UNTERNEHMEN TAIFUN

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Part I Fundamentals

Chapter 1

Quantum Mechanics

Hierzu ist es notwendig, die Energy nicht als eine stetige unbeschränkt teilbare, sondern als eine discrete, ause einer ganzen Zahl von endlichen gleichen Teilen zusammengesetzte Grösse aufzufassen.

— Max Planck

1.1 Classical Mechanics

The formalism used in quantum mechanics largely stems from William Rowan Hamilton's formulation of classical mechanics. Through the process of canonical quantisation any classical model of a physical system is turned into a quantum mechanical model.

In Hamilton's formulation of classical mechanics, a complete description of a system of N particles is described by a set of canonical coordinates $q = (\vec{q}_1, \dots, \vec{p}_N)$ and corresponding conjugate momenta $p = (\vec{p}_1, \dots, \vec{p}_N)$. Together, each pair of coordinate and momentum form a point $\xi = (q, p)$ in phase space, which is a space of all possible states of the system. Moreover, pairs of generalised coordinates and conjugate momenta are canonical if they satisfy the Poisson brackets so that $\{q_i, p_k\} = \delta_{ij}$. The Poisson bracket of two functions is defined as

$$\{f,g\} = \frac{\partial f}{\partial q} \frac{\partial g}{\partial g} - \frac{\partial f}{\partial p} \frac{\partial g}{\partial q}.$$
 (1.1)

The governing equations of motion in a classical system is Hamilton's equations,

$$\dot{q} = \frac{\partial}{\partial p} \mathcal{H}(q, p) \tag{1.2}$$

$$\dot{p} = -\frac{\partial}{\partial q} \mathcal{H}(q, p) \tag{1.3}$$

where $\mathcal{H}(q,p)$ is the Hamiltonian, a function for the total energy of the system. Hamilton's equations may also be stated in terms of the Poisson brackets,

$$\frac{dp_i}{dt} = \{p_i, \mathcal{H}\}, \ \frac{dq_i}{dt} = \{q_i, \mathcal{H}\}. \tag{1.4}$$

A system consisting of N of equal mass m, subject forces caused by an external potential, as well as acting on each other with forces stemming from a central potential $w(q_i j)$ has the following Hamiltonian,

$$\mathcal{H}(q,p) = \mathcal{T}(q) + \mathcal{V}(p) + \mathcal{W}(p) = \frac{1}{2m} \sum_{i} |\vec{p}_{i}|^{2} + \sum_{i} v(\vec{r}_{i}) + \frac{1}{2} \sum_{i < j} w(\vec{r}_{ij}).$$
 (1.5)

This Hamiltonian conveniently contains several parts - the kinetic energy, the external potential energy and the interaction energy; denoted by \mathscr{T} , \mathscr{V} and \mathscr{W} respectively,

1.2 The Dirac-von Neumann Postulates

This is the TL;DR version of Quantum Mechanics.

Hilbert Space A quantum state of an isolated physical system is described by a vector with unit norm in a Hilbert space, a complex vector space quipped with a scalar product.

Observables Each physical observable of a system is accociated with a *hermitian* operator acting on the Hilbert space. The eigenstates of each such operator define a *complete*, *orthonormal* set of vectors.

With O an operator, hermiticity means,

$$\langle \phi | \hat{O}\psi \rangle = \langle \hat{O}\phi | \psi \rangle \equiv \langle \phi | \hat{O} | \psi \rangle.$$
 (1.6)

Completness means,

$$\sum_{i} |i\rangle \langle i| = 1. \tag{1.7}$$

Orthonormal means,

$$\langle i|j\rangle = \delta_{ij}.\tag{1.8}$$

Time Evolution The time evolution of the state vector, $|\psi\rangle = |\psi(t)\rangle$, is given by the Schrödinger equation¹.

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = \hat{H} |\psi(t)\rangle.$$
 (1.9)

Measurements Physically measurable values, associated with an observable \hat{O} are defined by the eigenvalues o_n of the observable,

$$\hat{O}|n\rangle = o_n|n\rangle. \tag{1.10}$$

The probability for finding a particular eigenvalue in the measurement is

$$p_n = |\langle n|\psi\rangle|^2,\tag{1.11}$$

with the system in state $|\psi\rangle$ before the measurement, and $|n\rangle$ as the eigenstate corresponding to the eigenvalue o_n .

 $^{^1{\}rm In}$ the Schrödinger picture.