III. Basic Quantum Mechanics

(….. to Schrödinger and Heisenberg)

1. Wave function and *Schrödinger Equation*

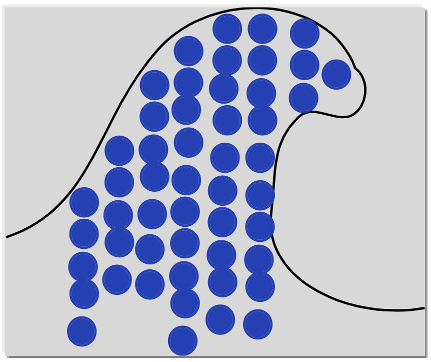

Figure 1: Water waves have a granular character. The macroscopic wave guides microscopic water molecules.

The major insight derived from experimental observations by a number of physicists (Planck, Bohr, de Broglie, Schrödinger and Heisenberg) in the early part of the 20th century is that

- All physical entities have a dual character: They can appear as particles (massive or mass-less) or as waves, depending on the method of their observation.
- Particles are guided/organized along a degree of freedom *x* by associated wave functions $\psi(x,t)$ which behave according to the rules of wave mechanics.
- The wave function is a stochastic function, in that the differential **probability** to find a particle at time *t* in an element d*x* around *x* is given by

$$dP = |\psi(x,t)|^2 \cdot dx \quad (1)$$

.

$$P = \int_{-\infty}^{+\infty} dP(x,t) = \int_{-\infty}^{+\infty} dx |\psi(x,t)|^2 = \int_{-\infty}^{+\infty} dx\, \psi(x,t)^* \cdot \psi(x,t) = 1 \quad (2)$$

This implies that the proper wave function has to be normalized, or normalizable, to represent a probability (amplitude). Equation 2 is a special case of a more generally defined **scalar product** between two wave functions, $\psi(x,t)$ and $\varphi(x,t)$,

$$\left\langle \psi(x,t) \middle| \varphi(x,t) \right\rangle := \int_{-\infty}^{+\infty} dx\, \psi(x,t)^* \cdot \varphi(x,t) \qquad (3)$$

This scalar product is zero for any two "**orthogonal**" functions. In fact, orthogonality is defined through this relation.

A complication arises for "continuum" wave functions, corresponding to the continuum of kinetic energies available to free particles. For such wave functions, the scalar product (Equ. 3) of two functions $\psi_p(x,t)$ and $\psi_{p'}(x,t)$

$$\left\langle \psi_p(x,t) \middle| \psi_{p'}(x,t) \right\rangle := \int_{-\infty}^{+\infty} dx\, \psi_p(x,t)^* \cdot \psi_{p'}(x,t) \propto \delta\left(p - p'\right) \qquad (4)$$

defines a distribution, the so-called "delta function." The normalization integral of Equ. 2 gives a corresponding result.
Such distributions appear as parts of integrands in an integral, where they work as projectors of the integrand evaluated for zero argument of the delta function.

- Each experimental observable A is represented by a quantum mechanical (differential) operator $\hat{A}$ that, when applied to a wave function, "projects" out an average expectation value of the observable,

$$A = \left\langle \hat{A} \right\rangle = \int_{-\infty}^{+\infty} dx \psi^*(x,t) \hat{A}\, \psi(x,t) \qquad (5)$$

- For non-relativistic entities, the wave function is a solution to the time dependent ***Schrödinger Equation***

$$i\hbar\frac{\partial}{\partial t}\psi(x,t)=\hat{H}\,\psi(x,t) \qquad (6)$$

where $\hat{H}=\hat{K}+\hat{V}$ is the Hamiltonian total energy operator, a sum of kinetic and potential energy operators.

- For stationary states, the wave function is solution to an **eigen-value problem** involving the time-independent ***Schrödinger Equation***

$$i\hbar\frac{\partial}{\partial t}\psi(x,t)=\hat{H}\,\psi(x,t)\equiv E\,\psi(x,t) \qquad (7)$$

where E is the total energy **eigen-value**, the energy of the state of the system described by the wave function $\psi(x,t)$.

- For independent degrees of freedom, *x, y, z,* the corresponding wave function factorizes,

$$\Psi(\vec{r},t)=\psi(x,t)\cdot\phi(y,t)\cdot\varphi(z,t) \qquad (8)$$

into a product of independent wave functions, one for every degree of freedom.

- Operators for systems that evolve along independent degrees of freedom are sums of individual operators

$$\hat{A}(\vec{r})=\hat{A}_x+\hat{A}_y+\hat{A}_z \qquad (9)$$

each one of which operates only on one degree of freedom.

For example, the momentum operator for a particle in a three-dimensional system can be written as,

$$\hat{p} = \frac{\hbar}{i}\vec{\nabla} = \frac{\hbar}{i}\begin{pmatrix} \frac{\partial}{\partial x} \\ \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} \end{pmatrix} = \hat{p}_x + \hat{p}_y + \hat{p}_z \tag{10}$$

Correspondingly, the Hamilton operator is represented by

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta = -\frac{\hbar^2}{2m}\left\{\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right\} \tag{11}$$

- operatorsstationary states, the wave function is solution to an eigen-value problem involving the time-independent ***Schrö-dinger Equation***

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}\,\psi(x,t) \equiv E\,\psi(x,t) \tag{12}$$

Possible scenario:

Free particle, spatially not localized → traveling wave
Bound particle, spatially localized → standing wave