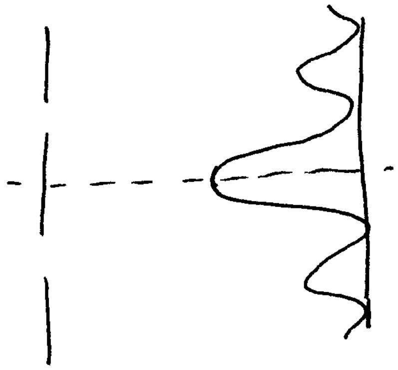
Chapter 2 Wave-particle duality and the SE (Schrödinger equation)

Old QM:

Concepts	Experiment
photons carry momentum and energy	Compton scattering
electrons carry momentum and energy (particles) + diffract	Davisson-Germer
angular momentum quantized (Bohr)	Stern-Gerlach
Correspondence principle:	classical results at $n \gg$

2-1 Diffraction and interference are not collective effects of many photons but are properties of each single photon

Classical two-slit experiment:



the interference pattern is observed even if photons are sent one by one

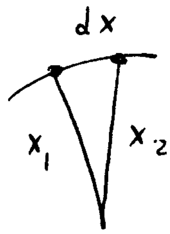
The resolution of the paradox is to assume that each photon interferes with itself

$$\underset{\substack{\uparrow \\ \text{electric} \\ \text{field of a} \\ \text{single photon}}}{\vec{e}(\vec{r},t)} = \underset{\substack{\uparrow \\ \text{electric} \\ \text{field from} \\ \text{slit 1}}}{\vec{e}_1(\vec{r},t)} + \underset{\substack{\uparrow \\ \text{electric} \\ \text{field from} \\ \text{slit 2}}}{\vec{e}_2(\vec{r},t)}$$

Two possible approaches to introduce "non-locality" to the particle world:

* make classical observables operators (Heisenberg)

  example: $\frac{d}{dx}$ is non local because derivative depends on two points



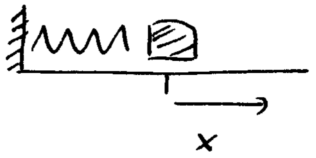
* describe state of particles with wave functions (Schrödinger)

  "wave mechanics"

One needs to formulate an equation for waves that will reproduce known "particle" properties.

Harmonic motion:

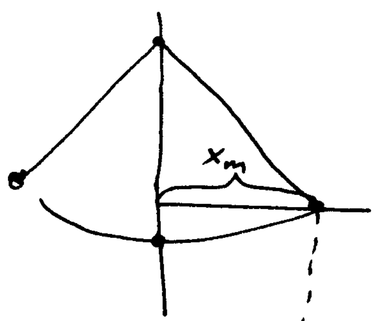
$$m\ddot{x} + kx^2 = 0$$

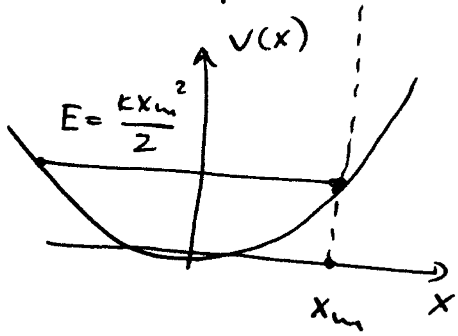


$$x(t) = x_m \cos(\omega t + \varphi)$$

amplitude (x_m), frequency (ω), phase (φ)

$$\omega = \sqrt{\frac{k}{m}}$$





at x_m: $K(x_m) = 0$

$$V(x_m) = \frac{kx_m^2}{2}$$

at $x = 0$: $K(0) = K_0 = K_{max}$

$$V(0) = 0$$

$$V(x) = \frac{kx^2}{2}$$

Equation of motion: $\underbrace{\frac{dp}{dt}}_{m\ddot{x}} = -\frac{\partial V(x)}{\partial x} = -kx$

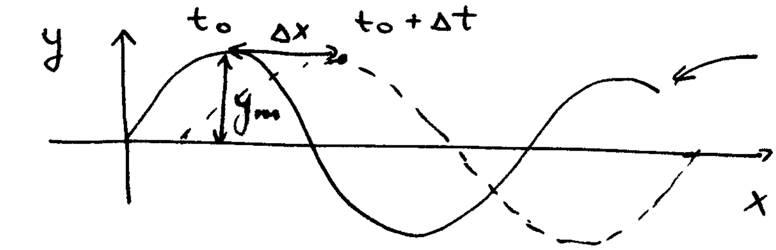
$$p = m\dot{x} = -m\omega x_m \sin(\omega t + \varphi)$$

Energy: $E = \frac{p^2}{2m} + \frac{kx^2}{2} =$

$$= \frac{kx_m^2}{2}\left[\cos^2(\omega t + \varphi) + \underbrace{\frac{m\omega^2}{k}}_{1}\sin^2(\omega t + \varphi)\right] = \frac{kx_m^2}{2}$$

Wave motion:

$y(x,t) \leftarrow$ displacement



traveling wave

Equation of wave motion:

$$\frac{1}{v^2}\frac{d^2 y(x,t)}{dt^2} = \frac{d^2 y(x,t)}{dx^2}, \quad \boxed{v = \frac{\Delta x}{\Delta t}}$$

velocity $\rightarrow v$

Solution:

wave vector, angular frequency

$$y(x,t) = \underbrace{y_m}_{\text{amplitude}} \sin(k\underset{\uparrow}{x}\ -\ \omega \underset{\nwarrow}{t})$$

position, time

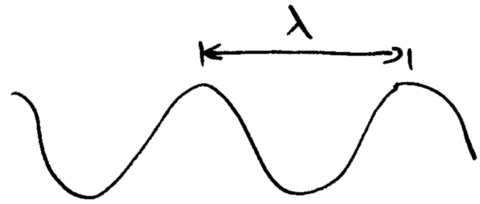
Substitute:

$$-\frac{\omega^2}{v^2} y_m \sin(kx-\omega t) = -y_m k^2 \sin(kx-\omega t)$$

$\omega = vk \leftarrow$ wave dispersion relation

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

$\uparrow$ wavelength



$\omega = 2\pi \nu \leftarrow$ frequency

Particle motion (Hamiltonian dynamics)

Energy of a particle

$$E = E(p,x) = \frac{p^2}{2m} + V(x)$$

kinetic energy   potential energy

$E(p,x) = H(p,x)$ ← Hamiltonian as a function of p and x variables

Equation of motion:

$$\dot{x} = \frac{\partial H(p,x)}{\partial p} = \frac{p}{m}, \quad p = m\dot{x} = m v$$

(definition of momentum

$$\dot{p} = -\frac{\partial H(p,x)}{\partial x} = -\frac{\partial V(x)}{\partial x}$$

(Newton's equation of motion

Example:

$$H(p,x) = \frac{p^2}{2m} + mgx$$

(particle in the gravitational field)

$$\dot{p} = m\ddot{x} = -\frac{\partial V(x)}{\partial x} = -mg$$

$$\dot{x} = \dot{x}_0 - gt$$

$$x(t) = x_0 + v_0 t - \frac{gt^2}{2}$$

Problem: construct equations to give Newton's law **and** interference in corresponding limits (Schrödinger)

2-2 Classical approach to wave/particle duality. Wave packets.

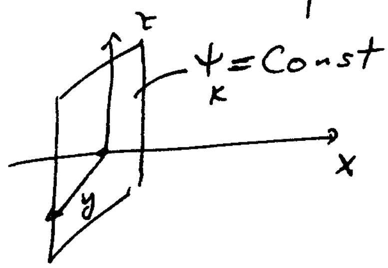
Harmonic wave: $\psi_k(x,t) = A\, e^{i(kx-\omega t)} + B\, e^{-i(kx-\omega t)}$

For light: $\omega = ck$ ← in vacuum

$\omega = \frac{c}{n} k$ ← in a medium

n: refractive index

Plane wave: amplitude constant in the y,z-plane



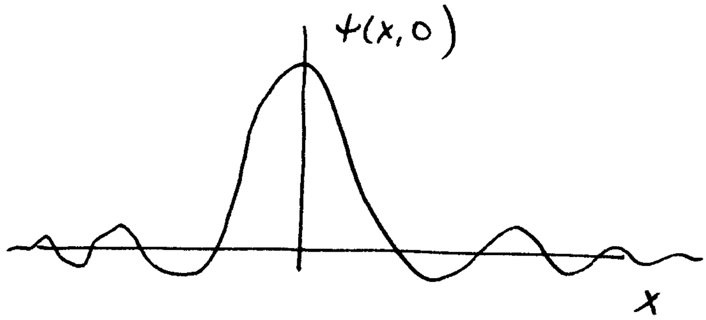
Wave packet: superposition of plane waves

$$\psi(x,t) = \int_{-\infty}^{\infty} dk\, \underline{\underline{A(k)}}\, e^{i(kx-\omega t)}$$

$A(k)$: amplitude as a function of wavevector

Gaussian packet: $A(k) = \exp\left[-\alpha(k-k_0)^2/2\right]$

$$\psi(x,0) = \sqrt{\frac{2\pi}{\alpha}}\, e^{ik_0 x - x^2/2\alpha}$$



$$\frac{|\psi(\Delta x, 0)|^2}{|\psi(0,0)|^2} = \frac{1}{e}, \qquad \Delta x = \sqrt{\alpha}$$

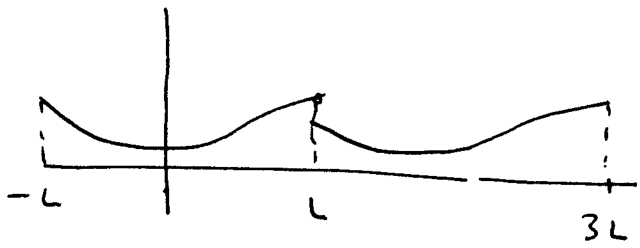
$$\frac{|A(\Delta k)|^2}{|A(0)|^2} = \frac{1}{e}, \qquad \Delta k = \frac{1}{\sqrt{\alpha}}$$

$$\boxed{\Delta x \, \Delta k \approx 1} \longleftarrow \text{independent of } \alpha$$

Fourier transformation

$$\psi(x,0) = \int_{-\infty}^{\infty} dk\, A(k) e^{ikx}$$ represents infinite-interval Fourier transformation

Fourier transformation applies to periodic functions, i.e. to functions satisfying periodically replicated boundary conditions



$$f(x) = f(x+2L)$$

function defined in the interval $(-L, L)$ can be periodically replicated

For any $x \in [-L, L]$

$$f(x) = \sum_{n=0}^{\infty} A_n \cos\frac{\pi n x}{L} + \sum_{n=1}^{\infty} B_n \sin\frac{\pi n x}{L}$$

Fourier series

<u>why $n=1$</u> ?

Complex exponents representation:

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{i\pi n x/L}$$

Orthonormality relation:

$$\frac{1}{2L}\int_{-L}^{L} dx\, e^{in\pi x/L} e^{-im\pi x/L} = \delta_{nm} = \begin{cases} 1, & m=n \\ 0, & m\neq n \end{cases}$$

Kronecker symbol

$$\int_{-L}^{L} e^{-\frac{i\pi n x}{L}} f(x)\,dx = \sum_{m=-\infty}^{\infty} a_m \int_{-L}^{L} e^{\frac{i\pi m x}{L} - \frac{i\pi n x}{L}} dx$$

$$= \sum_{m=-\infty}^{\infty} 2L\,\delta_{nm}\, a_m = 2L\, a_n$$

$$\boxed{a_n = \frac{1}{2L}\int_{-L}^{L} dx\, f(x)\, e^{-\frac{i\pi n x}{L}}}$$

From infinite sum to infinite integral:

$$f(x) = \sum_{n=-\infty}^{\infty} a_n e^{\frac{i\pi n x}{L}} \underset{\substack{\| \\ 1}}{\Delta n} = \frac{L}{\pi} \sum a_n e^{\frac{i\pi n x}{L}} \frac{\pi \Delta n}{L} =$$

$$= \sum \frac{A(k)}{\sqrt{2\pi}} \Delta k \, e^{ikx}, \quad \text{where} \quad k = \frac{\pi n}{L}$$

$$A(k) = \frac{L a_n}{\pi} \sqrt{2\pi}$$

In the limit $L \to \infty$, $\Delta k \to 0$ and one can replace the sum with an integral:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dx$$

$$A(k) = \sqrt{2\pi} \frac{L}{\pi} \frac{1}{2L} \int_{-L}^{L} f(x) e^{-\frac{i\pi n x}{L}} dx$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx} f(x) \, dx$$

<u>Integral Fourier transformation</u>:

$$\boxed{f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} A(k) e^{ikx} dk, \quad A(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx}$$

Dirac delta function

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{+ikx} \int_{-\infty}^{\infty} dy\, f(y)\, e^{-iky}$$

$$= \int_{-\infty}^{\infty} dy\, f(y) \left[\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(x-y)}\, dk \right]$$

same function !

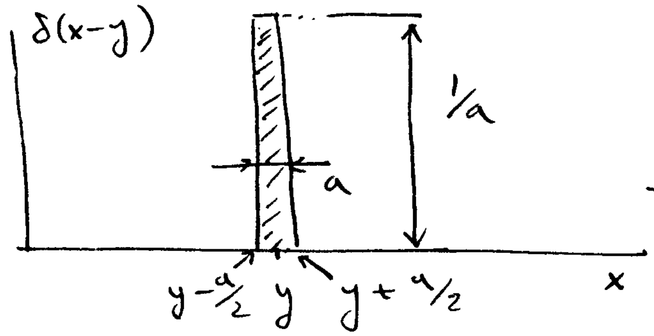
what is this ?

$$\boxed{\delta(x-y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk\, e^{ik(x-y)}}$$

← Dirac delta function

Definition :

$$\delta(x-y) = \begin{cases} \frac{1}{a}, & |x-y| \le \frac{a}{2} \\ 0, & |x-y| > \frac{a}{2} \end{cases}$$



$$\int_{-\infty}^{\infty} \delta(x-y)\, dx = 1$$

↑ area

Dirac function acts to pin-point a given value :

$$f(a) = \int \delta(x-a)\, f(x)\, dx$$

See Suppl. 2A, eq (2A-16) − (2A-32) for more mathematical properties

Movement of a wave packet

One needs to know the dispersion relation,

$\omega = \omega(k)$:

$$\omega(k) = \omega(k_0) + (k-k_0)\left(\frac{\partial\omega}{\partial k}\right)_{k_0} - \frac{1}{2}(k-k_0)\left(\frac{\partial^2\omega}{\partial k^2}\right)_{k_0}$$

$$v_g = \left(\frac{\partial\omega(k)}{\partial k}\right)_{k=k_0} \leftarrow \text{group velocity}$$

Look at the end of section 2-2 for a more mathematical description of how the wave packet spreads out with time.

For plane electromagnetic waves, $\omega(k) = ck$ and $v_g \equiv c$.

2-3 The probability interpretation

Ideas and requirements:

× in order to obtain interference, a particle (electron) must be described by a wave amplitude

× interference follows from a cross term of two possible events:

$$\psi_1 + \psi_2 \rightarrow (\psi_1+\psi_2)^2 = \underbrace{\psi_1^2 + \psi_2^2}_{\text{independent events}} + \underbrace{2\psi_1\psi_2}_{\text{interference}}$$

Phase/coherence issue:

two-slit experiment with a source of decoherence

$$\Psi(x,t) = \underbrace{e^{i\Phi}}_{\text{random phase}} \Psi_1(x,t) + \Psi_2(x,t)$$

$$|\Psi(x,t)|^2 = \underbrace{|\Psi_1(x,t)|^2 + |\Psi_1(x,t)|^2}_{\text{superposition of intensities}} +$$

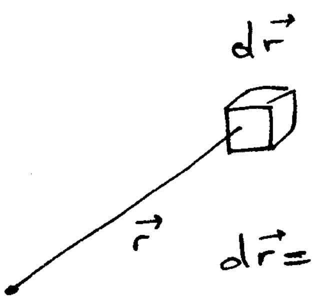
$$+ e^{i\Phi}\Psi_1\Psi_2^* + e^{-i\Phi}\Psi_2\Psi_1^* =$$

$$= I_1 + I_2 + 2\cos\Phi \, Re(\Psi_1\Psi_2^*) + 2\sin\Phi \, Im(\Psi_1\Psi_2^*)$$

$$\langle|\Psi(x,t)|^2\rangle_\Phi = I_1 + I_2 \leftarrow \text{no interference !}$$

Since $|\Psi_1+\Psi_2|^2$, when normalized, corresponds to probability, the function $|\Psi|^2$ should have the property of probability density

Max Born: The probability of finding an electron in the volume $d\vec{r}$

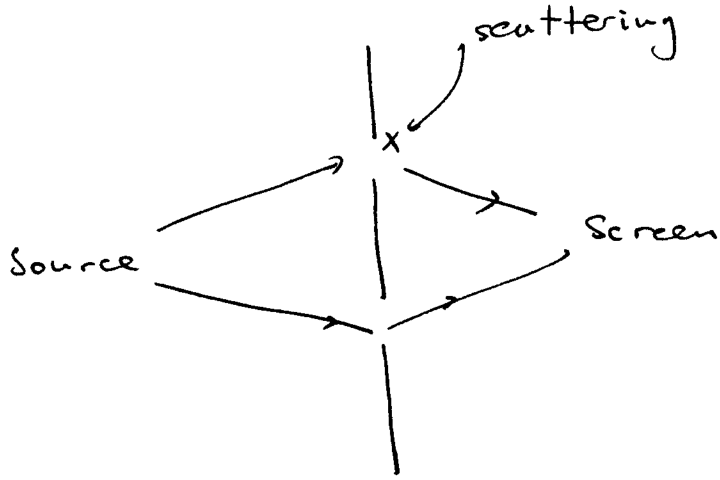


$$dW = \underbrace{P(\vec{r},t)}_{\text{probability density}} d\vec{r} = |\Psi(\vec{r},t)|^2 d\vec{r}$$

$d\vec{r} = dx\,dy\,dz$

× Probability in QM is a statement of fundamental limitations of gaining knowledge about the quantum world

× The experimental outcome depends on experimental setup: knowing about the actual trajectory eliminates interference



If some experiment (scattering) allows one to decide which trajectory did the electron go, the interference is eliminated

$$P(x,t) = |\Psi_1(x,t)|^2 + |\Psi_2(x,t)|^2$$

What we observe in the quantum experiment depends on how we "look" at the event!