IF/UFRJ
Graduate Quantum Mechanics I
2023/2 – Raimundo

Problem Set #4

28/8/2023 – Due on 4/9/2023 by 12:00 noon

1. The Hamiltonian for a particle of mass m in one-dimensional motion is

$$\mathcal{H} = \frac{P^2}{2m} + V(X), \tag{1}$$

where X and P are the usual position and momentum operators, respectively, satisfying $[X, P] = i\hbar$, and $V(X)$ is the potential. Let the eigenvectors of $\mathcal{H}$ be denoted by $|\phi_n\rangle$, with eigenvalues E_n, where n is a discrete index.

(a) Show that

$$\langle \phi_n | P | \phi_{n'} \rangle = \alpha_{n,n'} \langle \phi_n | X | \phi_{n'} \rangle, \tag{2}$$

where $\alpha_{n,n'}$ depends on the difference between E_n and $E_{n'}$. Determine $\alpha_{n,n'}$. [*Hint: consider the commutator* $[X, \mathcal{H}]$.]

(b) Assume $|\phi_n\rangle$ is a bound state. What can you conclude about $\langle P \rangle$?

(c) If $\mathcal{H}$ is even, the eigenstates $\{|\phi_n\rangle\}$ may be chosen to have definite parity (can you show this?). In this case, what can you conclude about $\langle \phi_n | P | \phi_{n'} \rangle$?

(d) Using the closure relation for this basis, show that

$$\sum_{n'} (E_n - E_{n'})^2 \left| \langle \phi_n | X | \phi_{n'} \rangle \right|^2 = \frac{\hbar^2}{m^2} \langle \phi_n | P^2 | \phi_n \rangle, \tag{3}$$

where n' runs over all states.

(e) Consider a one-dimensional harmonic oscillator. Given that $\langle P^2 \rangle$ is finite, what restrictions must be imposed on the left-hand side (LHS) of Eq. (3)?

(f) Consider a one-dimensional potential box. Given that $\langle P^2 \rangle$ is finite, what restrictions must be imposed on the left-hand side (LHS) of Eq. (3)?

2. Let $\mathcal{H}$ be the Hamiltonian operator for a physical system, with eigenvectors denoted by $|\phi_n\rangle$, with eigenvalues E_n, where n is a discrete index.

   (a) Show that for an arbitrary operator A, one has

   $$\langle\phi_n|[A,\mathcal{H}]|\phi_n\rangle = 0. \tag{1}$$

   (b) Specializing to one dimension, assume $\mathcal{H}$ is given by Eq. (1) of Prob. 1. Then,

      (i) Express the commutators $[\mathcal{H}, P]$, $[\mathcal{H}, X]$, and $[\mathcal{H}, XP]$ in terms of X and P.

      (ii) Show that the expectation value of the momentum vanishes, i.e.,

      $$\langle\phi_n|P|\phi_n\rangle = 0. \tag{2}$$

      (iii) Establish a relation between the expectation value of the kinetic energy,

      $$\langle K\rangle = \frac{1}{2m}\langle\phi_n|P^2|\phi_n\rangle, \tag{3}$$

      and the expectation value

      $$\langle W\rangle \equiv \langle\phi_n|X\frac{dV}{dX}|\phi_n\rangle. \tag{4}$$

      (iv) Given that $\langle V\rangle = \langle\phi_n|V(X)|\phi_n\rangle$, what is the relation between $\langle V\rangle$ and $\langle K\rangle$, when $V(X) = V_0X^\lambda$, with $\lambda = 2, 4, 6, \ldots; V_0 > 0$?

   (c) Discuss your results.

3. Virial theorem.

   (a) In a one-dimensional problem, consider a particle with a Hamiltonian

   $$\mathcal{H} = \frac{P^2}{2m} + V(X), \tag{1}$$

   where the potential energy is

   $$V(X) = \lambda X^n. \tag{2}$$

      (i) Calculate the commutator $[\mathcal{H}, XP]$.

      (ii) If there is one, or more, stationary states $|\varphi\rangle$ for the potential V, show that the mean values $\langle T\rangle$ and $\langle V\rangle$, of the kinetic and potential energies in these states satisfy the relation

      $$2\langle T\rangle = n\langle V\rangle. \tag{3}$$

(b) In a three-dimensional problem, $\mathcal{H}$ is written

$$\mathcal{H} = \frac{\mathbf{P}^2}{2m} + V(\mathbf{R}). \tag{4}$$

(i) Calculate the commutator $[\mathcal{H}, \mathbf{R} \cdot \mathbf{P}]$.

(ii) Assume that $V(\mathbf{R})$ is a homogeneous function of n-th order in the variables X, Y, Z. [Recall that a homogeneous function V of the n-th degree in the variables x, y, z by definition satisfies the relation

$$V(\alpha x, \alpha y, \alpha z) = \alpha^n V(x, y, z), \tag{5}$$

and satisfies Euler's identity,

$$x\frac{\partial V}{\partial x} + y\frac{\partial V}{\partial y} + z\frac{\partial V}{\partial z} = nV(x, y, z).] \tag{6}$$

What relation necessarily exists between the mean kinetic energy and the mean potential energy of the particle in a stationary state?

(iii) Apply this to a particle moving in a Coulomb potential $V(r) = -e^2/r$.

(c) Consider a system of N particles with positions $\mathbf{R}_i$ and momenta $\mathbf{P}_i$, $i = 1, 2, \ldots, N$. When their potential energy is a homogeneous function of n-th degree of the set of components X_i, Y_i, Z_i, can the results obtained above be generalised?

(d) Discuss your results.