PH3102 Quantum Mechanics Assignment 1

Instructor: Dr. Siddhartha Lal Autumn Semester, 2025

Start Date: August 22, 2025 Submission Deadline: August 28, 2025 .

Submit your answers to the Tutor at the start of the tutorial.

1 The Ehrenfest and quantum Virial theorems

The outcome of measurement of any observable in quantum mechanics cannot be predicted with certainty for a typical state of the quantum system. It can be any of the possible eigenvalues of the operator $\hat{\Omega}$ corresponding to the observable. One then defines expectation value of an operator in any given state, which is nothing but a statistical average. It has been shown in class to be given by: $\langle\hat{\Omega}\rangle = \langle\psi|\,\hat{\Omega}\,|\psi\rangle$ where $|\psi\rangle$ is a normalised state of the system.

(a) The expectation value, in general, depends on time, since the state of the system evolves with time. Show that the expectation value changes with time according to the formula:

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\Omega}\rangle_{|\psi\rangle} = \frac{1}{i\hbar}\Big\langle[\hat{\Omega},\hat{H}]\Big\rangle_{|\psi\rangle} + \Big\langle\frac{\partial\hat{\Omega}}{\partial t}\Big\rangle_{|\psi\rangle} \tag{1}$$

where $[\hat{\Omega},\hat{H}] = \hat{\Omega}\hat{H} - \hat{H}\hat{\Omega}$ is the commutator. This result is known as the **Ehrenfest theorem** in quantum mechanics. The $|\psi\rangle$ on the subscript is just to denote that the expectation value is taken with respect to the state $|\psi\rangle$.

Hint: You may use the Schrödinger equation which governs the time evolution of the state of the system:

$$i\hbar\frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t} = \hat{H}\,|\psi(t)\rangle\ . \tag{2}$$

(b) Now, for the case of a state $|\psi\rangle$ being an eigenket of the Hamiltonian $\hat{\mathcal{H}}$ and for an operator $\hat{\Omega}$ that does not depend explicitly on time, show (using the above result):

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\Omega}\rangle_{|\psi\rangle} = 0\ . \tag{3}$$

This is why quantum states that are eigenkets of the Hamiltonian are called **stationary states**: they yield expectation values, as well as probability densities, that do not change with time.

(c) (i) A general Hamiltonian for a single particle in 3D is given by:

$$\hat{\mathcal{H}} = \frac{\hat{p}^2}{2m} + V(\hat{r})\ , \tag{4}$$

where $\hat{p}$ is the momentum operator in 3D and has position space representation given by $\hat{p} = -i\hbar\nabla$. Starting with operator $\hat{\Omega} \equiv \hat{r}\hat{p}$ and using the results of parts (a) and (b), show that:

$$2\langle T\rangle = \langle\vec{r}\nabla V\rangle\ . \tag{5}$$

This result is known as **quantum viral theorem** and was first derived by Vladimir Fock (known for Fock space, Hartee Fock method etc.).

(ii) Using the above theorem and the central potential $V(r) = \frac{-e^2}{4\pi\epsilon r}$, show that:

$$\langle T\rangle = -\frac{1}{2}\langle V\rangle\ . \tag{6}$$

Note: this is a result from Bohr's theory of Hydrogen atom that you have verified even without solving the corresponding Schrödinger equation!

2 Gaussian distribution.

Consider the Gaussian distribution

$$\rho(x) = A \exp^{-\lambda(x-a)^2} \ ,$$

where A, a, and λ are positive real constants.

(i) Find the normalisation constant A.

(ii) Find $\langle x \rangle$, $\langle x^2 \rangle$, and the standard deviation.

(iii) Sketch the graph of $\rho(x)$.

3 Dirac–Delta and Heaviside step functions.

(i) Prove that

$$\delta(cx) = \frac{1}{|c|}\,\delta(x) \ ,$$

where c is a constant.

(ii) Let $\theta(x)$ be the Heaviside step function:

$$\theta(x) = \begin{cases} 1, & x > 0, \\ 0, & x < 0. \end{cases}$$

Show that

$$\frac{d}{dx}\,\theta(x) = \delta(x).$$