

From classical physics to quantum mechanics via the Ehrenfest theorem.

Related information you may find at:

<https://farside.ph.utexas.edu/teaching/qmech/Quantum/node36.html>

Hope I can help you with learning quantum mechanics.

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Prerequisite

The commutator of two operators (matrices) A, B :

$$[A, B] := AB - BA$$

The position operator X multiplies any functions applied to by x :

$$Xf(x) = x \cdot f(x)$$

The differentiation operator D derives any functions with respect to x :

$$Df(x) = \frac{d}{dx}f(x)$$

The commutator of D and X :

$$\begin{aligned} [X, D]f(x) &= \\ XDf(x) - DXf(x) &= \\ x \frac{d}{dx}f(x) - \frac{d}{dx}(xf(x)) &= \\ x \frac{d}{dx}f(x) - f(x) - x \frac{d}{dx}f(x) &= -f(x) \end{aligned}$$

In other words:

$$[X, D] = -1$$

Position and momentum classical

A particle moving along the x -axis has position x and momentum p .

The particle is moving on the x -axis in a potential $V(x)$.

We use the potential:

$$V(x) = a \cdot x^2$$

Note: This is the potential of the harmonic oscillator.

The Hamiltonian $h(x, p)$ describes the total energy of the particle, the sum of kinetic energy and potential energy:

$$h(x, p) = \frac{p^2}{2m} + V(x)$$

The speed of the particle:

$$\frac{dx}{dt} = \frac{\partial h}{\partial p} = \frac{p}{m}$$

The force acting on the particle:

$$\frac{dp}{dt} = -\frac{\partial h}{\partial x} = -\frac{dV(x)}{dx}$$

Note: x and p are observables that can be measured (exactly).

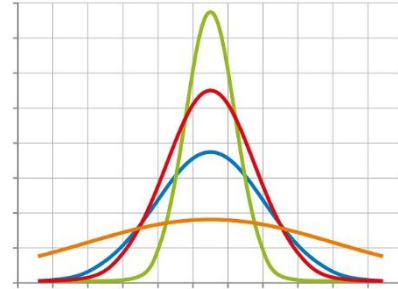
Position and momentum quantum

X and P are operators. The state of the particle becomes a vector $|\psi\rangle$ in Hilbert space of square integrable functions $L^2(\mathbb{R}, \mathbb{C})$. The function $\psi(x)$ is named wave function.

The operator X corresponds to the observable x , the operator P to the observable p .

The set of eigenfunctions of the operator X are elements $\{|x\rangle, x \in \mathbb{R}\}$. The corresponding eigenvalues are the position of the particle, x .

$|x\rangle$, the position of the particle, is not part of the Hilbert space of square integrable functions $L^2(\mathbb{R}, \mathbb{C})$. This causes that the position of the particle cannot be measured exactly. The position after measurement (after the application of the operator) must be a more or less sharp localized square integrable function – a wave function.



Ehrenfest

We transform the Classical Hamiltonian into the Quantum one:

$$h(x, p) = \frac{p^2}{2m} + V(x) \rightarrow H = \frac{P^2}{2m} + V(X)$$

The Ehrenfest Theorem states:

$$\frac{d}{dt}\langle A \rangle = \frac{1}{i\hbar}\langle [A, H] \rangle$$

Note: $\langle A \rangle$ denotes the expectation value (average).

Note: The operator A has no explicit time dependency.

Note: If A commutes with H , the expectation value of A does not change with time.

From the Ehrenfest Theorem we get the Ehrenfest equations:

$$\begin{aligned} \frac{d\langle X \rangle}{dt} &= \left\langle \frac{\partial H}{\partial P} \right\rangle = \frac{\langle P \rangle}{m} \\ \frac{d\langle P \rangle}{dt} &= -\left\langle \frac{\partial H}{\partial X} \right\rangle = -\frac{d}{dx}\langle V(X) \rangle \end{aligned}$$

We combine the Ehrenfest Theorem and the Ehrenfest equations:

$$\begin{aligned} \frac{d\langle X \rangle}{dt} &= \frac{\langle P \rangle}{m}, \quad \frac{d\langle X \rangle}{dt} = \frac{1}{i\hbar}\langle [X, H] \rangle \rightarrow \frac{\langle P \rangle}{m} = \frac{1}{i\hbar}\langle [X, H] \rangle \\ \frac{d\langle P \rangle}{dt} &= -\frac{d}{dx}\langle V(X) \rangle, \quad \frac{d\langle P \rangle}{dt} = \frac{1}{i\hbar}\langle [P, H] \rangle \rightarrow -\frac{d}{dx}\langle V(X) \rangle = \frac{1}{i\hbar}\langle [P, H] \rangle \end{aligned}$$

We take the first equation:

$$\frac{\langle P \rangle}{m} = \frac{1}{i\hbar}\langle [X, H] \rangle$$

We check the commutator.

$$[X, H] = XH - HX =$$

$$\begin{aligned}
X \left(\frac{P^2}{2m} + V(X) \right) - \left(\frac{P^2}{2m} + V(X) \right) X &= \\
\frac{XP^2}{2m} + XV(X) - \frac{P^2X}{2m} - V(X)X &= \\
\frac{XP^2}{2m} - \frac{P^2X}{2m} + XV(X) - V(X)X &
\end{aligned}$$

We examine the second part $XV(X) - V(X)X$:

$$\begin{aligned}
XV(X) &= xV(X) = xax^2 = ax^3 \\
V(X)X &= ax^2x = ax^3 \\
XV(X) - V(X)X &= 0
\end{aligned}$$

We get:

$$[X, H] = \frac{1}{2m} [X, P^2]$$

We disassemble this:

$$\frac{1}{2m} [X, P^2] = \frac{1}{2m} [X, P]P + P[X, P]$$

We go back to the first equation:

$$\frac{\langle P \rangle}{m} = \frac{1}{i\hbar} \langle [X, H] \rangle \rightarrow \frac{\langle P \rangle}{m} = \frac{1}{i\hbar} \frac{1}{2m} \langle [X, P]P + P[X, P] \rangle$$

This equation is valid if:

$$[X, P] = i\hbar \cdot id$$

Note: we work with operators (matrices), id is the identity matrix.

From the prerequisite we have:

$$[X, D] = -1$$

If we assign: $P := -i\hbar D$ we get:

$$\frac{\langle P \rangle}{m} = \frac{1}{i\hbar} \langle [X, H] \rangle$$

We check whether the second equation holds with this P :

$$-\frac{d}{dx} \langle V(X) \rangle = \frac{1}{i\hbar} \langle [P, H] \rangle$$

We check the commutator:

$$\begin{aligned}
[P, H] &= PH - HP = \\
P \left(\frac{P^2}{2m} + V(X) \right) - \left(\frac{P^2}{2m} + V(X) \right) P &= \\
P \frac{P^2}{2m} + PV(X) - \frac{P^2}{2m} P - V(X)P &=
\end{aligned}$$

$$P \frac{p^2}{2m} - \frac{p^2}{2m} P + PV(X) - V(X)P =;$$

Note: $PP^2 = P^2P$

$$\begin{aligned} PV(X) - V(X)P &= \\ -i\hbar DV(X) - V(X)(-i\hbar D) &=; \end{aligned}$$

Note: we need a function $f(x)$ the operators are applied to:

$$\begin{aligned} -i\hbar \left(\frac{d}{dx}(ax^2) - (ax^2) \left(\frac{d}{dx} \right) \right) f(x) &= \\ -i\hbar \left(\frac{d}{dx}((ax^2)f(x)) - (ax^2) \left(\frac{d}{dx} f(x) \right) \right) &= \\ -i\hbar \left(2axf(x) + ax^2 \frac{d}{dx} f(x) - ax^2 \frac{d}{dx} f(x) \right) &= \\ -i\hbar 2axf(x) & \end{aligned}$$

In other words:

$$[P, H] = -i\hbar 2ax = -i\hbar \frac{d}{dx} \langle V(X) \rangle$$

We check the second equation:

$$\begin{aligned} -\frac{d}{dx} \langle V(X) \rangle &= \frac{1}{i\hbar} \langle [P, H] \rangle \rightarrow \\ -\frac{d}{dx} \langle V(X) \rangle &= \frac{1}{i\hbar} \langle -i\hbar \frac{d}{dx} \langle V(X) \rangle \rangle \rightarrow \\ \frac{d}{dx} \langle V(X) \rangle &= \frac{d}{dx} \langle \langle V(X) \rangle \rangle \end{aligned}$$

Note: the average of an average remains the same.

Note: This will work with every potential that can be expressed in polynomial functions of x .

Result: If we set $P := -i\hbar D$ the Ehrenfest equations for our scenario are valid. The momentum operator, the equivalence to the classical momentum becomes the differentiation operator, multiplied by $-i\hbar$.

We can treat results of classical processes as averages of quantum processes and try to find the corresponding quantum operators. This may work but must not work in every case.