Quantum Mechanics

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Wave Mechanics

- ✓ We study the properties of the wave function !

  - ✓ In classical physics the wave function was apparently a wave in space which could be visualized, at least to a certain extent.

  - ✓ In QM, the wave function is not an objectively real entity, the wave function does not represent waves occurring in some material substance.

  - ✓ The wave mechanics offers a fairly direct route to some of the more important features of quantum mechanics !

The Probability Interpretation of the Wave Function

$|\Psi(x,t)|^2\,\delta x$ = Probability of observing the particle in the small region **$(x, x + \delta x)$** at time **t** !

$\Psi(x,t)$ → Probability amplitude

- ✓ **What this interpretation means in a practical sense ?**

  - ✓ Can be arrived at in a number of ways !

- ➢ The conventional one uses the notion of 'Ensemble of identically prepared systems' !

Probability amplitude

Ensamble

✓ The collection of identical copies of the same system all prepared in the same fashion is known as an ensemble.

➢ We then assume that, at time **t** after the start of the preparation procedure, the state of each particle will be given by the same wave function **ψ(x, t).**

Example: a simple system, consisting of just one particle !

✓ Now suppose we measure the position of the particle for such an ensamble !

➢ Invariably we will find that we get different results for the measurement of position, though each run of the experiment is supposedly identical to every other run. Moreover, the results vary in a random fashion.

Probability amplitude

- ❖ The manner in which the measured values of position are scattered is determined by the wave function $\psi(x,t)$!

- ❖ The scatter of values are quantified by the probability distribution

$$P(x, t) = |\psi(x, t)|^2$$

What do we get from P(x,t) ?

✓ It does not give the chances of a particle being observed at a precise position **x !**

✓ We can measure whether the particle position lies in an interval δx or not in each run of the experiment .

✓ If we do the experiment N times, we can count up the number of particles for which the value of x lies in the range $(x, \ x + \delta x)$. Call this number **$\delta N(x)$**.

$\delta N/N$ => probability of observing the particle in the mentioned region.

If N is made large, then $\frac{\delta N}{N} \approx P(x, t)\, \delta x$ and $\frac{\delta N}{N \delta x} \approx P(x, t)$

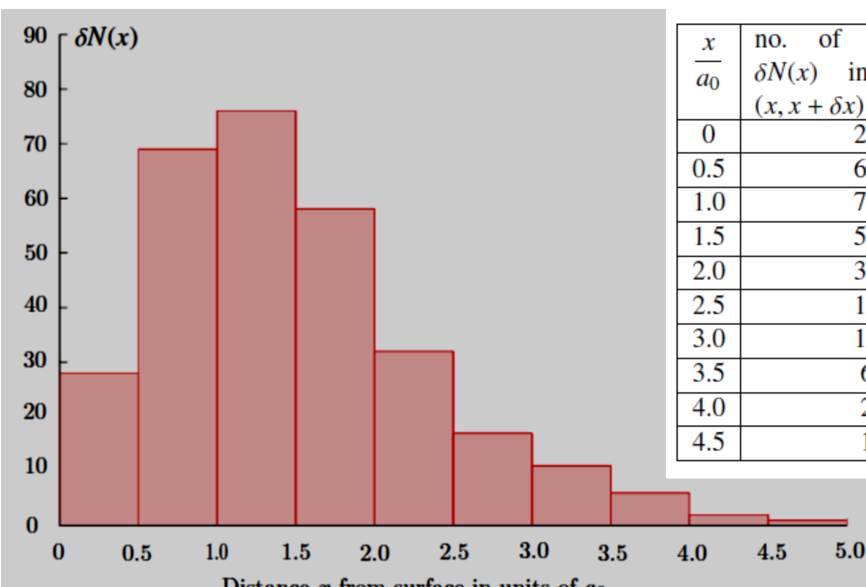
An example

An electron placed in the region x > 0 adjacent to the surface of liquid helium is attracted to the surface by its oppositely charged 'image' inside the surface. However, the electron cannot penetrate the surface (it is an infinitely high potential barrier). The wave function for the electron, in its lowest energy state, can be shown to be given by

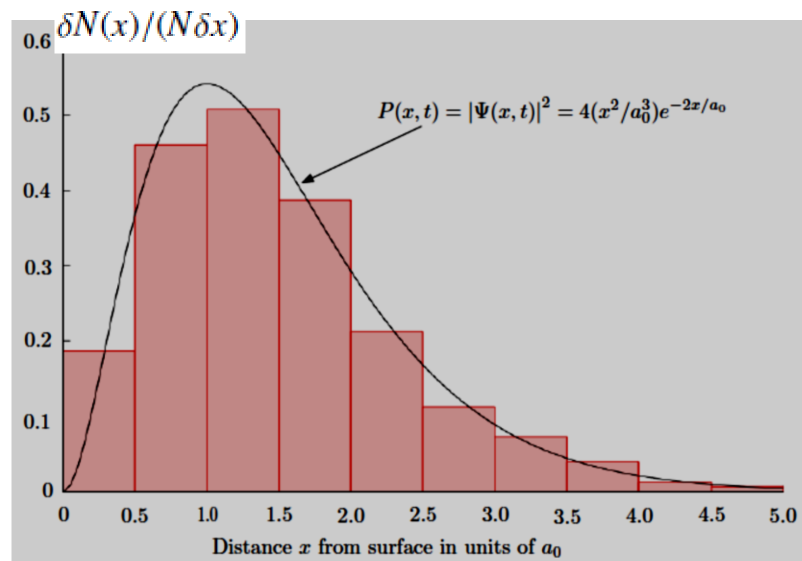
$$\Psi(x,t) = 2\, a_0^{-1/2}\, (x/a_0)\, e^{-\frac{x}{a_0}}\, e^{i\omega t} \quad \text{for} \quad x > 0$$

$$= 0 \quad \text{for} \quad x < 0$$

An experiment is conducted with the aim of measuring the distance of the electron from the surface. Suppose x can be measured with an accuracy $\pm\, a_0/4$.



$\frac{x}{a_0}$	no. of detections $\delta N(x)$ in interval $(x, x+\delta x)$
0	28
0.5	69
1.0	76
1.5	58
2.0	32
2.5	17
3.0	11
3.5	6
4.0	2
4.5	1



Normalization

- ✓ The probability interpretation given above tells us the probability of finding the particle in **a small interval δx**.

- ✓ We can calculate the probability of finding the particle in a finite range by dividing this range into segments of size x and simply adding together the contributions from each such segment.

- ✓ Hence, the probability of finding the particle in a finite range $a < x < b$, will be given by the integral $\int_a^b |\psi(x,t)|^2 \, dx$

- ✓ From this it immediately follows that the probability of finding the particle somewhere in the range $-\propto < x < \propto$ must be unity.

- ✓ After all, the particle is guaranteed to be found somewhere. Mathematically, this can be stated as $\int_{-\propto}^{\propto} |\psi(x,t)|^2 \, dx = 1$.

The wave function is said to be 'normalized to unity'.

Time dependent Schroedinger Equation

It is not possible to derive the Schroedinger equation !

✓ The experimental evidence discussed earlier suggests that it ought to have the properties like:

Linearity :

If $\psi_1(x, t)$ and $\psi_2(x, t)$ are solutions, then $b_1\,\psi_1(x, t) + b_2\,\psi_2(x, t)$ must also be a solution for any choice of the constants b_1 and b_2.

Dispersion relation:

For a free particle , the wave function $e^{i(k\,x - \omega\,t)}$ ought to be a solution of the Schroedinger equation if and only if $\frac{\hbar^2 k^2}{2m} = \hbar\omega \quad (\frac{P^2}{2m} = E)$.

This reasoning leads directly to the time-dependent Schroedinger equation for a free particle: $\frac{-\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = i\,\hbar\,\frac{\partial\psi}{\partial t}$

For particles moving through a potential $V(x)$

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

Time independent Schroedinger Equation

✓ The time-dependent Schrödinger equation tells you ψ (x, t) if you know ψ(x, 0).

➢ It is an equation of motion and does not say anything (directly) about quantisation or energy levels.

✓ The equation is satisfied by any wave function of the form

$$\psi(x,t) = \sum_n A_n\, e^{i(k_n x - \omega_n t)}$$

Contains various angular frequencies, it cannot have a precise energy.

✓ The energy may take any of the values $E_n = \hbar\omega_n$, for which $|A_n|^2 \neq 0$

A wave function with a precise energy, often known as an energy eigenfunction, is any solution of the time-dependent Schroedinger equation involving only a single angular frequency: $\psi(x,t) = e^{i(kx - \omega t)}$ **, the only possible energy is** $\hbar\omega$

A single-frequency trial solution of the form $\psi(x,t) = \phi(x)e^{i\omega t}$ ⇨

$$-\frac{\hbar^2}{2m}\frac{\partial^2\phi}{\partial x^2} + V\phi = E\phi$$

The time independent Schrödinger equation

Probability current

- ✓ A quantum particle such as an electron produces electric current because of its motion.

Associated with the flow of its probability

- ✓ The form of the **wave function** that describes the state of a particle determines these currents.

- ✓ Using the definition of probability density $\rho = |\psi|^2$

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial t}|\psi|^2 = \frac{\partial \psi}{\partial t}\psi^* + \frac{\partial \psi^*}{\partial t}\psi$$

From time dependent Schroedinger equation

$$\frac{\partial \rho}{\partial t} = \frac{i\hbar}{2m}\left(\psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2}\right)$$

$$= -\frac{i\hbar}{2m}\frac{\partial}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

Conservation equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$$

$$j = -\frac{i\hbar}{2m}\left(\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x}\right)$$

probability current

The rate of change of total probability P(t) of finding the particle inside a volume V is equal to the total flux of j through the boundary S.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} = 0$$

In 3D

Expectation value

✓ $|\psi(x,t)|^2$ is a normalized probability density for the particle to be found in some region in space, it can be used to calculate various statistical properties of the position of the particle.

In order to understand it better, we will make use again the **'ensemble of identically prepared systems'**

✓ The number of particles with position in the range **x** to **x + δx** => $\delta N(x)$

✓ The fraction of particles that are observed to lie in this range will then be $\delta N/N$

✓ The mean or average value of all these results $\bar{x}(t) = \sum_{All\ \delta x} x \frac{\delta N}{N}$

✓ This mean will be an approximation to the mean value that would be found if the experiment were repeated an infinite number of times !

In the limit $\delta x \to 0$, $\langle x(t) \rangle = \int_{-\infty}^{\infty} x\, P(x,t)\, dx = \int_{-\infty}^{\infty} x\, |\psi(x,t)|^2\, dx$

Expectation value of x

$$\langle f(x) \rangle = \int_{-\infty}^{\infty} f(x)\, |\psi(x,t)|^2\, dx$$

For any function f(x)

Example

- ✓ We can use the data from the previous example of liquid helium (slide 5) and calculate the average value of the distance of the electron from the surface of the liquid helium !

$\frac{x}{a_0}$	no. of detections $\delta N(x)$ in interval $(x, x+\delta x)$
0	28
0.5	69
1.0	76
1.5	58
2.0	32
2.5	17
3.0	11
3.5	6
4.0	2
4.5	1

$$< x > \approx \bar{x} = 0\,\frac{28}{300} + 0.5\,a_0\,\frac{69}{300} + a_0\,\frac{76}{300} + 1.5\,a_0\,\frac{58}{300} + 2\,a_0\,\frac{32}{300} + 2.5\,a_0\,\frac{17}{300} + 3\,a_0\,\frac{11}{300} + 3.5\,a_0\,\frac{6}{300} + 4\,a_0\,\frac{2}{300} + 4.5\,a_0\,\frac{1}{300} = 1.24\,a_0$$

- ✓ The results can be compared with that follows for the expectation value calculated from the wave function for the particle:

$$\Psi(x,t) = 2\,a_0^{-1/2}\,(x/a_0)\,e^{-\frac{x}{a_0}}\,e^{i\omega t} \quad \text{for} \quad x > 0$$

$$= 0 \quad \text{for} \quad x < 0$$

$$< x > = \int_{-\infty}^{\infty} x\,|\psi(x,t)|^2\,dx = 1.5\,a_0$$

Calculation of Δx

✓ We can calculate the uncertainty in the position of the particle !

- The uncertainty is a measure of how widely the results of the measurement of the position of the electron are spread around the mean value.

- As is the case in the analysis of statistical data, this is done in terms of the usual statistical quantity, the standard deviation, written σ_x .

Now, $\overline{(\Delta x)^2} \approx \sum_{\text{all } \delta x} (x - \bar{x})^2 \frac{\delta N}{N}$

Average value obtained from the data

✓ In the limit of an infinite number of measurements, the uncertainty is

$$\sigma_x^2 = \langle (\Delta x)^2 \rangle = \langle (x - \langle x \rangle)^2 \rangle = \langle x^2 \rangle - \langle x \rangle^2$$

$1.24\ a_0$

✓ In our example, from the data $\sigma_x \approx 0.87\ a_0$

✓ From the theory we have $\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - 2.25\ {a_0}^2$

$\langle x^2 \rangle = \int_{-\infty}^{\infty} \psi^* x^2 \psi \, dx = 3\ {a_0}^2$

$\sigma_x = 0.87\ a_0$

Momentum expectation value

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt}$$

Slide 9

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

$$\frac{d}{dt}\int x|\psi|^2 dx = \int x \frac{\partial}{\partial t}|\psi|^2 dx = \frac{i\hbar}{2m}\int x \frac{\partial}{\partial x}\left[\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right] dx$$

Integrate by parts

$$= -\frac{i\hbar}{2m}\int_{-\infty}^{\infty} \frac{\partial x}{\partial x}\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right) dx + \frac{i\hbar}{2m}\, x\left(\psi^* \frac{\partial \psi}{\partial x} - \frac{\partial \psi^*}{\partial x}\psi\right)\Bigg|_{-\infty}^{\infty}$$

$\frac{\partial x}{\partial x} = 1$

$$\int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x}\psi\, dx = -\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx + \psi^*\psi\Big|_{-\infty}^{\infty}$$

$\psi^*\psi\Big|_{-\infty}^{\infty} = 0$

= 0, since $\psi(\pm\infty) = 0$

$$= -\frac{i\hbar}{m}\int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$$

Our final result: $\langle p \rangle = m \frac{d\langle x \rangle}{dt} = -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \psi}{\partial x} dx$

$$\langle p \rangle = \int \psi^* \left(-i\hbar \frac{\partial}{\partial x}\right)\psi\, dx$$

Variable p -> $-i\hbar \frac{\partial}{\partial x}$