

## Wave-particle duality

In classical mechanics a state of a physical system is described using position and momentum. Microscopically we consider a system of particles. If we know the position and velocity of each particle at time  $t$  then we can, in principle, determine their positions and momenta at any other time. The answer comes from Newton's second law of motion:

$$\vec{F}_i = m_i \frac{d^2 \vec{r}_i}{dt^2},$$

where  $\vec{F}_i$  is the force that acts on particle  $i$ .

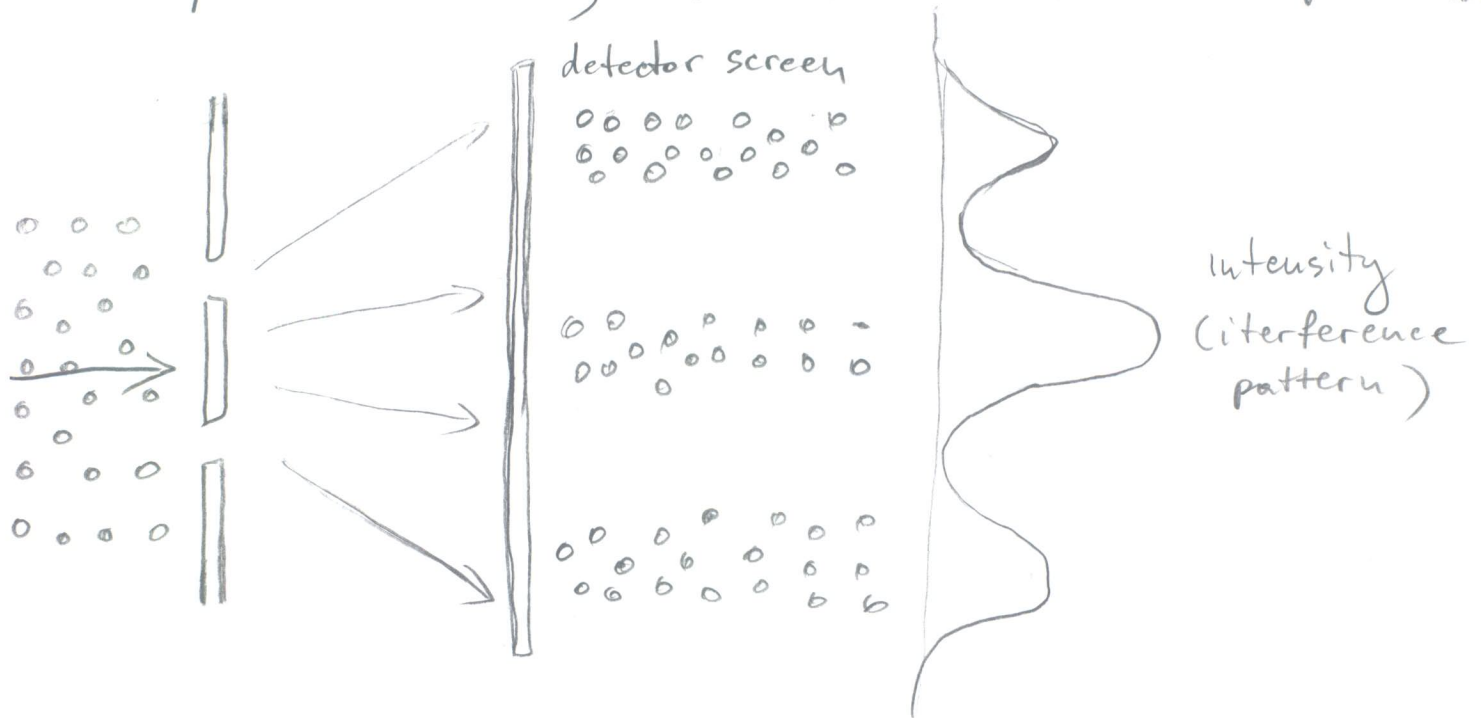
In quantum mechanics we ask the same question - what is the mechanical state of the system at time  $t$  - but the answer is tricky because position and momentum are not the right variables to describe the system.

Numerous experiments performed at the microscopic level (say at the level of atoms) have shown that quantum particles - electrons, protons, neutrons, photons, etc. do not just exhibit the properties of particles as we know it. They also behave as waves under certain circumstances. So in a way neither the concept of a particle, nor the concept of a wave separately can fully describe the behavior of quantum scale objects. However, together they can. This fact is referred to as the wave-particle duality.

Louis de Broglie postulated that not only light but also matter as we know it exhibit wave-particle duality. Interestingly enough, de Broglie's idea was not really based on experimental evidence, rather it stemmed from considerations inspired by Einstein's theory of relativity. The experimental evidence followed soon, however.

$$E = h\nu = \hbar\omega \quad \vec{p} = \hbar\vec{k} \quad \text{or} \quad p = \frac{h}{\lambda}$$

One of the most well known demonstrations of wave-particle duality is the double slit experiment



In this experiment electrons (protons, photons, etc.) are shot one at a time all over the screen with two parallel slits. The second (detector) screen registers where the electrons end up. What is observed in this experiment is the interference pattern yet on the detector screen each electron arrives as a particle.

# The Schrödinger equation

In quantum mechanics the object that describes the state of the system is the wave function (sometimes the terms state vector or ket are used). It is a function of both position and time:

$$\Psi = \Psi(x, t)$$

The number of coordinates corresponds to the number of degrees of freedom. For example, for a motion of a single quantum particle in 3D we would have  $\Psi(x, y, z, t)$ . On the other hand, if we deal with two particles constrained to move in a plane then the wave function depends on four spatial and one time variable:  $\Psi = \Psi(x_1, y_1, x_2, y_2, t)$

The wave function is obtained by solving the Schrödinger equation:

$$i\hbar \frac{\partial \Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi(x, t)}{\partial x^2} + V \Psi(x, t)$$

where  $\hbar$  is the Planck constant divided by  $2\pi$ ,  $m$  is the mass of the particle and  $V(x, t)$  is the potential.

The Schrödinger equation plays the role of Newton's second law in quantum mechanics. It describes the time evolution of the wave function. Given suitable initial conditions (say  $\Psi(x, 0)$ ) it allows, in principle, to determine  $\Psi$  at any given time.

Let us examine a few key properties of the Schrödinger equation.

- a) The Schrödinger equation (SE) is postulated, not derived. The existing "inspirations", e.g. based on opto-mechanics analogies cannot be treated as rigorous mathematical derivations.
- b) The wave function provides the most complete description that can be given to a physical system.
- c) The SE by itself does not say directly what exactly the wave function is, i.e. it does not provide any interpretation or assigns any physical meaning to the wave function.
- d) The SE is a partial differential equation, 1st order in time and 2nd order in spatial coordinates.
- e) To find a solution of the SE (assuming that  $V(x,t)$  is given) it is necessary to know the initial conditions (say  $\psi(x, t=0)$ ) and the boundary conditions (e.g.  $\psi \rightarrow 0$  when  $x \rightarrow \pm\infty$ )
- f) The SE is linear. That means the superposition principle holds — a sum of two solutions is also a solution.
- g) The SE admits wave-like solutions if  $V$  does not depend on time explicitly. Hence, it can describe waves and is called the wave equation.

Indeed if we assume  $V = V_0$  and put

$$\xi = x - vt \quad \text{or} \quad x = \xi + vt \quad (\text{here } v \text{ is a constant})$$

then we get

$$\frac{\partial}{\partial t} = \underbrace{\frac{\partial x}{\partial t}}_0 \frac{\partial}{\partial x} + \frac{\partial \xi}{\partial t} \frac{\partial}{\partial \xi} \Rightarrow \frac{\partial}{\partial t} = -v \frac{\partial}{\partial \xi}$$

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x} \frac{\partial}{\partial \xi} + \underbrace{\frac{\partial t}{\partial x}}_0 \frac{\partial}{\partial t} \Rightarrow \frac{\partial}{\partial x} = \frac{\partial}{\partial \xi}$$

So the SE

$$i\hbar \frac{\partial \Psi}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V_0 \right) \Psi$$

is transformed into

$$-i\hbar v \Psi'_{\xi}(\xi) = -\frac{\hbar^2}{2m} \Psi''_{\xi\xi}(\xi) + V_0 \Psi(\xi)$$

The latter equation depends only on  $\xi$ , not on  $x$  or  $t$  individually. Thus, one can indeed find wave-like solutions. They wind up looking like  $e^{ik\xi}$

h)  $\Psi$  is in general a complex function. By itself it cannot represent a physically measurable quantity. It should be emphasized that the complex nature of  $\Psi$  is fundamental, it is not merely a matter of mathematical convenience such as in the case of Maxwell's equations where we sometimes look for complex electric and magnetic fields knowing that the actual solution is obtained by taking the real (or complex) part of  $\vec{E}$  or  $\vec{B}$  that we find.

# The statistical interpretation of the wave function

The interpretation of the wave function was provided by Max Born. He argued that the absolute square of it

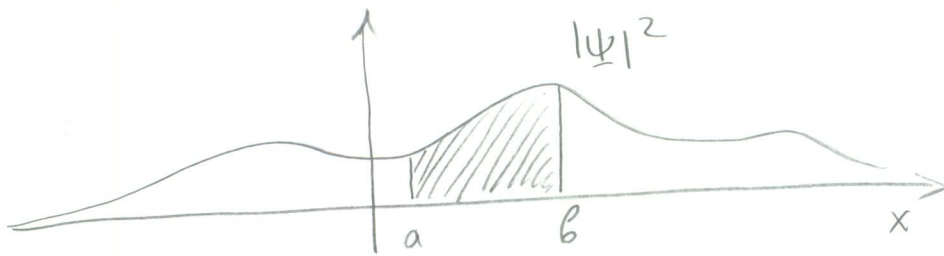
$$\Psi^*(x,t)\Psi(x,t) = |\Psi(x,t)|^2$$

represents the probability density, i.e. the probability per unit volume that a particle is found at the position  $x$  at the time  $t$ .

Here we should stress the difference between the classical mechanics and the quantum mechanics.

In the classical mechanics a particle has a definite position at any given moment of time. In quantum mechanics the particle no longer has a definite position at the time  $t$ . We can only define the probability of finding it at any particular region of space.

$$P(a < x < b, t) = \int_a^b |\Psi(x,t)|^2 dx$$



Hence at least in the Born interpretation of quantum mechanics there is inherent indeterminacy. We do not know exactly where the particle is. While this fact has caused a lot of discomfort it nevertheless does not affect our ability to do calculations and correctly predict the experiment.

One of the important points in quantum theory is

the fact that it is impossible to do a measurement of a system without altering its state. The usual interpretation is that the wave function collapses (or gets projected) upon the measurement. If a repeated and exactly the same measurement is made the outcome of the measurement is the same because the state (i.e. the wave function) has already been projected onto a particular eigenstate corresponding to the measured value.

Since the probability of finding a particle anywhere must be 1 (or 100%) the wave function must obey the normalization condition, namely

$$\int_{-\infty}^{+\infty} |\Psi(x,t)|^2 dx = 1$$

Here the integration is over all accessible space. If the particle is constrained to move within a certain region, say  $A \leq x \leq B$ , then the  $(-\infty, +\infty)$  integration interval would need to be replaced with  $(A, B)$ , i.e.

$$\int_A^B |\Psi(x,t)|^2 dx = 1$$

If we deal with a particle moving in multiple dimensions (say in 3D) the integration must be over the entire accessible multidimensional space:

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\Psi(x,y,z,t)|^2 dx dy dz = 1$$

If we deal with multiple particles the integration is extended to all degrees of freedom, e.g. for

two particles we have

$$\int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} |\Psi(x_1, y_1, z_1, x_2, y_2, z_2, t)|^2 dx_1 dy_1 dz_1 dx_2 dy_2 dz_2 = 1$$

To shorten the notation we will often write it as

$$\int_{-\infty}^{+\infty} |\Psi(\vec{r}_1, \vec{r}_2, t)|^2 d\vec{r}_1 d\vec{r}_2$$

or  $\int_{-\infty}^{+\infty} |\Psi|^2 d\tau$  where  $\tau$  denotes the volume

of the multidimensional space we work with.

In the beginning of the lecture we have written the Schrödinger equation in 1D. The generalization for 3D case is obvious:

$$i\hbar \frac{\partial \Psi(\vec{r}, t)}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi(\vec{r}, t) + V(\vec{r}, t) \Psi(\vec{r}, t)$$

Similarly if we have several particles in a system the Schrödinger equation becomes

$$i\hbar \frac{\partial \Psi(\vec{r}_1, \dots, \vec{r}_n, t)}{\partial t} = \left[ -\frac{\hbar^2}{2m} (\nabla_{\vec{r}_1}^2 + \nabla_{\vec{r}_2}^2 + \dots + \nabla_{\vec{r}_n}^2) + V(\vec{r}_1, \dots, \vec{r}_n, t) \right] \Psi(\vec{r}_1, \dots, \vec{r}_n, t)$$

In the end let us show that the wave function stays normalized at any moment of time, not just at any given instant (say at  $t=0$ ). In other words we want to show that  $P(-\infty < x < +\infty, t)$  is 1 for

any  $t$ .

$$\text{If } P(t) = \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx \quad \text{then} \quad \frac{dP}{dt} = \frac{d}{dt} \int_{-\infty}^{+\infty} |\Psi(x, t)|^2 dx =$$
$$= \int_{-\infty}^{+\infty} \frac{\partial}{\partial t} |\Psi(x, t)|^2 dx$$



Note that

$$\frac{\partial |\Psi|^2}{\partial t} = \frac{\partial \Psi^* \Psi}{\partial t} = \Psi^* \frac{\partial \Psi}{\partial t} + \frac{\partial \Psi^*}{\partial t} \cdot \Psi$$

From the Schrödinger equation we also have

$$\frac{\partial \Psi}{\partial t} = \frac{i\hbar}{2m} \frac{\partial^2 \Psi}{\partial x^2} - \frac{i}{\hbar} V \Psi \Rightarrow \frac{\partial \Psi^*}{\partial t} = -\frac{i\hbar}{2m} \frac{\partial^2 \Psi^*}{\partial x^2} + \frac{i}{\hbar} V \Psi^*$$

(here we assumed that  $V$  is real), Then

$$\frac{\partial |\Psi|^2}{\partial t} = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial^2 \Psi}{\partial x^2} - \frac{\partial^2 \Psi^*}{\partial x^2} \Psi \right) = \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right]$$

and, finally,

$$\frac{dP}{dt} = \int_{-\infty}^{+\infty} \frac{\partial}{\partial x} \left[ \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \right] dx = \frac{i\hbar}{2m} \left( \Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x} \Psi \right) \Big|_{-\infty}^{+\infty}$$

$\Psi(x,t)$  and  $\Psi^*(x,t)$  must vanish at  $x \rightarrow \pm\infty$ , otherwise the area under the curve would be infinite and the wave function would not be normalizable at all. Hence

$$\frac{dP}{dt} = 0 \quad \text{and} \quad P = \text{const} = 1$$