Quantum Mechanics I, Sheet 7, Spring 2013

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Exercises starting with (*) are optional.

I. (*) FUNCTIONAL CALCULUS AND GENERALIZED COMMUTATORS

Consider an analytic function $F : \mathbb{C} \to \mathbb{C}$ so that

$$F(x) = \sum_{n=0}^{\infty} f_n x^n \,.$$

The function $F(\hat{A})$ of an operator $\hat{A}$ is then defined as

$$F(\hat{A}) = \sum_{n=0}^{\infty} f_n \hat{A}^n \,.$$

1. Let $|\psi\rangle$ be an eigenvector of $\hat{A}$ with eigenvalue a. Prove that $|\psi\rangle$ is an eigenvector of $F(\hat{A})$ with eigenvalue $F(a)$.
2. If $\big[\hat{B}, \hat{A}\big] = 0$, we directly obtain that $\big[\hat{B}, F(\hat{A})\big] = 0$. Prove by induction that if $\big[\hat{B}, \hat{A}\big] \neq 0$, but $\big[\big[\hat{B}, \hat{A}\big], \hat{A}\big] = 0$ then

$$\big[\hat{B}, \hat{A}^n\big] = n\big[\hat{B}, \hat{A}\big]\hat{A}^{n-1} \,,$$

   and deduce the relation

$$\big[\hat{B}, F(\hat{A})\big] = \big[\hat{B}, \hat{A}\big]F'(\hat{A}) \,.$$

3. Since $\big[\hat{X}, \hat{P}\big] = \mathrm{i}\hbar$, deduce the explicit expression of the commutators $\big[\hat{X}, T(\hat{P})\big]$ and $\big[\hat{P}, V(\hat{X})\big]$.

II. EHRENFEST THEOREM AND HAMILTON'S EQUATIONS

In this exercise we consider a particle in three dimensions in a potential V, and the aim is to link and see the differences between classical and quantum mechanics. The classical Hamiltonian is

$$\mathcal{H} = \frac{\mathbf{p}^2}{2m} + V(\mathbf{q}) \,,$$

where $\mathbf{p} = (p_1, p_2, p_3)$ and $\mathbf{q} = (q_1, q_2, q_3)$ are the generalized coordinates. The quantum Hamiltonian is

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{q}}) \,,$$

where $\hat{\mathbf{p}} = (\hat{p}_1, \hat{p}_2, \hat{p}_3)$ and $\hat{\mathbf{q}} = (\hat{q}_1, \hat{q}_2, \hat{q}_3)$ are the momentum and position operators.

A. Poisson brackets and commutators

The Poisson bracket of two classical observables is defined as

$$\{A, B\} = \sum_{i=1}^{3} \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right) ,$$

and the commutator between two quantum observables by

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

1. Prove that the classical observables satisfy

$$\{q_i, q_j\} = 0 , \qquad \{p_i, p_j\} = 0 , \qquad \{q_i, p_j\} = \delta_{ij} .$$

2. By using the representation where

$$\hat{q}_i \psi(\mathbf{q}) = q_i \psi(\mathbf{q}) , \qquad \hat{p}_i \psi(\mathbf{q}) = -\mathrm{i}\hbar \frac{\partial}{\partial q_i} \psi(\mathbf{q}) ,$$

show that

$$\left[\hat{q}_i, \hat{q}_j\right] = 0 , \qquad \left[\hat{p}_i, \hat{p}_j\right] = 0 , \qquad \left[\hat{q}_i, \hat{p}_j\right] = \mathrm{i}\hbar\delta_{ij} .$$

B. Ehrenfest theorem

1. By using Hamilton's equations

$$\dot{q}_i = \frac{\partial \mathcal{H}}{\partial p_i} , \qquad \dot{p}_i = -\frac{\partial \mathcal{H}}{\partial q_i} ,$$

show that the evolution of a classical observable $A = F(\mathbf{q}, \mathbf{p}, t)$ is given by

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial t} + \{A, \mathcal{H}\} .$$

2. For an quantum observable $\hat{A}$ evolving under the action of the Hamiltonian $\hat{H}$, prove that

$$\frac{\mathrm{d}}{\mathrm{d}t}\langle \hat{A} \rangle = \left\langle \frac{\partial \hat{A}}{\partial t} \right\rangle + \frac{1}{\mathrm{i}\hbar} \left\langle [\hat{A}, \hat{H}] \right\rangle .$$

C. Hamilton's equations

1. Deduce the quantum evolution equation of $\langle \hat{\mathbf{q}} \rangle$ and $\langle \hat{\mathbf{p}} \rangle$ and compare to the corresponding Hamilton's equations.

[*Hint:* Use the following relation derived in the first exercise

$$\left[\hat{\mathbf{p}}, V(\hat{\mathbf{q}})\right] = -\mathrm{i}\hbar \nabla V(\hat{\mathbf{q}}) .$$

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2. If the potential V is quadratic, prove that the quantum-classical correspondence

$$\langle \hat{\mathbf{q}} \rangle \leftrightarrow \mathbf{q} , \qquad \langle \hat{\mathbf{p}} \rangle \leftrightarrow \mathbf{p} ,$$

provides an exact analogy. Understand why this is not true for a generic potential.

III. EVOLUTION OPERATOR

The time-evolution of a quantum state $|\psi(t)\rangle \in \mathcal{E}$ where $\mathcal{E}$ is an Hilbert space is given by the Schrödinger equation

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

where $\hat{H}(t) = \hat{H}(t)^\dagger$ is the Hamiltonian of the system.

1. Show that the operator $\hat{U}(t) : \mathcal{E} \to \mathcal{E}$ defined as $\hat{U}(t)|\psi(0)\rangle = |\psi(t)\rangle$ is linear. The operator $\hat{U}(t)$ defined that way is called the evolution operator.

2. Check that the evolution operator satisfies the following differential equation

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t) = \hat{H}(t)\hat{U}(t)\,, \qquad \hat{U}(0) = \hat{I}.$$

   This equation also defines the evolution operator uniquely.

3. (*) Prove that the evolution operator $\hat{U}(t)$ is unitary.

   [*Hint:* Prove that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{U}(t)^\dagger \hat{U}(t)\right) = 0\,.$$

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4. In particular, if the Hamiltonian is time-independent, show that the evolution operator is explicitly given by

$$\hat{U}(t) = \mathrm{e}^{-\mathrm{i}\hat{H}t/\hbar}\,.$$

5. (*) Can you explain, why if $\hat{H}(t)$ is time-dependent, the evolution operator is not given by

$$\exp\left\{\frac{-\mathrm{i}}{\hbar}\int_0^t \hat{H}(s)\,\mathrm{d}s\right\}\,,$$

   as for an ordinary differential equation?