Mathematical Tripos Part 1B — Dr. Eugene A. Lim
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QUANTUM MECHANICS

Example Sheet 3

1. A particle moving in three dimensions is confined within a box $0 < x < a$, $0 < y < b$, $0 < z < c$. (The potential is zero inside and infinite outside.) By considering a stationary state wavefunction of the form $\chi(x, y, z) = f_1(x)f_2(y)f_3(z)$, show that the allowed energies are

$$\frac{\hbar^2\pi^2}{2m}\left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\right).$$

What is the degeneracy of the first excited energy level when $a = b = c$?

2. The isotropic 3-dimensional quantum harmonic oscillator has potential $U(x, y, z) = \frac{1}{2}m\omega^2(x^2 + y^2 + z^2)$. Find the stationary states in the form $A(x)B(y)C(z)$. Hence show that the energy levels are $E = \left(\frac{3}{2} + N_x + N_y + N_z\right)\hbar\omega$, where N_x, N_y, N_z are non-negative integers.

How many linearly independent states have energy $E = \left(\frac{3}{2} + N\right)\hbar\omega$? Show that the ground state is spherically symmetric and find one state with $N = 2$ that is also spherically symmetric.

3. As a model for the deuterium nucleus (a bound state of a proton and a neutron) consider a particle in the 3-dimensional square-well potential

$$U(r) = \begin{cases} -U_0 & r < a \\ 0 & r > a \end{cases}$$

with $U_0 > 0$. Show how to find the spherically symmetric bound-state wavefunctions. Is there always a bound state? [*You may use* $\nabla^2\psi = r^{-1}d^2(r\psi)/dr^2$.]

4. Using the relation $[\hat{L}_1, \hat{L}_2] = i\hbar\hat{L}_3$ and its cyclic permutations, satisfied by the orbital angular momentum operators, show that $[\hat{L}_3, \hat{\mathbf{L}}^2] = 0$, where $L^2 = \hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2$, and hence show that the eigenfunctions of $\hat{L}_3$ with eigenvalues $m\hbar$ can be chosen to be eigenfunctions of $\hat{\mathbf{L}}^2$ too.

Show that the expectation value $\langle[\hat{L}_3, \hat{L}_1\hat{L}_2]\rangle$ vanishes in any eigenstate of $\hat{L}_3$. Hence show, by evaluating $[\hat{L}_3, \hat{L}_1\hat{L}_2]$, that $\langle\hat{L}_1^2\rangle = \langle\hat{L}_2^2\rangle$ in any eigenstate of $\hat{L}_3$. Given a state in which $\hat{L}_3$ has eigenvalue $m\hbar$ and $\hat{\mathbf{L}}^2$ has eigenvalue $\ell(\ell + 1)\hbar^2$, show that $\langle\hat{L}_1^2\rangle = \frac{1}{2}\hbar^2\left(\ell(\ell + 1) - m^2\right)$.

5. Show that the 2×2 matrices

$$\hat{S}_1 = \frac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad \hat{S}_2 = \frac{1}{2}\hbar\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad \hat{S}_3 = \frac{1}{2}\hbar\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

satisfy the commutation relations of angular momentum ($[\hat{S}_1, \hat{S}_2] = i\hbar\hat{S}_3$ and cyclic permutations). Show that there are two linearly independent eigenvectors $\psi_\pm$ of $\hat{S}_3$ with eigenvalues $\pm s\hbar$, where s is a number that you should determine. Show that the vectors $\psi_\pm$ are also eigenvectors of $S^2 = \hat{S}_1^2 + \hat{S}_2^2 + \hat{S}_3^2$, and that both have eigenvalue $s(s + 1)\hbar^2$.

6. The Hamiltonian of a quantum system suddenly changes by a finite amount. Show that the wavefunction must change continuously if the time-dependent Schrödinger equation is to be valid throughout the change.

Show that the ground-state wavefunction for a hydrogenic atom (a bound state of one electron and a nucleus of charge Ze, with Z a positive integer) takes the form

$$\psi_0(r) = \frac{1}{\sqrt{\pi a^3}}\, e^{-r/a} \,,$$

and determine the dependence of the constant a on Z. Such a hydrogenic atom is in its ground state. The nucleus emits an electron, suddenly changing to one with charge $(Z+1)e$. Compute the probability that if the energy is now measured, the atom will still be found in its ground state.

7. An atom of atomic number Z has Z electrons in stationary states that we may assume, as a first approximation, to be those of one electron in a hydrogenic atom with some effective value of Z (less than the actual value, to allow for screening of the electric charge on the nucleus by other electrons). In other words, we have states labelled by the same quantum numbers n, ℓ, m as in the hydrogen atom, and with each energy level having the same degeneracies ($E = E_n$, independent of both ℓ and m). Moreover, because the electron is a particle of spin 1/2 there are *two* degenerate electron states for each one allowed by the Schrödinger equation. Given that each state can be occupied by just one electron (Pauli exclusion principle), and that in the atomic ground state the lowest energy electron states are occupied (compatibly with this principle), show that the $n = 1$ level is filled for atomic number $Z = 2$, i.e. a Helium atom.

If we assume that Helium is chemically inert because of its filled energy level, then we might guess that the element in the periodic table for which both the $n = 1$ and $n = 2$ levels are filled will also be chemically inert. What is the atomic number of this element? What everyday use of it provides evidence that it is indeed chemically inert?

8. Suppose two operators $\hat{A}$ and $\hat{B}$ do not commute, but they individually commute with the Hamiltonian, i.e.

$$[\hat{A}, \hat{H}] = 0 \;,\; [\hat{B}, \hat{H}] = 0.$$

Prove that the energy eigenstates are, in general, degenerate.

9. Show that, given that the canonical commutation relationship of the position and momentum operators in one dimension $[\hat{x}, \hat{p}] = i\hbar$, the following are true

$$[\hat{x}, \hat{p}^n] = i\hbar n \hat{p}^{n-1}$$

and

$$[\hat{p}, \hat{x}^n] = -i\hbar n \hat{x}^{n-1}.$$

Given the Hamiltonian for the Simple Harmonic Oscillator

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

Use the relations derived above to calculate $[\hat{H}, \hat{x}]$ and $[\hat{H}, \hat{p}]$.