A_1 + B_1\epsilon & B_2\epsilon \\ B_2\epsilon & A_2 \end{pmatrix},$$

where all quantities are real and ϵ is a small parameter. To first order in ϵ, what are the allowed energies in the cases (a) $A_1 \neq A_2$, and (b) $A_1 = A_2$?
Obtain the exact eigenvalues and recover the results of perturbation theory by expanding in powers of ϵ.

Qu 3. The harmonic oscillator with mass m and angular frequency ω is perturbed by $\delta H = \epsilon x^2$. (a) What is the exact change in the ground-state energy? Expand this change in powers of ϵ up to order ϵ^2. (b) Show that the change given by first-order perturbation theory agrees with the exact result to $\mathcal{O}(\epsilon)$ (c) Show that the first-order change in the ground state is $|b\rangle = -(\epsilon\ell^2/\sqrt{2}\hbar\omega)|E_2\rangle$. (d) Show that second-order perturbation theory yields an energy change $E_c = -\epsilon^2\hbar/4m^2\omega^3$ in agreement with the exact result.

Qu 4. The harmonic oscillator is perturbed by $\delta H = \epsilon x$. Show that the perturbed Hamiltonian can be written

$$H = \frac{1}{2m}\left(p^2 + m^2\omega^2 X^2 - \frac{\epsilon^2}{\omega^2}\right),$$

where $X = x + \epsilon/m\omega^2$ and hence deduce the exact change in the ground-state energy. Interpret these results physically.
What change in energy eigenvalues does first-order perturbation theory give? From perturbation theory determine the coefficient b_1 of the unperturbed first-excited state in the perturbed ground state. Discuss your result in relation to the exact ground state of the perturbed oscillator.

Qu 5. The harmonic oscillator is perturbed by $\delta H = \epsilon x^4$. Show that the first-order change in the energy of the nth excited state is

$$\delta E = 3(2n^2 + 2n + 1)\epsilon \left(\frac{\hbar}{2m\omega}\right)^2.$$

Hint: express x in terms of $A + A^\dagger$.

Qu 6. The infinite square-well potential $V(x) = 0$ for $|x| < a$ and ∞ for $|x| > a$ is perturbed by the potential $\delta V = \epsilon x/a$. Show that to first order in ϵ the energy levels of a particle of mass m are unchanged. Show that even to this order the ground-state wavefunction *is* changed to

$$\psi_1(x) = \frac{1}{\sqrt{a}}\cos(\pi x/2a) + \frac{16\epsilon}{\pi^2 E_1 \sqrt{a}} \sum_{n=2,4,} (-1)^{n/2} \frac{n}{(n^2-1)^3} \sin(n\pi x/2a),$$

where E_1 is the ground-state energy. Explain physically why this wavefunction does not have well-defined parity but predicts that the particle is more likely to be found on one side of the origin than the other. State with reasons but without further calculation whether the second-order change in the ground-state energy will be positive or negative.

Qu 7. An atomic nucleus has a finite size, and inside it the electrostatic potential $\Phi(r)$ deviates from $Ze/(4\pi\epsilon r)$. Take the proton's radius to be $a_p \simeq 10^{-15}$m and its charge density to be uniform. Then treating the difference between Φ and $Ze/(4\pi\epsilon_0 r)$ to be a perturbation on the Hamiltonian of hydrogen, calculate the first-order change in the ground-state energy of hydrogen. Why is the change in the energy of any P state extremely small? Comment on how the magnitude of this energy shift varies with Z in hydrogenic ions of charge Z. Hint: exploit the large difference between a_p and a_0 to approximate the integral you formally require.

Qu 8. A particle of mass m moves in the potential $V(x, y) = \frac{1}{2}m\omega^2(x^2 + y^2)$, where ω is a constant. Show that the Hamiltonian can be written as the sum $H_x + H_y$ of the Hamiltonians of two identical one-dimensional harmonic oscillators. Write down the particle's energy spectrum. Write down kets for two stationary states in the first-excited level in terms of the stationary states $|n_x\rangle$ of H_x and $|n_y\rangle$ of H_y. Show that the nth excited level is $n + 1$ fold degenerate.
The oscillator is disturbed by a small potential $H_1 = \lambda xy$. Show that this perturbation lifts the degeneracy of the first excited level, producing states with energies $2\hbar\omega \pm \lambda\hbar/2m\omega$. Give expressions for the corresponding kets.
The mirror operator M is defined such that $\langle x, y|M|\psi\rangle = \langle y, x|\psi\rangle$ for any state $|\psi\rangle$. Explain physically the relationship between the states $|\psi\rangle$ and $M|\psi\rangle$. Show that $[M, H_1] = 0$. Show that $MH_x = H_y M$ and thus that $[M, H] = 0$. What do you infer from these commutation relations?

Qu 9. The Hamiltonian for a hydrogen atom in a uniform magnetic field with flux density B along z is approximately

$$H = \frac{\hat{\mathbf{p}}^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r} + \frac{\hbar e B}{2m}(L_z + \sigma_z)$$

where $\hbar L_z$ and $(\hbar/2)\sigma_z$ are operators representing respectively the z-components of the orbital and spin angular momentum of the electron.

Discuss how the terms involving B arise. What is the justification for omitting a term in B^2?

What quantum numbers label eigenstates of this Hamiltonian?

Draw a diagram showing the energies of a representative selection of these eigenstates as a function of magnetic field.

Further Quantum Mechanics: Problem Set 2.

Easter vacation and Trinity term weeks 1 – 2

Qns. 3 – 8 are taken from the book by Binney and Skinner. † denotes relatively advanced material.

Qu. 1 (*From 2013 A3 paper.*) The electron in a hydrogen-like ion has a Hamiltonian

$$H = -\frac{\hbar^2}{2m}\nabla^2 - \frac{Ze^2}{4\pi\epsilon_0}\frac{1}{r}$$

and eigenstates $|n, l, m\rangle$.
(a) Explain the origin of each term in the Hamiltonian, and the meaning of each of the quantum numbers n, l and m. On which quantum number does the energy depend? For $n = 2$, what values may l and m take?
(b) By considering the electric dipole selection rules or otherwise, identify which of the matrix elements $\langle 2, l', m'|z|2, l, m\rangle$ are non-zero.
(c) A small static electric field of strength $\mathcal{E}$ is applied in the z direction. Write down the perturbation Hamiltonian. Calculate its non-zero matrix elements for the basis of states with $n = 2$.
(d) Identify the linear combinations of the $n = 2$ states that diagonalise the perturbation Hamiltonian and calculate the energy shifts. Hence sketch the $n = 2$ energy levels before and after the application of the perturbation. In each case, label the eigenstates and give the magnitude of any energy differences.

[The integral $\int_0^\infty \rho^n e^{-\rho}\mathrm{d}\rho = n!$. The normalised states $|n, l, m\rangle = u_n^l(r)\mathrm{Y}_l^m(\theta, \phi)$, with

$$u_2^0(r) = \frac{2e^{-r/2a_Z}}{(2a_Z)^{3/2}}\left(1 - \frac{r}{2a_Z}\right), \qquad u_2^1(r) = \frac{e^{-r/2a_Z}}{\sqrt{3}(2a_Z)^{3/2}}\frac{r}{a_Z}, \qquad a_Z = \frac{4\pi\epsilon_0\hbar^2}{Zme^2},$$

and $\mathrm{Y}_0^0(\theta, \phi) = \sqrt{\frac{1}{4\pi}}$, $\mathrm{Y}_1^0(\theta, \phi) = \sqrt{\frac{6}{8\pi}}\cos\theta$, $\mathrm{Y}_1^{\pm1}(\theta, \phi) = \mp\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm\mathrm{i}\phi}$.]

Qu. 2.† State and prove the *variational theorem* in quantum mechanics.

Use this theorem to prove that in a one-dimensional system an attractive potential always has a bound state, by taking the following steps. We define an attractive potential $V(x)$ to be one that has finite range a and is negative on average, meaning that

$$V(x) = 0 \quad \text{for} \quad |x| \geq a \qquad \text{and} \qquad \int_{-a}^{a} \mathrm{d}x\, V(x) = -v_0$$

with $v_0 > 0$. Consider a function $f(y)$ that has its maximum at $x = 0$, is non-negative, and approaches zero for $y \to \pm\infty$, with the properties

$$\int_{-\infty}^{\infty} \mathrm{d}y |f(y)|^2 = 1 \quad \text{and} \quad \int_{-\infty}^{\infty} \mathrm{d}y \left|\frac{\mathrm{d}f(y)}{\mathrm{d}y}\right|^2 = 1\,.$$

For the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

use the (unnormalised) trial wavefunction $\psi(x) = f(x/\lambda)$ with variational parameter λ to show that

$$\langle H\rangle \equiv \frac{\int_{-\infty}^{\infty}\mathrm{d}x\,\psi^*(x)\hat{H}\psi(x)}{\int_{-\infty}^{\infty}\mathrm{d}x\,|\psi(x)|^2} < 0$$

for sufficiently large λ. How is the situation different for a three-dimensional system?

Qu 3.
In the β decay H^3 (1 proton + 2 neutrons in the nucleus) $\to (\mathrm{He}^3)^+$ (2 protons + 1 neutron in the nucleus), the emitted electron has a kinetic energy of 16 keV. We will consider the effects on the motion of the atomic electron, i.e. the one orbiting the nucleus, which we assume is initially in the ground state of H^3.

Show by a brief justification that the perturbation is sudden, by considering the location of the emitted electron at a time around $\tau = 5 \times 10^{-17}$ s after emission. How does τ compare with the time-scale on which the wavefunction changes?
Show that the probability for the electron to be left in the ground state of $(\mathrm{He}^3)^+$ is $2^3(2/3)^6 \simeq 0.7$.

Qu 4. At early times ($t \sim -\infty$) a harmonic oscillator of mass m and natural angular frequency ω is in its ground state. A perturbation $\delta H = \mathcal{E} x \mathrm{e}^{-t^2/\tau^2}$ is then applied, where $\mathcal{E}$ and τ are constants.
What is the probability according to first-order theory that by late times the oscillator transitions to its second excited state, $|2\rangle$?
Show that to first order in δH the probability that the oscillator transitions to the first excited state, $|1\rangle$, is

$$P = \frac{\pi \mathcal{E}^2 \tau^2}{2m\hbar\omega} \mathrm{e}^{-\omega^2\tau^2/2},$$

Plot P as a function of τ and comment on its behaviour as $\omega\tau \to 0$ and $\omega\tau \to \infty$.

Qu 5. Write down the selection rules for radiative transitions in the electric dipole approximation. Draw an energy level diagram for hydrogen (use the vertical direction for energy, and separate the states horizontally by angular momentum ℓ). Show how the selection rules apply to hydrogen by marking allowed transitions on your diagram.

Qu 6. With $|nlm\rangle$ a stationary state of hydrogen, which of these matrix elements is non-zero?

$$\begin{array}{lll} \langle 100|z|200\rangle & \langle 100|z|210\rangle & \langle 100|z|211\rangle \\ \langle 100|z|300\rangle & \langle 100|z|310\rangle & \langle 100|z|320\rangle \\ \langle 100|x|200\rangle & \langle 100|x|210\rangle & \langle 100|x|211\rangle \end{array}$$

Qu 7. With $|nlm\rangle$ a stationary state of hydrogen, and given that

$$Y_{10}(\theta,\phi) = \sqrt{\frac{6}{8\pi}}\cos\theta \quad Y_{11}(\theta,\phi) = -\sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{i\phi} \quad Y_{1-1}(\theta,\phi) = \sqrt{\frac{3}{8\pi}}\sin\theta\,\mathrm{e}^{-i\phi},$$

show that

$$\begin{array}{rcl} \langle 100|(x-iy)|211\rangle & = & -\sqrt{2}\langle 100|z|210\rangle \\ \langle 100(x-iy)|21-1\rangle & = & 0. \end{array}$$

Write down the values of $\langle 100|(x+iy)|21-1\rangle$ and $\langle 100|(x+iy)|211\rangle$ and hence show that with

$$|\psi\rangle \equiv \frac{1}{\sqrt{2}}(|211\rangle - |21-1\rangle),$$

$\langle 100|x|\psi\rangle = -\langle 100|z|210\rangle$. Explain the physical significance of this result.

Qu 8. Derive the selection rules

$$\begin{array}{rcll} \langle n'l'm'|x_+|nlm\rangle & = & 0 \quad \text{unless} & m' = m+1 \\ \langle n'l'm'|x_-|nlm\rangle & = & 0 \quad \text{unless} & m' = m-1. \end{array}$$

where $x_\pm = x \pm iy$. From this selection rule one infers that when the atom sits in a magnetic field along the z axis and the spectrometer looks along the z axis, the detected photons will be circularly polarised. Show that linearly polarised photons *can* be detected from an atom that's in a magnetic field.
From the above rules it might be argued that photons emitted along the z axis will be circularly polarised even in the absence of a magnetic field. Why is this argument bogus?

Further Quantum Mechanics: Problem Set 3.

Trinity term weeks 2-3

Questions 1 and 2 are adapted from Shankar. † denotes relatively advanced material.

Qu 1. A system has n non-degenerate single-particle states. These states account for all the degrees of freedom of the particle – position and (if relevant) spin. The states are occupied by a number p of similar non-interacting particles, without any constraints except for those arising from symmetry under particle exchange. How many distinct many-particle states are there for the p-particle system in the following cases:

(i) if the particles are distinguishable;

(ii) if the particles are identical fermions and $p = n$;

(iii) if the particles are identical bosons and $p = n = 2$;

(iv) if the particles are identical bosons and $p = n = 3$?

Qu 2. Consider two identical, non-interacting particles, each of mass m, with coordinates x_1, x_2. They are confined to a box of length L, so that $0 \leq x_1, x_2 \leq L$.

Suppose the particles are identical spin-zero bosons. What is the wavefunction $\psi(x_1, x_2)$ if the system is in an eigenstate with total energy: (i) $\hbar^2\pi^2/mL^2$, or (ii) $5\hbar^2\pi^2/2mL^2$?

Suppose alternatively that the particles are identical spin-half fermions: for the same values of total energy write down a complete set of possible wavefunctions, as products of space and spin factors.

Qu 3. He: ionisation energy. The ionization energy is the energy required to remove one electron from an atom or ion in its ground state, leaving it in the ground state of the next higher ionization stage. (The energy is often quoted in eV and referred to as an ionization potential.)
If we make the (poor) approximation of ignoring the electron-electron repulsion altogether, what value (in eV) is obtained for the ionization potential of the ground state in helium? How much additional energy would then be required to remove the second electron? Assuming these estimates have been made as accurately as reasonably possible within their respective assumptions, state the degree of accuracy of each of these two results (i.e. how close they may be expected to be to the true first and second ionization energies for helium.)

To do better, use the variational method. Using hydrogen-like wavefunctions for both electrons: $\psi_{1s} = \sqrt{Z^3/\pi a_0^3}\,\exp(-Zr/a_0)$, where Z is an adjustable parameter distinct from the nuclear charge, show that

$$\langle \frac{1}{r_1} + \frac{1}{r_2} \rangle = \frac{2Z}{a_0}.$$

Using also $\langle p_1^2 + p_2^2 \rangle = 2Z^2\hbar^2/(a_0^2)$ and $\langle 1/r_{12} \rangle = 5Z/(8a_0)$, show that the mean energy as a function of Z is given in terms of the Rydberg R by

$$E(Z) = -2R\left(4Z - Z^2 - 5Z/8\right).$$

Complete the variational procedure, and hence obtain an upper limit for the ground state energy, and a lower limit for the ionization energy of helium.

Qu 4. Two of the energy levels in Helium have the standard notation $1s2s\,{}^1S_0$ and $1s2s\,{}^3S_1$. Explain every part of this notation. The difference in the notation for the two levels stresses a difference in the spin part of the wavefunction, but the spatial part is also different: what is the important distinguishing feature between the two spatial wavefunctions?

Qu 5.† Consider the following two Stern-Gerlach experiments.

A is a beam of atoms with spin-1/2 with the spin alined along the $+x$-axis. B is a beam of similar unpolarised atoms. A and B are separately passed through a Stern-Gerlach apparatus aligned along z. In each case you get two emerging beams coming out of the Stern-Gerlach experiment.

Is there any difference between the two cases? If so, how could you detect that experimentally?

Write down density matrices in the z-basis to describe the beams A and B before passage through the Stern-Gerlach apparatus. Use these density matrices to evaluate $\langle \hat{s}_x \rangle$ and $\langle \hat{s}_z \rangle$ for each beam.