Quantum Mechanics I, Correction Sheet 7, Spring 2013

Responsible for this sheet: J. Guillod (julien.guillod@unige.ch), office 212, Sciences I

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Prof. D. van der Marel (dirk.vandermarel@unige.ch)
Tutorials: J. Guillod (julien.guillod@unige.ch), O. E. Peil (oleg.peil@unige.ch)

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. Therefore, for all $n \in \mathbb{N}$, we have,

$$\hat{A}^n|\psi\rangle = a^n|\psi\rangle \,.$$

so by definition of $F(\hat{A})$,

$$F(\hat{A})|\psi\rangle = \sum_{n=0}^{\infty} f_n \hat{A}^n|\psi\rangle = \sum_{n=0}^{\infty} f_n a^n|\psi\rangle = F(a)|\psi\rangle \,,$$

and $|\psi\rangle$ is an eigenvector of $F(\hat{A})$ with eigenvalue $F(a)$.

2. If $\big[[\hat{B}, \hat{A}], \hat{A}\big] = 0$, we prove by induction that

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

The base case is $n = 1$. For the inductive step, by assuming the relation true of n, we have

$$\begin{aligned}
\big[\hat{B}, \hat{A}^{n+1}\big] &= \hat{B}\hat{A}^n\hat{A} - \hat{A}^n\hat{A}\hat{B} = \hat{B}\hat{A}^n\hat{A} - \hat{A}^n\hat{B}\hat{A} + \hat{A}^n\hat{B}\hat{A} - \hat{A}^n\hat{A}\hat{B} \\
&= \big[\hat{B}, \hat{A}^n\big]\hat{A} + \hat{A}^n\big[\hat{B}, \hat{A}\big] = n\big[\hat{B}, \hat{A}\big]\hat{A}^n + \hat{A}^n\big[\hat{B}, \hat{A}\big] \\
&= (n+1)\,\big[\hat{B}, \hat{A}\big]\hat{A}^n \,,
\end{aligned}$$

since $\big[\hat{B}, \hat{A}\big]$ commutes with $\hat{A}$. For a general function, we obtain

$$\big[\hat{B}, F(\hat{A})\big] = \sum_{n=0}^{\infty}\big[\hat{B}, f_n\hat{A}^n\big] = \sum_{n=0}^{\infty} f_n\big[\hat{B}, \hat{A}^n\big] = \big[\hat{B}, \hat{A}\big]\sum_{n=0}^{\infty} n f_n \hat{A}^{n-1} = \big[\hat{B}, \hat{A}\big]F'(\hat{A}) \,,$$

because by definition,

$$F'(x) = \sum_{n=0}^{\infty} n f_n x^{n-1} \,.$$

3. If $\left[\hat{X},\hat{P}\right] = \mathrm{i}\hbar$, then we deduce

$$\left[\hat{X},T(\hat{P})\right] = \left[\hat{X},\hat{P}\right]T'(\hat{P}) = \mathrm{i}\hbar T'(\hat{P})\,,$$

and

$$\left[\hat{P},V(\hat{X})\right] = \left[\hat{P},\hat{X}\right]V'(\hat{X}) = -\mathrm{i}\hbar V'(\hat{X})\,.$$

These two relations will be used in the next exercise.

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. By definition of the Poisson bracket, we obtain

$$\begin{aligned}
\{q_i,q_j\} &= \sum_{k=1}^{3}\left(\frac{\partial q_i}{\partial q_k}\frac{\partial q_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial q_j}{\partial q_k}\right) = \sum_{k=1}^{3}(\delta_{ik}0 - 0\delta_{jk}) = 0\,,\\
\{p_i,p_j\} &= \sum_{k=1}^{3}\left(\frac{\partial p_i}{\partial q_k}\frac{\partial p_j}{\partial p_k} - \frac{\partial p_i}{\partial p_k}\frac{\partial p_j}{\partial q_k}\right) = \sum_{k=1}^{3}(0\delta_{jk} - \delta_{ik}0) = 0\,,\\
\{q_i,p_j\} &= \sum_{k=1}^{3}\left(\frac{\partial q_i}{\partial q_k}\frac{\partial p_j}{\partial p_k} - \frac{\partial q_i}{\partial p_k}\frac{\partial p_j}{\partial q_k}\right) = \sum_{k=1}^{3}(\delta_{ik}\delta_{jk} - 0) = \delta_{ij}\,.
\end{aligned}$$

2. In the representation given by

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

we have

$$\begin{aligned}
\left[\hat{q}_i, \hat{q}_j\right]\psi(\mathbf{q}) &= \hat{q}_i\hat{q}_j\psi(\mathbf{q}) - \hat{q}_j\hat{q}_i\psi(\mathbf{q}) = q_iq_j\psi(\mathbf{q}) - q_jq_i(\mathbf{q}) = 0\,,\\
\left[\hat{p}_i, \hat{p}_j\right]\psi(\mathbf{q}) &= \hat{p}_i\hat{p}_j\psi(\mathbf{q}) - \hat{p}_j\hat{p}_i\psi(\mathbf{q}) = -\hbar^2\frac{\partial}{\partial q_i}\frac{\partial}{\partial q_j}\psi(\mathbf{q}) + \hbar^2\frac{\partial}{\partial q_j}\frac{\partial}{\partial q_i}\psi(\mathbf{q}) = 0\,,\\
\left[\hat{q}_i, \hat{p}_j\right]\psi(\mathbf{q}) &= \hat{q}_i\hat{p}_j\psi(\mathbf{q}) - \hat{p}_j\hat{q}_i\psi(\mathbf{q}) = -\mathrm{i}\hbar q_i\frac{\partial}{\partial q_j}\psi(\mathbf{q}) + \mathrm{i}\hbar\frac{\partial}{\partial q_j}\left(q_i\psi(\mathbf{q})\right)\\
&= -\mathrm{i}\hbar q_i\frac{\partial}{\partial q_j}\psi(\mathbf{q}) + \mathrm{i}\hbar q_i\frac{\partial}{\partial q_j}\psi(\mathbf{q}) + \mathrm{i}\hbar\frac{\partial q_i}{\partial q_j} = \mathrm{i}\hbar\delta_{ij}\,.
\end{aligned}$$

The commutation relations between position and momentum operators in quantum mechanics are the analog of the Poisson brackets between position and momentum in classical mechanics.

B. Ehrenfest theorem

1. By using the chain rule, the evolution of a classical observable $A = F(\mathbf{q}, \mathbf{p}, t)$ is given by

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{\partial A}{\partial t} + \sum_{i=1}^{3}\left(\frac{\partial A}{\partial q_i}\dot{q}_i + \frac{\partial A}{\partial p_i}\dot{p}_i\right) = \frac{\partial A}{\partial t} + \sum_{i=1}^{3}\left(\frac{\partial A}{\partial q_i}\frac{\partial \mathcal{H}}{\partial p_i} - \frac{\partial A}{\partial p_i}\frac{\partial \mathcal{H}}{\partial q_i}\right) = \frac{\partial A}{\partial t} + \{A, \mathcal{H}\}\ ,$$

where we used Hamilton equations,

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

2. The evolution of the expectation value of a quantum observable $\hat{A}$ evolving under the action of the Hamiltonian $\hat{H}$, is

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{A}\rangle &= \frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\hat{A}|\psi(t)\rangle = \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle + \left(\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi(t)|\right)\hat{A}|\psi(t)\rangle + \langle\psi(t)|\hat{A}\left(\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle\right)\\
&= \langle\psi(t)|\frac{\partial\hat{A}}{\partial t}|\psi(t)\rangle - \frac{1}{\mathrm{i}\hbar}\langle\psi(t)|\hat{H}\hat{A}|\psi(t)\rangle + \frac{1}{\mathrm{i}\hbar}\langle\psi(t)|\hat{A}\hat{H}|\psi(t)\rangle\\
&= \left\langle\frac{\partial\hat{A}}{\partial t}\right\rangle + \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{A}, \hat{H}\right]\right\rangle\ ,
\end{aligned}$$

where we used the Schrödinger equation and its adjoint,

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

C. Hamilton's equations

1. By applying Ehrenfest theorem and the conclusions of the first exercise, we have

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{q}}\rangle &= \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{\mathbf{q}}, \hat{H}\right]\right\rangle = \frac{1}{2\mathrm{i}\hbar m}\left\langle\left[\hat{\mathbf{q}}, \hat{\mathbf{p}}^2\right]\right\rangle = \frac{1}{m}\langle\hat{\mathbf{p}}\rangle\ ,\\
\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\mathbf{p}}\rangle &= \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{\mathbf{p}}, \hat{H}\right]\right\rangle = \frac{1}{\mathrm{i}\hbar}\left\langle\left[\hat{\mathbf{p}}, V(\hat{\mathbf{q}})\right]\right\rangle = -\langle\nabla V(\hat{\mathbf{q}})\rangle\ .
\end{aligned}$$

For the classical system, the Hamilton's equations are given by

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{q} = \frac{1}{m}\mathbf{p}\,, \qquad\qquad \frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p} = -\nabla V(\mathbf{q})\,.$$

2. For a quadratic potential

$$V(\mathbf{q}) = \frac{m\omega^2}{2}\mathbf{q}^2 \qquad \Rightarrow \qquad \nabla V(\mathbf{q}) = m\omega^2\mathbf{q}\,,$$

and therefore the quantum-classical correspondence

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

provides an exact analogy. This correspondence is not true for a generic potential. For example for a quartic one,

$$V(\mathbf{q}) = \frac{\lambda}{4}\mathbf{q}^4 \qquad \Rightarrow \qquad \nabla V(\mathbf{q}) = \lambda\mathbf{q}^3\,,$$

and consequently

$$\langle\nabla V(\hat{\mathbf{q}})\rangle = \lambda\left\langle\hat{\mathbf{q}}^3\right\rangle \neq \lambda\left\langle\hat{\mathbf{q}}\right\rangle^3 \leftrightarrow \lambda\mathbf{q}^3\,.$$

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. The evolution operator $\hat{U}(t) : \mathcal{E} \to \mathcal{E}$ is defined as $\hat{U}(t)|\psi(0)\rangle = |\psi(t)\rangle$. This operator is linear because if

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

then

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle\,, \qquad \text{with} \qquad |\psi(t)\rangle = \alpha|a(t)\rangle + \beta|b(t)\rangle\,,$$

which prove that

$$\begin{aligned}\hat{U}(t)\left(\alpha|a(0)\rangle + \beta|b(0)\rangle\right) &= \hat{U}(t)|\psi(0)\rangle = |\psi(t)\rangle \\ &= \alpha|a(t)\rangle + \beta|b(t)\rangle = \alpha\hat{U}(t)|a(0)\rangle + \beta\hat{U}(t)|b(0)\rangle\,.\end{aligned}$$

2. By using the Schrödinger equation, we have

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)|\psi(0)\rangle = \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle = \hat{H}(t)\hat{U}(t)|\psi(0)\rangle\,,$$

and also by definition,

$$\hat{U}(0)|\psi(0)\rangle = |\psi(0)\rangle\,.$$

Since the last two relations are valid for all $|\psi(0)\rangle \in \mathcal{E}$, the evolution operator satisfies the following differential equation

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

This equation also defines the evolution operator uniquely.

3. (*) By using the differential equation satisfied by the evolution operator and its conjugate, we have

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\left(\hat{U}(t)^\dagger\hat{U}(t)\right) &= \left(\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)^\dagger\right)\hat{U}(t) + \hat{U}(t)^\dagger\left(\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\hat{U}(t)\right)\\ &= -\left(\hat{H}(t)\hat{U}(t)\right)^\dagger\hat{U}(t) + \hat{U}(t)^\dagger\hat{H}(t)\hat{U}(t) = 0\,,\end{aligned}$$

and

$$\hat{U}(0)^\dagger\hat{U}(0) = \hat{I}^\dagger\hat{I} = \hat{I}\,,$$

which together prove that

$$\hat{U}(t)^\dagger\hat{U}(t) = \hat{I}\,.$$

Strictly speaking, to prove that $\hat{U}(t)$ is unitary, it remains to show that $\hat{U}(t)\hat{U}(t)^\dagger = \hat{I}$. In fact this is automatically true by the fact that $\hat{U}(t)$ is surjective: for all $|\psi(t)\rangle \in \mathcal{E}$ there exists $|\psi(0)\rangle \in \mathcal{E}$ such that $|\psi(t)\rangle = \hat{U}(t)|\psi(0)\rangle$ and therefore,

$$\hat{U}(t)\hat{U}(t)^\dagger|\psi(t)\rangle = \hat{U}(t)\hat{U}(t)^\dagger\hat{U}(t)|\psi(0)\rangle = \hat{U}(t)|\psi(0)\rangle = |\psi(t)\rangle\,.$$

4. If the Hamiltonian is time-independent, the evolution operator satisfies the linear differential equation

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

Since this differential equation is linear it is sufficient to check that

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

is a solution:

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

5. (*) If $\left[\hat{H}(t), \hat{H}(s)\right] = 0$, then the evolution operator is given as for an ordinary differential equation by

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

However, if the Hamiltonian does not commute at different times, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\int_0^t \hat{H}(s)\,\mathrm{d}s\right)^2 = \hat{H}(t)\int_0^t \hat{H}(s)\,\mathrm{d}s + \int_0^t \hat{H}(s)\,\mathrm{d}s\,\hat{H}(t) \neq 2\hat{H}(t)\int_0^t \hat{H}(s)\,\mathrm{d}s\,,$$

and the evolution operator does not satisfies the differential equation.