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

$$\frac{\hbar^2\pi^2}{2m}\Big(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2}\Big) \qquad \text{for integers } n_i > 0\ .$$

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

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

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

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 $E = \left(N + \frac{3}{2}\right)\hbar\omega$? Show that the ground state is spherically symmetric and find a state with $N = 2$ that is also spherically symmetric.

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

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{Q}\rangle_\Psi = \langle\, [\hat{Q}, \hat{H}]\,\rangle_\Psi$$

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

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

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

4. Let $\hat{A}$ and $\hat{B}$ be hermitian operators. Show that $i[\hat{A}, \hat{B}]$ is hermitian.

Given a normalised state ψ, consider $\|\,(\hat{A} + i\lambda\hat{B})\psi\,\|^2$ with λ a real variable and deduce that

$$\langle\hat{A}^2\rangle\langle\hat{B}^2\rangle \geq \tfrac{1}{4}\,|\,\langle\, i[\hat{A}, \hat{B}]\,\rangle\,|^2\,,$$

with all expectation values taken in the state ψ. Hence derive the generalised uncertainty relation:

$$\Delta A\,\Delta B \geq \tfrac{1}{2}\,|\,\langle\,[\hat{A}, \hat{B}]\,\rangle\,|\ .$$

5. **(a)** Let $\psi(r)$ be a wavefunction that depends only on the radial coordinate r (in three dimensions). Write down an expression for $\nabla\psi$ and deduce that $\nabla^2\psi = \psi'' + (2/r)\psi' = (r\psi)''/r$. Show that $\hat{\mathbf{p}}^2\psi = (\hat{p}_r)^2\psi$, where $\hat{p}_r$ is a first-order differential operator involving r. Is $\hat{p}_r$ hermitian?

(b) The time-independent Schrödinger Equation for an electron in a Hydrogen atom is

$$-\frac{\hbar^2}{2m_e}\nabla^2\psi - \frac{e^2}{4\pi\epsilon_0}\frac{1}{r}\,\psi = E\psi\,.$$

Verify 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?

6. Let $\phi(r)$ be any spherically symmetric wavefunction. Show, using Cartesian coordinates, that $\hat{L}_3\,\phi = 0$. Show that $\phi(r)$ is also an eigenstate of $\hat{L}^2$. [*Recall that* $\partial r/\partial x_i = x_i/r$.]

Now calculate the results obtained by applying $\hat{L}_3$ and $\hat{L}_3^2$ to each of the wavefunctions

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

From your answers, deduce that each $\psi_i(\mathbf{x})$ is an eigenfunction of $\hat{L}^2$ with eigenvalue $2\hbar^2$. Find linear combinations of the wavefunctions $\psi_i(\mathbf{x})$ that are also eigenfunctions of $\hat{L}_3$; what are the eigenvalues?

7. (a) A particle of mass μ moves in a spherically symmetric potential $U(r)$ in three dimensions.

Show that $\psi(\mathbf{x}) = R(r)Y(\theta,\varphi)$ is an energy eigenstate iff (i) $Y(\theta,\varphi)$ is an eigenfunction of $\hat{L}^2$, with eigenvalue $\hbar^2\ell(\ell{+}1)$, say, and (ii) $\chi(r) = rR(r)$ satisfies the radial Schrödinger equation with effective potential

$$U(r) \;+\; \frac{\hbar^2\ell(\ell{+}1)}{2\mu r^2}\,.$$

[*You may quote properties of* $\hat{L}^2$ *that you need, including its relation to* ∇^2.]

(b) A three-dimensional oscillator of mass μ is governed by the potential $U(r) = \frac{1}{2}\mu\omega^2 r^2$.

Setting $\ell = 0$ in part (a), deduce the energy levels of the oscillator for this value of the angular momentum. [*You may quote results for a one-dimensional oscillator.*]

For general ℓ, re-express the radial Schrödinger equation for $\chi(r)$ as a differential equation for $f(y)$, where $\chi(r) = f(y)\,e^{-y^2/2}$ and $y = (\mu\omega/\hbar)^{1/2}r$. Find all solutions of the form $f(y) = Cy^\alpha$ and determine the corresponding energy eigenvalues (you need not calculate C).

(c)* *If time permits* : Use a power series approach to find all solutions for $f(y)$ in part (b) that give normalisable energy eigenstates. What are the allowed values of ℓ at each energy?

8. Use the commutation relations for orbital angular momentum $[\,\hat{L}_1,\,\hat{L}_2\,] = i\hbar\hat{L}_3$ (and cyclic permutations) to show that $[\,\hat{L}_3,\,\hat{L}^2\,] = 0$.

Prove that $\langle\,[\,\hat{L}_3,\,\hat{A}\,]\,\rangle = 0$ when the expectation value is taken in any eigenstate of $\hat{L}_3$, for any operator A. Hence, by evaluating $[\,\hat{L}_3,\,\hat{L}_1\hat{L}_2\,]$, deduce that $\langle\,\hat{L}_1^2\,\rangle = \langle\,\hat{L}_2^2\,\rangle$ in any eigenstate of $\hat{L}_3$.

Now consider a joint eigenstate for which $\hat{L}_3$ has eigenvalue $\hbar m$ and $\hat{L}^2$ has eigenvalue $\hbar^2\ell(\ell{+}1)$. Show that $\langle\,\hat{L}_1^2\,\rangle = \langle\,\hat{L}_2^2\,\rangle = \frac{1}{2}\hbar^2(\,\ell(\ell{+}1) - m^2\,)$ in this state.

Check that this result is consistent with the generalised uncertainty relation for ΔL_1 and ΔL_2.

9. Consider the $2{\times}2$ hermitian matrices defined by

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

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 $\hbar^2 s(s+1)$, respectively, for a certain positive number s.

10. 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 Example **5** above, 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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