Schrödinger's wave equation?

The Schrödinger's aquation is
a very useful relation.

It solves many problems for quantum mechanical particles that have mass, such as electrons moving much slower than the velocity of light but behaving like waves.

emilio.scalise@unimib.it

Electrons as waves

de Broglie model: electron wavelength is given by

$$\lambda = \frac{h}{p}$$

With *p* the electron moment and the Planck's constant

$$h = 6.62606957 \times 10^{-34}\, J\, s$$

emilio.scalise@unimib.it

Electrons as waves

Helmholtz wave equation

$$\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + k^2\psi = 0 \qquad \text{with} \qquad k = \frac{2\pi}{\lambda}$$

This is working for simple (monochromatic) waves, and has solutions like:

$$\mathrm{e}^{\mathrm{i}kx}, \mathrm{e}^{-\mathrm{i}kx}, \cos(kx), \sin(kx)$$

emilio.scalise@unimib.it

Helmholtz wave equation in 3D

$$\nabla^2\psi \equiv \frac{\delta^2\psi}{\delta x^2} + \frac{\delta^2\psi}{\delta y^2} + \frac{\delta^2\psi}{\delta z^2} = -k^2\psi$$

and has solutions like:

$$\mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}, \cos(\boldsymbol{k}\cdot\boldsymbol{r}), \sin \boldsymbol{k}\cdot\boldsymbol{r})$$

$\boldsymbol{k}$ and $\boldsymbol{r}$ are vectors

emilio.scalise@unimib.it

From Helmholtz to Schrödinger

de Broglie model:

$$\lambda = \frac{h}{p}$$

definition:

$$k = \frac{2\pi}{\lambda}$$

Then: $$k = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

We can rewrite the Helmholtz equation

$$\nabla^2 \psi = -\frac{p^2}{\hbar^2}\psi$$

or

$$-\hbar^2 \, \nabla^2 \psi = p^2 \psi$$

emilio.scalise@unimib.it

From Helmholtz to Schrödinger

We can divide both ides by he mass

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \underbrace{\frac{p^2}{2m}}_{\text{Kinetic Energy}}\psi$$

In general:

$$E_{TOT} = E_{kin} + V(\boldsymbol{r})$$

emilio.scalise@unimib.it

From Helmholtz to Schrödinger

So:

$$E_{kin} = \frac{p^2}{2m} = E_{TOT} - V(\boldsymbol{r})$$

Helmholtz wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = \frac{p^2}{2m}\psi$$

becomes:

Schrödinger wave equation

$$-\frac{\hbar^2}{2m}\nabla^2\psi = (E - V(\boldsymbol{r}))\psi$$

emilio.scalise@unimib.it

Schrödinger's time independent equation

$$E\,\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(\boldsymbol{r})\right)\psi$$

emilio.scalise@unimib.it

Born's postulate

The probability P(**r**) of finding an electron near any specific point **r is proportional to the modulus squared**

$|\psi(\mathbf{r})|^2$ of the wavefunction $\psi(\mathbf{r})$

$$|\psi(\mathbf{r})|^2$$

is the "probability density"

emilio.scalise@unimib.it

Born's postulate

$|\psi(\mathbf{r})|^2$ is the "probability density"

For some very small (infinitesimal) volume $d^3\mathbf{r}$ around $\mathbf{r}$, the probability of finding the particle in that volume is

$$P(\mathbf{r})d^3\mathbf{r} \propto |\psi(\mathbf{r})|^2 d^3\mathbf{r}$$

The sum of such probabilities should equal to 1, i.e.,

$$\int P(\mathbf{r})d^3\mathbf{r} = 1$$

emilio.scalise@unimib.it

Normalization of the wfc

In general, solving the Schrödinger's equation will give some ψ for which $\int |\psi(\mathbf{r})|^2 d^3\mathbf{r} \neq 1$.

We will have to normalize the wfc. If we have that:

$$\int |\psi(\mathbf{r})|^2 d^3\mathbf{r} = \frac{1}{|a|^2}$$

Then we can multiply the wfc by a constant, obtaining the normalized wfc: $\psi_N = a\psi$

And now: $\int |\psi_N(\mathbf{r})|^2 d^3\mathbf{r} = 1$

emilio.scalise@unimib.it

Normalization of the wfc

Then we can multiply the wfc by a constant, obtaining the normalized wfc: $\psi_N = a\psi$

And now: $\int \left|\psi_N(\mathbf{r})\right|^2 d^3\mathbf{r} = 1$

The normalized wfc solve the problem of correspondence between probability density and modulus squared of the wfc, and it will still be a solution of the SE due to its **linearity**.

emilio.scalise@unimib.it

Linearity of quantum mechanics

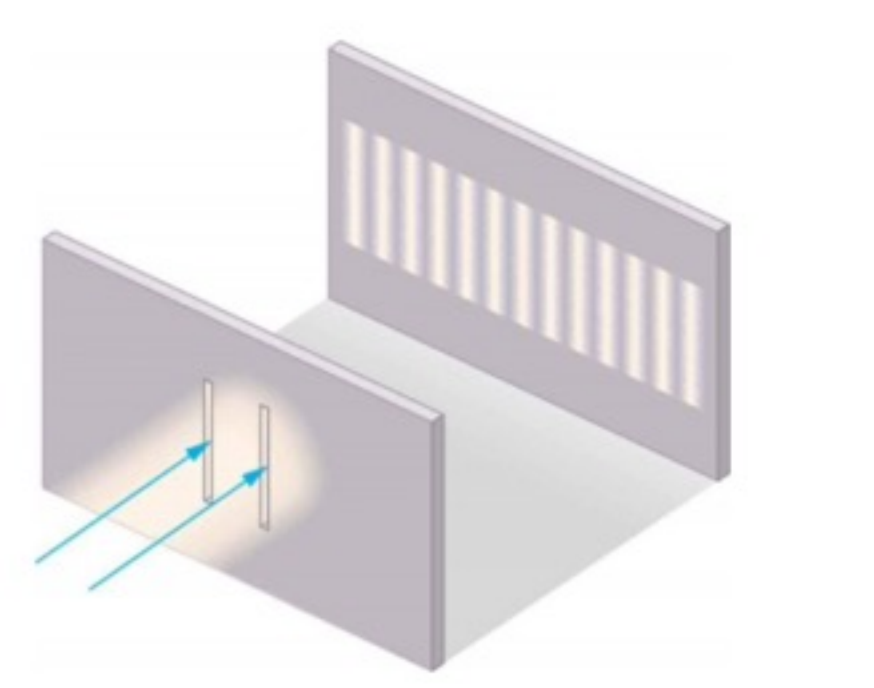
In Schrödinger's equation we could multiply both sides of the equation by a **constant** and the equation would still hold.

If ψ is a solution of Schrödinger's equation, also $a\,\psi$
Will solve the same equation because
Schrödinger's equation is linear

emilio.scalise@unimib.it

Diffraction by two slits

This is a key experiment that probed the wave behavior of light. The experiment in optics is known as Young's slits, after Thomas Young performed it in the very early 1800s



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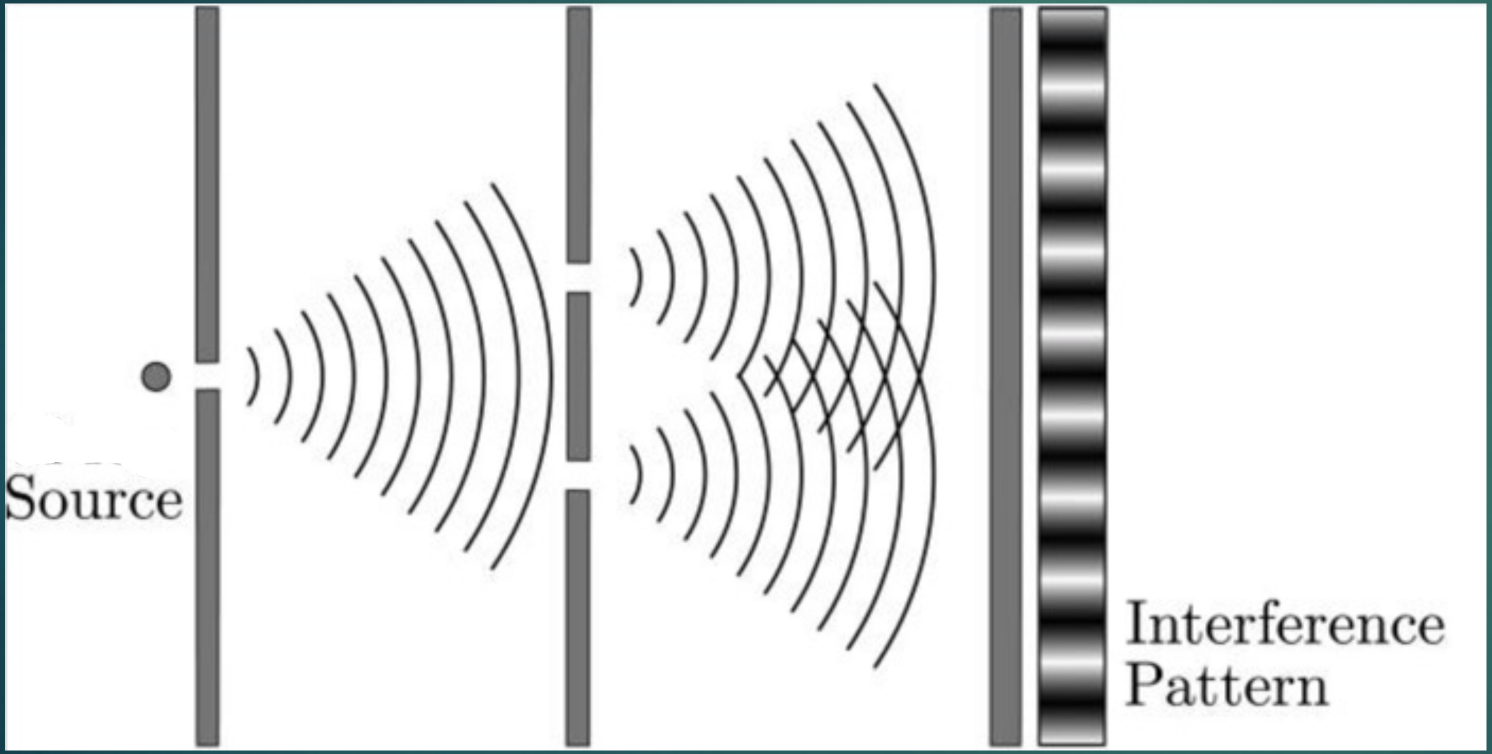
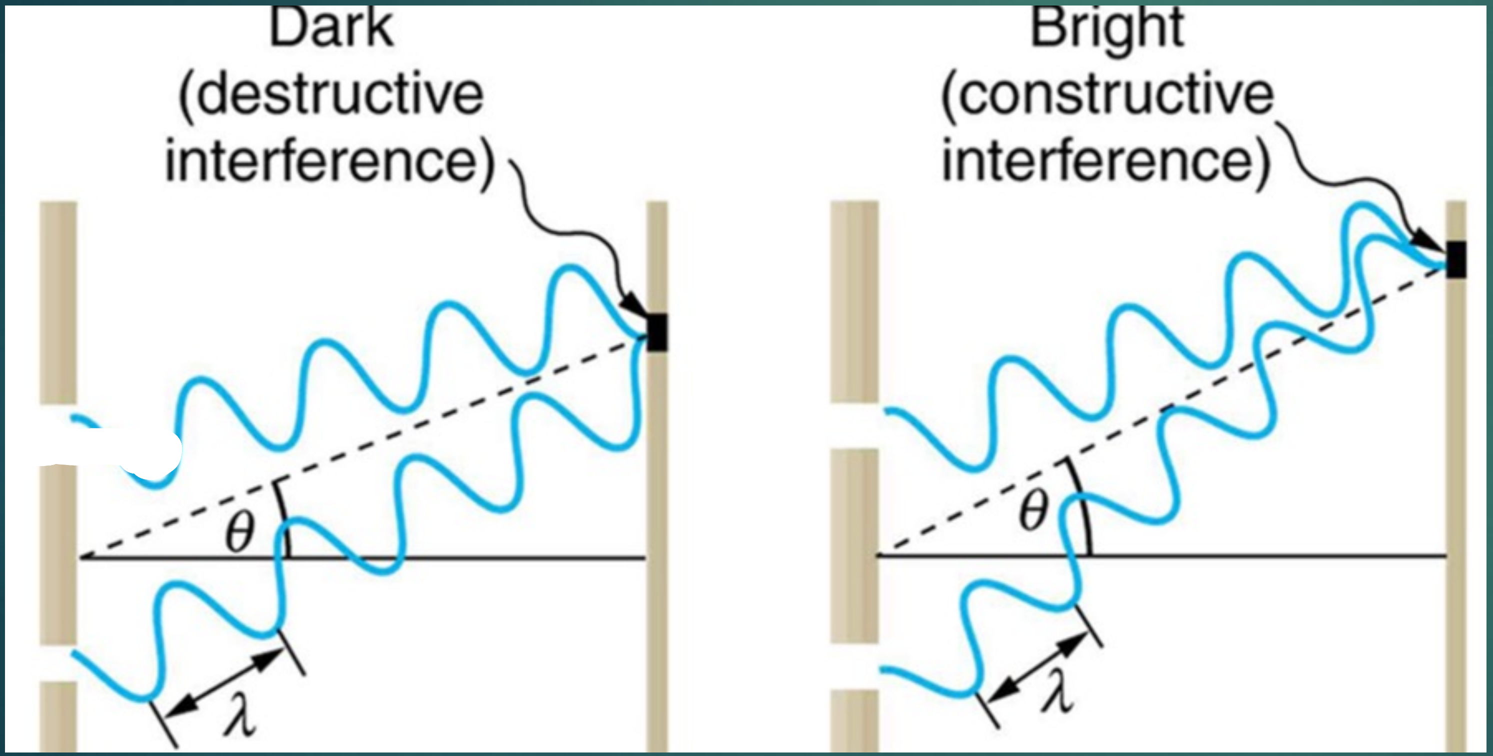
Diffraction by two slits



(bright spots: Interference Fringes)

emilio.scalise@unimib.it

Diffraction by two slits



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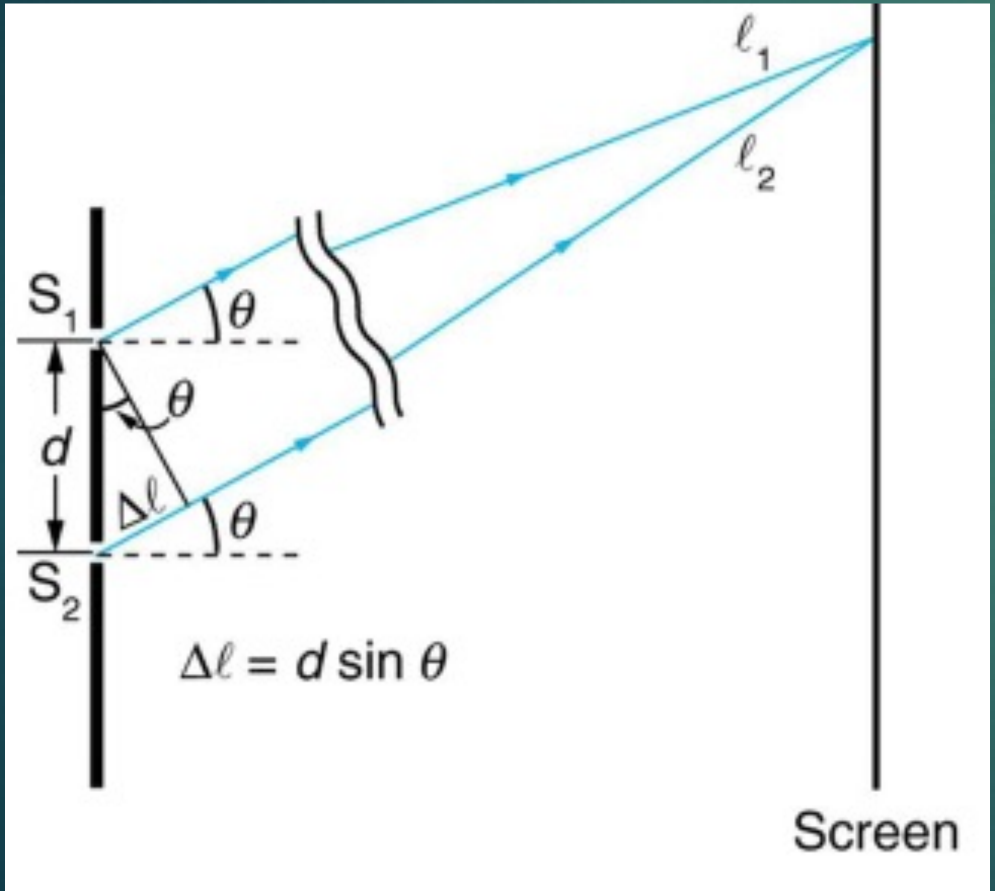
Diffraction by two slits



Constructive interference

$d \sin\theta = m\lambda$, for m = 0, 1, −1, 2, −2, . . .)

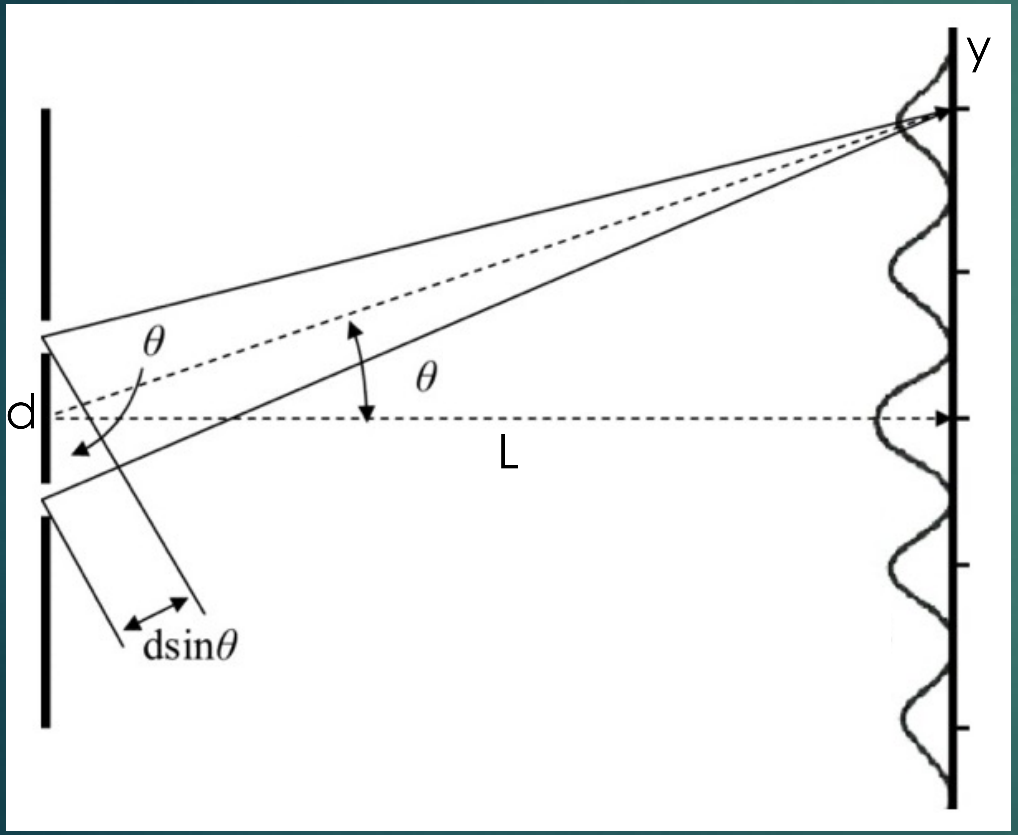
Destructive interference

d sinθ=(m+1/2)λ, for m=0,1,−1,2,−2,…

emilio.scalise@unimib.it

Diffraction by two slits

It enables us to measure the small wavelength!



Constructive interference

$$d \sin\theta = m\lambda$$

But: $\tan\theta = \frac{\Delta y}{L}$

and for small angle $\tan\theta = \sin\theta$

Thus: $y_m = L\,\frac{m\,\lambda}{d}$

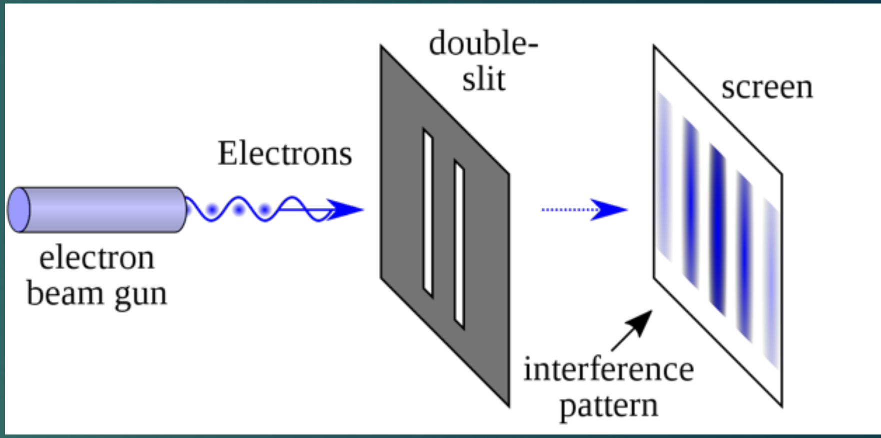
The distance between adjacent fringes is: $\Delta y = \frac{L\,\lambda}{d}$

emilio.scalise@unimib.it

Diffraction by two slits

It is still working with electrons!

If instead of thinking about **light waves** incident on two slits we think about an **electron** wave incident on those same two slits, we have some apparent problems.



A particle has to go through one slit or the other. **Surely a particle can not go through two slits.**

Part of our difficulty here is that we 'pretend' to have definite position for the particle

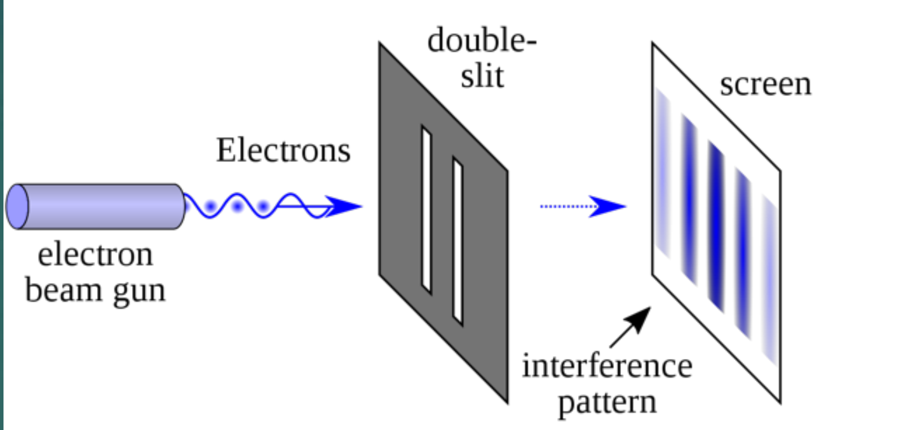
emilio.scalise@unimib.it

Diffraction by two slits

It is still working with electrons!

The quantum mechanical view of this is that the elctrons propagate as a **wave**… The act of hitting the screen causes a measurement of position to be made, according to Born's rule:

the wave function **collapses** into one with a definite position with a **probability** proportional to the modulus squared.



emilio.scalise@unimib.it