

Postulates⁽¹⁾ of mechanics

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	Postulates	
	Classical mechanics (CM)	Quantum mechanics (QM)
(1) Fundamental observables	x_j (position) and p_j (momentum) are independent real variables ⁽²⁾ Their conjugation coefficient is thus zero.	\hat{x}_j and \hat{p}_j are Fourier-conjugate hermitian (real) operators ⁽³⁾ Their conjugation coefficient ⁽⁴⁾ is \hbar
(2) State of the system ⁽⁵⁾	The state is uniquely specified as a function of time t by a trajectory $T(t) \hat{=} \{x_j(t), p_j(t)\}$ Note: a x - p pair of variables is needed.	The state is uniquely specified by a wavefunction ⁽⁶⁾ $ t\rangle \hat{=} \{\Psi^{(r)}(\hat{x}_j, t), \Psi^{(i)}(\hat{x}_j, t)\}$ Note: a $\Psi^{(r)}$ - $\Psi^{(i)}$ pair of functions is needed.
(3) Derived observables A	Real functions $A(x_j, p_j)$	Hermitian operators $\hat{A}(\hat{x}_j, \hat{p}_j)$
(4) Measurement of observables A	If a measurement of A is made at time t , A equals the real value $A(x_j(t), p_j(t))$ with 100% probability ($P(t)=1$).	If a measurement of A is made at time t , a real value A_n is obtained with probability $P_n(t)$ A_n must satisfy $\hat{A} \Psi_n(x_j) = A_n \Psi_n(x_j) \hat{=} \hat{A} n\rangle = A_n n\rangle$ The probability ⁽⁷⁾ is given by $P_n(t) = \langle n t\rangle ^2$
(5) Equation of motion	The energy, called Hamiltonian, is a real observable given by $H = \sum_j \frac{p_j^2}{2m} + V(x_j)$ The trajectory evolves in time according to $-\frac{\partial p_j}{\partial t} = \frac{\partial H}{\partial x_j}, \quad +\frac{\partial x_j}{\partial t} = \frac{\partial H}{\partial p_j}$	The Hamiltonian is a hermitian operator given by $\hat{H} = \sum_j \frac{\hat{p}_j^2}{2m} + V(\hat{x}_j)$ The wavefunction evolves according to $-\frac{\partial \Psi^{(i)}}{\partial t} = \frac{\hat{H}}{\hbar} \Psi^{(r)}, \quad +\frac{\partial \Psi^{(r)}}{\partial t} = \frac{\hat{H}}{\hbar} \Psi^{(i)}$
(6) Particles	Particles have intrinsic variables such as mass and charge. (There is no spin.) All classical particles are distinguishable	Particles have intrinsic variables such as mass, charge, <u>and spin</u> (an angular momentum). ⁽⁸⁾ Two types of indistinguishable quantum particles exist: 1) Fermions: $\hat{P} 12\rangle = - 12\rangle$, spin = $1/2, 3/2, 5/2 \dots$ 2) Bosons: $\hat{P} 12\rangle = + 12\rangle$, spin = $0, 1, 2, 3 \dots$

⁽¹⁾ In consistent mathematic systems, the analog of postulates are called “axioms,” such as Euclid’s axioms of plane geometry. IN chemistry and physics, postulates may have to be adopted based on experimental evidence, so we don’t call them axioms. The above postulates are complete, but for the sake of simplicity, some mathematical rigor has been left out for this undergraduate class.

(2) Each particle in 3-D space has 3 coordinates and momenta, so we use subscripts to distinguish different coordinates and momenta, as in $(x, y, z) = (x_1, x_2, x_3)$ for the coordinates of the first particle, $(x, y, z) = (x_4, x_5, x_6)$ for the coordinates of the second particle, etc.

(3) These types of technical terms are defined in the "Quantum Vocabulary". For example, "hermitian" basically just means "real."

(4) This constant is called "hbar" and has units of (position) times (momentum). It approximately equals $1.05 \cdot 10^{-34}$ (m)·(kg·m/s)

(5) The symbol " $\hat{=}$ " means "is equivalent to."

(6) For wavefunctions, " $|t\rangle$ " is an abstract notation invented by P. Dirac in the 1930s, to express the idea that wavefunctions can be equivalently written in terms of different variables, such as $\Psi(x) \hat{=} \Psi(p)$, but contain the same information. Think of the volume element in integration as an example of equivalence: $r^2 dr \cos\theta d\theta d\phi$ is equivalent to $dx dy dz$, but they are not the same!

(7) $|\langle n|t\rangle|^2$ is another bit of Dirac's shorthand that we will learn later. It means $|\int dx \Psi_n^*(x_j) \Psi(\hat{x}_j, t)|^2$, where $\Psi(\hat{x}_j, t) = \Psi^{(r)}(\hat{x}_j, t) + i \Psi^{(i)}(\hat{x}_j, t)$ and "i" is the imaginary number $\sqrt{-1}$. The $|\ |^2$ means "absolute value squared of what's between the vertical bars."

(8) spin and spin angle are just another momentum-coordinate pair, like p and x . It just turns out that in classical mechanics, they don't exist!

The operator \hat{P} , called the "permutation operator," takes two identical particles (e.g. 2 electrons), and switches them. You might expect that the wavefunction $|12\rangle$ for the two particles "1" and "2" would stay the same, but it switches sign! This is the property of fermions, such as protons and electrons. On the other hand, for bosons, such as photons or molecular vibrations, the wavefunction does not switch sign. One can prove from relativistic quantum field theory that only integer (0,1...) and half-integer ($1/2 \dots$) spins exist, and that they must have the permutation properties in postulate 6. However, this goes beyond what we have time to derive in this class. It is a postulate of non-relativistic (Schrödinger-Heisenberg) quantum mechanics.