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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* $\nabla^2\chi = r^{-1}d^2(r\chi)/dr^2$.]

4. Using the relation $[L_1, L_2] = i\hbar L_3$ and its cyclic permutations, satisfied by the orbital angular momentum operators, show that $[L_3, L^2] = 0$, where $L^2 = L_1^2 + L_2^2 + L_3^2$, and hence show that the eigenfunctions of L_3 with eigenvalues $m\hbar$ can be chosen to be eigenfunctions of L^2 too.

Show that the expectation value $\langle[L_3, L_1L_2]\rangle$ vanishes in any eigenstate of L_3. Hence show, by evaluating $[L_3, L_1L_2]$, that $\langle L_1^2\rangle = \langle L_2^2\rangle$ in any eigenstate of L_3. Given a state in which L_3 has eigenvalue $m\hbar$ and L^2 has eigenvalue $\ell(\ell + 1)\hbar^2$, show that $\langle L_1^2\rangle = \frac{1}{2}\hbar^2\left(\ell(\ell + 1) - m^2\right)$.

5. Show that the 2×2 matrices

$$S_1 = \frac{1}{2}\hbar\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \qquad S_2 = \frac{1}{2}\hbar\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \qquad S_3 = \frac{1}{2}\hbar\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

satisfy the commutation relations of angular momentum ($[S_1, S_2] = i\hbar S_3$ and cyclic permutations). Show that there are two linearly independent eigenvectors $\psi_\pm$ of 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 $S^2 = S_1^2 + S_2^2 + S_3^2$, 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

$$\chi_0(r) = \frac{1}{\sqrt{\pi a^3}}\, e^{-r/a} ,$$

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. Given two vector operators $\hat{\mathbf{A}}$ and $\hat{\mathbf{B}}$ and a scalar operator $\hat{H}$, show that

$$[\hat{H}, \hat{\mathbf{A}} \times \hat{\mathbf{B}}] = [\hat{H}, \hat{\mathbf{A}}] \times \hat{\mathbf{B}} + \hat{\mathbf{A}} \times [\hat{H}, \hat{\mathbf{B}}] .$$

Now let $\hat{H}$ be the Hamiltonian operator for a particle in a central potential:

$$\hat{H} = -\frac{\hbar^2}{2M}\nabla^2 + U(r) .$$

By taking $\hat{\mathbf{A}} = \mathbf{r}$ and $\hat{\mathbf{B}} = \hat{\mathbf{p}}$, show that $[\hat{H}, \hat{\mathbf{L}}] = \mathbf{0}$.

By instead taking $\hat{\mathbf{A}} = \hat{\mathbf{p}}$ and $\hat{\mathbf{B}} = \hat{\mathbf{L}}$ show that

$$\left[\hat{H}, \left(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}\right)\right] = \mathbf{r}\ (\mathbf{G} \cdot \hat{\mathbf{p}} + \hat{\mathbf{p}} \cdot \mathbf{G}) - ((\mathbf{r} \cdot \mathbf{G})\hat{\mathbf{p}} + \hat{\mathbf{p}}(\mathbf{r} \cdot \mathbf{G})) - i\hbar \mathbf{G}$$

where

$$\mathbf{G}(\mathbf{r}) = [\hat{H}, \hat{\mathbf{p}}] .$$

Use this result to compute $[\hat{H}, \hat{\mathbf{K}}]$, where

$$\hat{\mathbf{K}} = \frac{1}{2M}\left(\hat{\mathbf{p}} \times \hat{\mathbf{L}} - \hat{\mathbf{L}} \times \hat{\mathbf{p}}\right) + U(r)\,\mathbf{r} .$$

Hence show that $\hat{H}$ commutes with $\hat{\mathbf{K}}$ if

$$\mathbf{r} \cdot \boldsymbol{\nabla} U + U = 0 .$$

For what functions $U(r)$ is this condition satisfied?