Course: BSO 203 Instructor: S. Raychaudhuri

SESSION 2002-2003, SEMESTER I

PROBLEM SET V

Operators, Expectation Values and Uncertainties

1. A Hermitian operator $\hat{\vartheta}$ on the space of wavefunctions $\psi(\vec{x})$ is defined by the property

$$\int d^3\vec{x}\ \psi^*(\vec{x}) \left[\hat{\vartheta}\psi(\vec{x})\right] = \int d^3\vec{x}\ \left[\hat{\vartheta}\psi(\vec{x})\right]^* \psi(\vec{x})$$

where $\psi(\vec{x})$ is any wavefunction.

   (a) Using this property, verify that the operator $\hat{p} = -i\hbar\frac{\partial}{\partial x}$ is Hermitian.

   (b) Prove that the eigenvalues of a Hermitian operator must be real.

   (c) Prove that the non-degenerate eigenfunctions of a Hermitian operator define an orthonormal set. (This can be proved for degenerate eigenfunctions as well).

   (d) Solve the eigenvalue equation for the momentum operator and find the eigenvalues and eigenstates.

2. (a) If $\hat{\vartheta}$ is a Hermitian operator with orthonormal eigenfunctions satisfying

$$\hat{\vartheta}\ \phi_i(\vec{x}) = \lambda_i\ \phi_i(\vec{x})$$

   and an arbitrary wavefunction can be written

$$\psi_i(\vec{x}) = \sum_i\ c_i\ \phi_i(\vec{x})$$

   where the c_i are complex constants, then prove that the expectation value is given by

$$\langle\vartheta\rangle = \int d^3\vec{x}\ \psi^*(\vec{x}) \left[\hat{\vartheta}\psi(\vec{x})\right] = \sum_i\ |c_i|^2\ \lambda_i\ .$$

   (b) Establish that the Fourier integral is nothing but an expansion of the wavefunction in terms of eigenstates of momentum. Identify the expansion coefficients and prove that the sum of their squared moduli is unity.

   (c) Take the Fourier transform of the Schrödinger equation and establish an operator equivalence for the position operator in momentum space.

3. Consider a Gaussian wavefunction

$$\psi(x) = \frac{1}{(\pi\sigma)^{1/4}}\ e^{-x^2/2\sigma}\ .$$

   (a) Use Schrödinger's equation to find the potential $V(x)$ corresponding to this wavefunction.

(b) Calculate the uncertainty in position Δx with this wavefunction.

(c) Calculate the uncertainty in momentum Δp with this wavefunction.

(d) Find the uncertainty product.

(e) Calculate the overlap integral between a Gaussian wavefunction

$$\psi_1(x) = \frac{1}{(\pi\sigma)^{1/4}}\ e^{-(x-x_0)^2/2\sigma}\ .$$

and a Lorentzian wavefunction

$$\psi_2(x) = \sqrt{\frac{2\gamma}{\pi}}\ \frac{1}{x - x_0 + i\gamma}$$

and find the condition for it to be maximum for a given x_0.

4. (a) If $f(\hat{\vartheta})$ be an 'operator-valued' function expansible as a power series in $\hat{\vartheta}$ and

$$\hat{\vartheta}\ \phi_i(\vec{x}) = \lambda_i\ \phi_i(\vec{x})$$

show that

$$f(\hat{\vartheta})\ \phi_i(\vec{x}) = f(\lambda_i)\ \phi_i(\vec{x})\ .$$

(b) If we have a set of commuting variables $\{\hat{\vartheta}_k\}$, and these satisfy a relation

$$R\left(\hat{\vartheta}_1, \hat{\vartheta}_2, \ldots\right) = 0\ ,$$

show that the (simultaneous) eigenvalues λ_k satisfy the relation

$$R\left(\lambda_1, \lambda_2, \ldots\right) = 0\ .$$

This result is known in linear algebra as *Cayley's Theorem.*

(c) If Ψ is a simultaneous eigenstate of *all* variables, argue that we can do without it.

5. Define the *commutator* $\left[\hat{A}, \hat{B}\right]$ and the anticommutator $\left\{\hat{A}, \hat{B}\right\}$ of two operators $\hat{A}$ and $\hat{B}$ by

$$\left[\hat{A}, \hat{B}\right] = \hat{A}\hat{B} - \hat{B}\hat{A}\ , \qquad \left\{\hat{A}, \hat{B}\right\} = \hat{A}\hat{B} + \hat{B}\hat{A}\ .$$

Now establish the following identities.

(a) $\hat{A}\hat{B} = \frac{1}{2}\left(\left[\hat{A}, \hat{B}\right] + \left\{\hat{A}, \hat{B}\right\}\right)$.

(b) $\left[\hat{A}, \hat{B}\hat{C}\right] = \hat{B}\left[\hat{A}, \hat{C}\right] + \left[\hat{A}, \hat{B}\right]\hat{C} = \left\{\hat{A}, \hat{B}\right\}\hat{C} - \hat{B}\left\{\hat{A}, \hat{C}\right\}$

(c) $\left\{\hat{A}, \hat{B}\hat{C}\right\} = \hat{B}\left\{\hat{A}, \hat{C}\right\} + \left[\hat{A}, \hat{B}\right]\hat{C} = \left\{\hat{A}, \hat{B}\right\}\hat{C} - \hat{B}\left[\hat{A}, \hat{C}\right]$.

(d) $\left[\hat{A}, \left[\hat{B}, \hat{C}\right]\right] + \left[\hat{B}, \left[\hat{C}, \hat{A}\right]\right] + \left[\hat{C}, \left[\hat{A}, \hat{B}\right]\right] = 0$.
This result is known as *Jacobi's identity.*

(e) Do similar-looking identities appear anywhere else in your experience?