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 stationary state wavefunctions of the form $\psi(x, y, z) = X(x)Y(y)Z(z)$, show that the allowed energy levels are

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

for integers $n_i > 0$.

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

2. The isotropic 3-dimensional harmonic oscillator has potential $V(x_1, x_2, x_3) = \frac{1}{2} m \omega^2 (x_1^2 + x_2^2 + x_3^2)$. Find energy eigenstates of separable form in Cartesian coordinates, and hence show that the energy levels are

$$E = (n_1 + n_2 + n_3 + \frac{3}{2}) \hbar \omega$$

where $n_1, n_2, n_3$ are non-negative integers. (Assume results for the oscillator in one dimension.)

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

3. (i) Verify that $A \exp(ik \cdot x)$ is a simultaneous eigenstate of the components of momentum $\hat{p}$. Hence show that it is also an energy eigenstate for a free particle (vanishing potential).

(ii) Let $\Psi(x, t)$ be any solution of the time-dependent Schrödinger Equation with zero potential. Show that

$$\Psi(x - ut, t) \exp(ik \cdot x) \exp(-i\hbar k^2 t/2m)$$

is also a solution, provided $\hbar k = mu$ (where $m$ is the mass of the particle).

4. Suppose $Q$ is an observable that does not depend explicitly on time. Show that

$$i\hbar \frac{d}{dt} \langle Q \rangle = \langle [Q, H] \rangle \psi$$

where $\Psi(t)$ obeys the Schrödinger Equation. Apply this to the position and momentum of a particle in three dimensions, with Hamiltonian

$$H = \frac{1}{2m} \hat{p}^2 + V(\hat{x})$$

by calculating the commutator of $H$ with each component of $\hat{x}$ and $\hat{p}$. Compare the results with the classical equations of motion.

5. The time-independent Schrödinger Equation for an electron in a Hydrogen atom is

$$-\frac{\hbar^2}{2m} \nabla^2 \psi - \frac{e^2}{4\pi \epsilon_0 r} \psi = E\psi$$

Show that there is a spherically-symmetric energy eigenstate of the form

$$\psi(r) = Ce^{-r/a}$$

for a certain value of the constant $a$, and find the corresponding energy eigenvalue $E$.

Compute the value of $C$ required to normalise the wavefunction. What is the expectation value of the distance of the electron from the proton (which is assumed to be stationary at the origin) and how does this compare to the Bohr radius? [Recall that $\nabla^2 f = f'' + (2/r)f'$ for $f(r)$.]
6. As a model for the deuteron nucleus (a bound state of a proton and a neutron) consider a particle in the 3-dimensional square-well potential

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

with $U > 0$. Consider the radial Schrödinger equation for the special case of a spherically symmetric wavefunction. Is there always a spherically symmetric bound state solution?

7. Let $A$ and $B$ be hermitian operators. Show that $i[A, B]$ is hermitian.

Let $\Psi$ be any normalised state. Setting $\Phi = (A + i\lambda B)\Psi$ and considering $\langle \Phi, \Phi \rangle$ as a quadratic in the real variable $\lambda$, show that

$$\langle A^2 \rangle \langle B^2 \rangle \geq \frac{1}{2} \left| \langle i[A, B] \rangle \right|^2$$

(with all expectation values taken in the state $\Psi$). Hence derive the generalised Uncertainty Principle:

$$\Delta A \Delta B \geq \frac{1}{2} \left| \langle [A, B] \rangle \right|.$$ 

8. Let $\phi(r)$ be any spherically symmetric wavefunction. Show, using Cartesian coordinates, that $L_3 \phi = 0$. Show that $\phi(r)$ is also an eigenstate of $L^2$. [Recall that $\partial r / \partial x_i = x_i / r$.]

Now calculate the results obtained by applying $L_3$ and $L_3^2$ to each of the wavefunctions

$$\psi_i(x) = x_i \phi(r) \quad \text{with} \quad i = 1, 2, 3.$$ 

From your answers, deduce that each $\psi_i(x)$ is an eigenfunction of $L^2$ with eigenvalue $2\hbar^2$. Find linear combinations of the wavefunctions $\psi_i(x)$ that are also eigenfunctions of $L_3$; what are the eigenvalues?

9. Use the commutation relations for orbital angular momentum $[L_1, L_2] = i\hbar L_3$ (and cyclic permutations) to show that $[L_3, L^2] = 0$.

Prove that $\langle [L_3, A] \rangle = 0$ when the expectation value is taken in any eigenstate of $L_3$, for any operator $A$. Hence, by evaluating $[L_3, L_1 L_2]$, deduce that $\langle L_3^2 \rangle = \langle L_3^2 \rangle^2$ in any eigenstate of $L_3$. Now consider a joint eigenstate for which $L_3$ has eigenvalue $\hbar m$ and $L^2$ has eigenvalue $\hbar^2 (\ell(\ell+1))$. Show that $\langle L_1^2 \rangle = \langle L_3^2 \rangle = \frac{1}{2}\hbar^2 (\ell(\ell+1) - m^2)$ in this state.

10. Consider the $2 \times 2$ hermitian matrices defined by

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

Evaluate the commutators $[S_i, S_j]$ for all values of $i$ and $j$ (there are only three independent cases to consider) and calculate the matrix $S^2 = S_1^2 + S_2^2 + S_3^2$.

Write down simultaneous eigenvectors of $S_3$ and $S^2$ and hence show that their eigenvalues are $\pm \hbar s$ and $\hbar^2 (s + 1)$, respectively, for a certain positive number $s$.

11. Suppose that the Hamiltonian of a quantum system depends on a parameter that changes suddenly, at a certain time, by a finite amount. Show that the wavefunction must change continuously if the time-dependent Schrödinger equation is to be valid throughout the change.

In a hydrogenic atom, a single electron is bound to a nucleus of charge $Ze$, with $Z$ a positive integer. The normalised ground state wavefunction has the form

$$\psi(r) = \frac{c}{\sqrt{a^3}} e^{-r/a}.$$ 

From your answer to question 5, give the value of $c$ and find the dependence of $a$ on $Z$.

A hydrogenic atom is in its ground state when the nucleus emits an electron, suddenly changing its charge from $Ze$ to $(Z + 1)e$. Calculate the probability that a measurement of the energy of the atom after the emission will also find it to be in its ground state.

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