I. FROM CLASSICAL MECHANICS TO WAVE MECHANICS

We have ample experimental evidence that the laws of classical mechanics break down in the microscopic realm (later: action $p \cdot x \lesssim \frac{h}{2\pi}$). Examples: stability of atoms, atomic spectra and absorption, interaction of light with matter, nuclei, etc.

We need a generalized set of axioms which recovers classical mechanics in the limit $p \cdot x \gg \frac{h}{2\pi}$: <u>quantum mechanics</u>

We stay in the non-relativistic regime, i.e. particle velocities* $v \ll c$

* we will have to define this in quantum mechanics

I.1 AXIOMS OF QUANTUM MECHANICS

* Recall the fundamental principles of mechanics (cf. [ARNOLD])

(A) A particle (point mass) is described by its motion in $\mathbb{R}^3$, i.e. by a differentiable mapping $x : \underset{\text{time}}{\mathbb{R}} \to \underset{\text{space}}{\mathbb{R}^3}$

A system of N particles is described by the direct product of the motions $\mathbb{R} \to \mathbb{R}^{3N}$

(B) In inertial frames of reference the laws of classical mechanics are invariant under transformations with the Galilei group $\mathcal{G}(3,1)$ [Galileo's Principle of Relativity]

(C) The initial state of a system, i.e. the totality of positions and velocities of its particles at one moment in time uniquely determines all of its motion.

Essentially the axioms make classical mechanics a theory of second order differential equations whose solutions are the motions of systems of particles.

* We have to replace classical mechanics by the following set of axioms

(Q1) A system is described by a complex Hilbert Space $\mathcal{H}$; composite systems consisting of N subsystems are described by the direct product of the Hilbert Spaces of the subsystems. Each possible state of the system is described by a ray (or unit vector) $|\psi\rangle$.

(Q2) Observables, i.e. measurable physical quantities, are represented by linear, self-adjoint operators acting on $\mathcal{H}$. The possible outcomes of a measurement of an observable operator $\hat{O}$ are its eigenvalues λ_i.

(Q3) If a system is in a state $|\psi\rangle$ the probability to measure the value λ for an observable $\hat{O}$ is $w_\lambda = |\langle\phi_\lambda|\psi\rangle|^2$ where $|\phi_\lambda\rangle$ is the eigenstate for the eigenvalue λ. After the measurement the system will be in the state $|\phi_\lambda\rangle$ (collapse).

(Q4) There is a linear, unitary (projective) representation of the Galilei Group $\mathcal{G}(3,1)$ on $\mathcal{H}$ and the laws of quantum mechanics are invariant under Galilei transformations, except for time translations. The evolution of a system in time is given by the unitary Galilean time translation operator only between two measurements.

* We will not start from these axioms but slowly work towards establishing them.
  We will first "derive" wave mechanics in which a particular useful choice for $\mathcal{H}$ is made: $\mathcal{H}$ is a space of functions and its rays are interpreted as wave functions of the system.

* Classical mechanics should be contained in quantum mechanics as a suitable limit.

I.2 The Case for Matter Waves

I.2.1 Experimental Findings

* Discreteness of energy: in the microscopic world energy seems to exist in "quanta".

  - Planck's Blackbody radiation formula [1900]:

    energy density $u(\nu, T) = \frac{8\pi h \nu^3}{c^3} \frac{1}{e^{h\nu/kT} - 1}$

    T = temperature
    c = speed of light
    k = Boltzmann's constant

    He had to assume that oscillators in the body have a quantized energy spectrum $\boxed{E_i = n_i h\nu}$ $\quad n \in \mathbb{N}$

    $h = 6.6261 \times 10^{-34}\,\mathrm{Js} = 4.136 \times 10^{-15}\,\mathrm{eV\,s}$ is Planck's constant (dimension of action)

    High-/low-frequency limits:

    $$u(\nu, T) = \begin{cases} \xrightarrow{h\nu \ll kT} \frac{8\pi}{c^3} \nu^2 kT & \text{(Rayleigh)} \\ \xrightarrow{h\nu \gg kT} \frac{8\pi h\nu^3}{c^3} e^{-\frac{h\nu}{kT}} & \text{(Wien)} \end{cases}$$

    (Rayleigh) — classical result independent of h; small frequency ~ many quanta, i.e. discrete character not important

    (Wien) — proper quantum regime, few quanta

  - Photoelectric effect, Einstein [1905]:

    Energy in electromagnetic waves comes in quanta too: $\boxed{E = h\nu}$

    h is the same quantum of action.

  - Stable atoms with discrete energies, Bohr [1913]

    Let q_i be a set of generalized coord. and $p_i = \frac{\partial L}{\partial \dot{q}_i}$ the conjugate momenta.

    Then only phase space trajectories $p_i(q_i)$ with $\boxed{\oint p_i \, dq_i = n_i h}$

are allowed (Bohr's quantization condition).

Phenomenological success only for simple systems (harmonic oscillator, hydrogen atom).

- Absorption and emission spectra of atoms, Bohr and Sommerfeld [1916]

  Orbits satisfying Bohr's quantization condition are stable and do not absorb or emit radiation. However when transiting from one discrete energy level E_1 to another one E_2 one quantum of electromagnetic radiation of frequency

  $$\boxed{\nu = \frac{1}{h} |E_2 - E_1|}$$

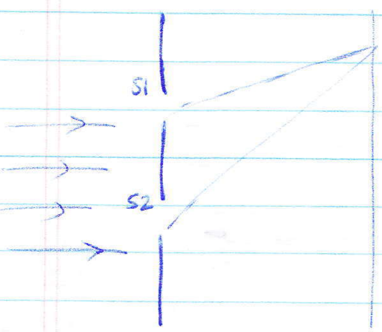
  is absorbed (if $E_2 > E_1$) or emitted (if $E_1 > E_2$)

* Interference and diffraction effects: first indication that particles can behave like waves. Beams of particles seem to resemble plane waves of wave length $\lambda = \frac{h}{p}$ where p = particle momentum.

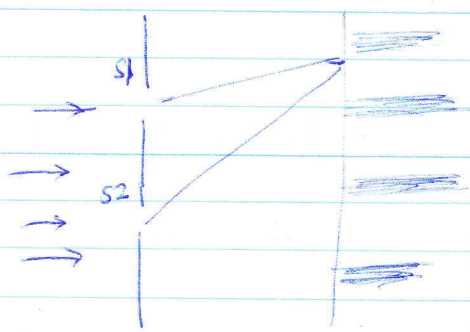
Postulated by de Broglie [1924]; experiment: Davisson and Germer [1927] electron scattering off Ni crystals.

* A particle – wave duality emerges for both matter (electrons, protons, etc.) and electromagnetic radiation (photons).

Preliminary resolution (example: double slit experiment)



A single particle or photon (quantum) can be detected. It goes either through S1 or S2.



Many quanta form an interference pattern.

I.e. the matter wave describes the statistical distribution.

Note: if $\lambda \ll x$ (typical length scale, e.g. slit distance here) then the wave character is irrelevant and classical mechanics could be restored.

$1 \gg \frac{\lambda}{x} = \frac{h}{xp} \Rightarrow$ wave aspects negligible for $xp \gg h$.

Hence h sets the scale for quantum effects to be important.

In other words, we expect classical mechanics to reemerge in the limit $h \to 0$.

* Example for successfull Bohr-Sommerfeld quantisation: hydrogen atom.

We need to analyze the phase space trajectory of classical motion in the Coulomb field, i.e. solutions to Kepler's problem. Here; only circular trajectories.

In suitable spherical coordinates $T = \left(\frac{1}{2}m\dot{r}^2 +\right) \frac{1}{2} m r^2 \dot{\phi}^2$, $U = -\frac{e^2}{4\pi\varepsilon_0 r}$

(note $\dot{r} = 0$)

$L = T - U$, $E = T + U$

Conjugate momentum for ϕ: $p_\phi = \frac{\partial L}{\partial \dot{\phi}} = m r^2 \dot{\phi} \equiv L$

$$\oint p_\phi \, d\phi = \int_0^{2\pi} m r^2 \dot{\phi} = 2\pi m r^2 \dot{\phi} \stackrel{!}{=} n h \quad \Rightarrow L_z = n\hbar \quad (n \in \mathbb{N})$$

where $\hbar = \frac{h}{2\pi}$

Hence Bohr-Sommerfeld means that angular momentum is quantized in multiples of $\hbar$ in this case.

Equation of motion for r: $\underbrace{m\ddot{r}}_{0} - \underbrace{m r \dot{\phi}^2}_{\frac{L^2}{mr^3}} + \frac{e^2}{4\pi\varepsilon_0 r^2} = 0 \Rightarrow L_z^2 = \frac{m e^2 r}{4\pi\varepsilon_0}$

Quantisation: $r = n^2 \frac{4\pi\varepsilon_0 \hbar^2}{m e^2}$

In particular the smallest radius is predicted to be

$$r_1 = \frac{4\pi\varepsilon_0 \hbar^2}{me^2} = 5.29 * 10^{-11}\, m$$

coincides with the full QM expression for the Bohr radius a_0

Energy: $$E = \frac{L_z^2}{2mr^2} - \frac{e^2}{4\pi\varepsilon_0 r} = \frac{1}{2}\frac{e^2}{4\pi\varepsilon_0 r} - \frac{e^2}{4\pi\varepsilon_0 r} = -\frac{1}{n^2}\frac{me^4}{2(4\pi\varepsilon_0)^2\hbar^2} = -\frac{1}{n^2}\frac{2\pi^2 me^4}{(4\pi\varepsilon_0)^2 h^2}$$

$$n=1: \quad E_1 = -\frac{me^4}{8h^2\varepsilon_0^2} = -13.6\text{ eV}$$

coincides with full QM expression for the Rydberg constant $-R_H$

Wave length of light emitted when electron changes state (or "orbit") from n_1 to n_2 $(n_1 > n_2)$

$$\lambda = \frac{c}{\nu} = \frac{hc}{E_1 - E_2}$$

($\lambda\nu = c$ for plane e.m. waves)

$$\frac{1}{\lambda} = \frac{R_H}{hc}\left(\frac{1}{n_2} - \frac{1}{n_1}\right)$$

Lyman series: $n_1 = 1$ [1906]

Balmer series: $n_1 = 2$ [1885]

I.2.2 Matter Waves and Wave Functions

* Interference and diffraction phenomena $\Longrightarrow$ free particles should be described by (travelling waves); de Broglie's equation $\lambda = \frac{h}{p}$ connects particle and wave properties.

* Bound particles only take certain energies: reminiscent of standing waves in classical physics (e.g. vibrating string or membrane). "Quantization" forced by boundary conditions.

* Thus we postulate: particles can be described by scalar fields $\psi(\vec{r},t) = \psi(x,y,z,t)$ called wave functions.

* The restriction to scalar fields is for simplicity only. Quantum theory allows fields with internal structure (vector fields, spinor fields etc.), see QM II course. So among other things we neglect spin of particles for now.

* We would like a probabilistic interpretation of ψ (recall the double slit experiment), but ψ can be negative (or even complex as we'll see) so ψ itself can not be a probability density. Following the guidance from electrodynamics where

not $\vec{E}$ and $\vec{B}$ but $|\vec{E}|^2$ and $|\vec{B}|^2$ determine the intensity (i.e. photons/(area × time)) we postulate that $|\psi(\vec{r},t)|^2$ is the probability density associated with ψ. The wave function ψ is the probability amplitude.

* Superposition Principle: If mater waves should exhibit interference effects as in optics we need the superposition principle to hold. Hence if $\psi_1(\vec{r},t)$ and $\psi_2(\vec{r},t)$ describe possible physical situations then $\psi(\vec{r},t) = \psi_1(\vec{r},t) + \psi_2(\vec{r},t)$ is also a possible physical solution.

Example: Double slit experiment. Suppose only one slit is open at a time. Then the particle going through slit i is described by wave function ψ_i. $(i=1,2)$. Intensities are given by $|\psi_1|^2$ and $|\psi_2|^2$ resp. When both slits are open the wave function is a superposition and the intensity is now $\propto |\psi_1+\psi_2|^2 \neq |\psi_1|^2 + |\psi_2|^2$

The interference pattern comes from the additional "interference term"

$\psi_1 \psi_2^* + \psi_1^* \psi_2$

Here $(\cdot)^*$ denotes complex conjugation. We have not yet decided whether wave fcts. have to be real or can be complex, see next subsection.

I.3 Plane Waves

* We are led to postulate that free particles with momentum $\vec{p}$ should be represented by plane waves with wave vector $\vec{k}$ and (angular) frequency ω.

Recall $k = \frac{2\pi}{\lambda}$ for a plane wave and we identify the direction of propagation of the wave with the direction of propagation of the particle: $\vec{k} \parallel \vec{p}$

Then from de Broglie: $\boxed{\vec{p} = \hbar \vec{k}}$

* The most general form of a plane wave is

$$\psi(\vec{r},t) = A\cos(\vec{k}\cdot\vec{r} - \omega t) + B\sin(\vec{k}\cdot\vec{r} - \omega t)$$

Experimental observation: we do not observe oscillations in intensity for single particles or beams of particles; moreover there should be translational invariance in the direction of $\vec{p}$

Thus a small translation along $\vec{p}$ by an amount $\vec{\delta} = \varepsilon \frac{\vec{k}}{k^2}$ should keep $|\psi|^2$ invariant:

(*) $\psi(\vec{r}+\vec{\delta},t) = a(\varepsilon)\,\psi(\vec{r},t)$ where $|a(\varepsilon)| = 1$ so $|\psi(\vec{r}+\vec{\delta},t)|^2 = |\psi(\vec{r},t)|^2$

for any choice of ε!

$$\Rightarrow \psi(\vec{r}+\vec{\delta},t) = A\cos(\vec{k}\cdot\vec{r} - \omega t + \varepsilon) + B\sin(\vec{k}\cdot\vec{r} - \omega t + \varepsilon)$$

$$= A\left[\cos(\vec{k}\cdot\vec{r} - \omega t)\cos\varepsilon - \sin(\vec{k}\cdot\vec{r} - \omega t)\sin\varepsilon\right] + B\left[\sin(\vec{k}\cdot\vec{r} - \omega t)\cos\varepsilon + \cos(\vec{k}\cdot\vec{r} - \omega t)\sin\varepsilon\right]$$

$B = \pm iA$ and $a(\varepsilon) = e^{\pm i\varepsilon}$ are solutions to (*)

Proof: ~~For~~ these choices $\psi(\vec{r}+\vec{\sigma},t) = A\left[\cos(\vec{k}\cdot\vec{r}-\omega t) \pm i\sin(\vec{k}\cdot\vec{r}-\omega t)\right]\cos\varepsilon$

$$\pm iA\left[\cos(\vec{k}\cdot\vec{r}-\omega t) \pm i\sin(\vec{k}\cdot\vec{r}-\omega t)\right]\sin\varepsilon$$

$$= \psi(\vec{r},t)\, e^{\pm i\varepsilon}$$

We choose $B = +iA$, $a = e^{i\varepsilon}$

Hence we are forced to the conclusion that wave functions in QM are complex valued. This is often summarized as:

"The phase of a single particle is not observable."

(If it were a real-valued sin or cos-wave it would be!)

* Hence $\boxed{\psi(\vec{r},t) = A\, e^{i(\vec{k}\cdot\vec{r}-\omega t)}}$ is the general form of a plane wave permitted in quantum mechanics.

* The (angular) frequency is yet undetermined. We expect it to be given by $\vec{k}$ as $\omega = \omega(\vec{k})$ in analogy to classical waves (dispersion relation).

If we postulate $\boxed{E = h\nu = \hbar\omega}$ as for photons

and use $E = \frac{p^2}{2m}$ for free particles* then

$$\hbar\omega = \frac{(\hbar k)^2}{2m} \implies \boxed{\omega = \frac{\hbar}{2m} k^2},$$

* This is another postulate and will be better motivated below.

Dispersion relation for free particles / plane waves.

I.4 Wave Packets

I.4.1 Fourier Transformations

* Recall that for a suitable function $f: \mathbb{R}^n \to \mathbb{C}$ (or $\mathbb{R}$) $(n \in \mathbb{N})$

we define the Fourier transformation as

$$\hat{f}(\vec{k}) = \frac{1}{\sqrt{2\pi}^n} \int_{\mathbb{R}^n} f(\vec{r})\, e^{-i\vec{k}\cdot\vec{r}}\, d^n r$$

"Suitable" usually means that f has to be integrable (L^1) or square-integrable (L^2)

$\hat{f}$ is again a function $\mathbb{R}^n \to \mathbb{C}$.

* Under certain conditions f can be recovered from $\hat{f}$ by an inverse Fourier transformation. Then

$$f(\vec{r}) = \frac{1}{\sqrt{2\pi}^n} \int_{\mathbb{R}^n} \hat{f}(\vec{k})\, e^{+i\vec{k}\cdot\vec{r}}\, d^n k$$

* Fourier transformation can be extended to a certain class of distributions (generalized functions), most notably Dirac's δ-function.

Recall δ is defined by $\int_I \delta(x) f(x)\, dx = f(0)$ for any open interval I containing 0.

$\int_I \delta(x) f(x)\, dx = 0$ for any other open interval.

for any arbitrary "test function" $f: \mathbb{R} \to \mathbb{R}$

Thus $\delta(x)$ can be seen as a "function" that is zero everywhere except for $x = 0$ where it diverges.

* We have $\hat{\delta}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x)\, e^{-ikx}\, dx = \frac{1}{\sqrt{2\pi}}$

More generally $\hat{\delta}_{x_0}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \delta(x-x_0)\, e^{-ikx} = \frac{1}{\sqrt{2\pi}}\, e^{-ikx_0}$

Conversely $\frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ikx_0}\, e^{ikx}\, dk = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{+ik(x-x_0)}\, dx = \delta(x-x_0)$

I.e. $\delta(x-x_0) \xleftrightarrow{\text{Fourier}} \frac{1}{\sqrt{2\pi}} e^{-ikx_0}$

* Parseval's Theorem:

Let $f, g: \mathbb{R}^n \to \mathbb{R}$ or $\mathbb{C}$ be integrable and square-integrable functions (L^1 and L^2), and let $\hat{f}, \hat{g}$ be their Fourier transforms.

Then
$$\int_{\mathbb{R}^n} f(x)\, g^*(x)\, d^n x = \int_{\mathbb{R}^n} \hat{f}(k)\, \hat{g}^*(k)\, d^n k$$

Proof: $\int_{\mathbb{R}^n} \hat{f}(k)\, \hat{g}^*(k)\, d^n k = \frac{1}{2\pi^n} \int_{\mathbb{R}^n} d^n x\, d^n x' \int dk\; e^{-ikx} f(x)\, e^{ikx'} g^*(x')$

$= \int_{\mathbb{R}^n} d^n x\, d^n x'\; \delta^{(n)}(x-x')\, f(x)\, g^*(x') = \int_{\mathbb{R}^n} d^n x\; f(x)\, g^*(x)$

* Corollary: Plancherel's Theorem

Under the same assumptions as above

$$\int_{\mathbb{R}^n} |f(x)|^2 \, d^n x = \int_{\mathbb{R}^n} |\hat{f}(k)|^2 \, d^n k$$

I.e. Fourier transformations preserve L^2-norms.

* Let $f: \mathbb{R} \to \mathbb{C}$ or $\mathbb{R}$ be differentiable so that the FT exist for both f and $f' = \frac{df}{dx}$. If $\hat{f}(k)$ is the FT of $f(x)$ then $\widehat{f'}(k) = ik\hat{f}(k)$.

I.e. under FT $k \longleftrightarrow -i\frac{d}{dx}$.

Proof: $$\widehat{f'} = \int_{\mathbb{R}} \left[\frac{d}{dx} f(x)\right] e^{-ikx} \, dx = \underbrace{f(x)e^{-ikx}\Big|_{-\infty}^{+\infty}}_{\substack{f(x) \xrightarrow[x\to\pm\infty]{} 0 \text{ for} \\ \text{(square) integrability}}} - \int_{-\infty}^{+\infty} f(x) \frac{d}{dx} e^{-ikx} \, dx$$

$$= ik \int_{\mathbb{R}} f(x) e^{-ikx} \, dx = ik\hat{f}(k).$$

* This generalizes in a trivial way to higher derivatives and multi-dimensional derivatives.

I.4.2 Fourier Analysis of Wave Packets

* A plane wave with wave vector $\vec{k}$ corresponds to particles with a sharply defined momentum $\vec{p} = \hbar\vec{k}$. But ~~they~~ plane waves are completely unlocalized in space. But this is not the only wave function allowed for free particles. Because of the superposition principle arbitrary sums of plane waves are also allowed (i.e. solutions to the yet unknown equations of motion).

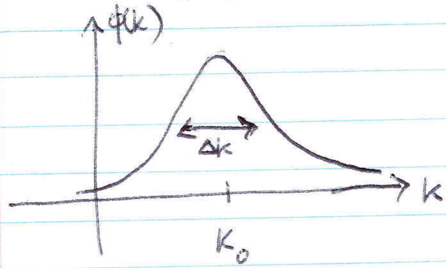
In general
$$\psi(\vec{r},t) = \frac{1}{\sqrt{2\pi}^3}\int \phi(\vec{k})\, e^{i(\vec{k}\cdot\vec{r} - \omega(k)t)}\, d^3k$$
is an allowed wave fct. with suitable ~~ϕ~~ (integrable) ϕ.

* Obviously $\phi(\vec{k})$ is the Fourier transformed of $\psi(\vec{r},0)$, i.e.
$$\phi(\vec{k}) = \frac{1}{\sqrt{2\pi}^3}\int \psi(\vec{r},0)\, e^{-i\vec{k}\cdot\vec{r}}\, d^3r$$

Because of $\vec{p} = \hbar\vec{k}$ $\phi(\vec{k})$ is also called the wave fct. in momentum space. First we restrict ourselves to 1-D waves for simplicity.

* For now analyze wave packets at a fixed time, say $t = 0$.

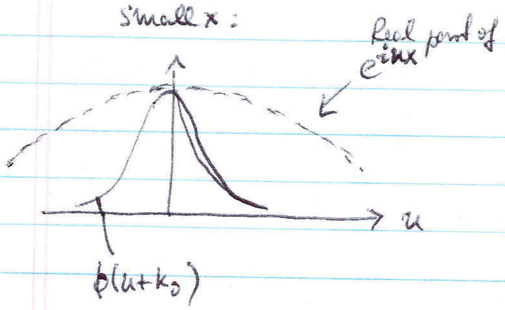
Let $\phi(k)$ (the distribution of "modes") resemble a function which is real and falls off from a peak at $k = k_0$ with a typical width Δk:



Then with $u = k - k_0$:
$$\psi(x,0) = \underbrace{\frac{1}{\sqrt{2\pi}}\, e^{ik_0x}}_{\text{plane wave with "average" momentum } k_0} \underbrace{\int_{-\infty}^{+\infty} \phi(u+k_0)\, e^{iux}\, du}_{\text{modulation } \bar{\psi}(x)}$$

$\Psi(x)$ is a fct. which goes to zero outside of an interval $\left(-\frac{\Delta x}{2}, \frac{\Delta x}{2}\right)$

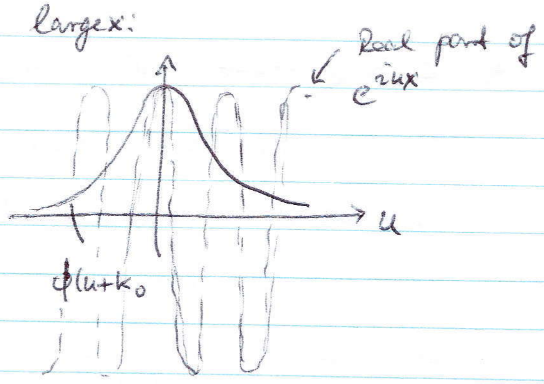
small x:



All of the important part of $\phi(u+k_0)$ is within one cycle of e^{iux} $\longrightarrow$ maximal contribution to the u-integral

$$x \cdot \Delta k \ll \pi$$

large x:



Many oscillations of e^{iux} within within Δk $\longrightarrow$ cancellation in the u-integral

$$x \cdot \Delta k \gg \pi$$

Hence $\Delta x \sim \frac{1}{\Delta k}$: the width Δx of the wave packet and the width of the mode distribution Δk are reciprocal to each other.

* We just obtained a ~~version~~ version of Heisenberg's uncertainty principle qualitatively!

$\Delta x \cdot \Delta k \sim \mathcal{O}(1)$ is a natural property of any wave phenomenon.

* We can make this uncertainty relation mathematically precise. Let $f: \mathbb{R} \to \mathbb{C}$ or $\mathbb{R}$ be a differentiable fct. for which the FT $\hat{f}$ exists. Furthermore let f have L^2-Norm unity, i.e. $\int_{\mathbb{R}} |f|^2 dx = 1$. Let $x_0 \in \mathbb{R}$, $k_0 \in \mathbb{R}$ be arbitrary points. We define the variation of f around x_0 as

$$(\Delta x)^2 = \int_{\mathbb{R}} (x-x_0)^2 |f(x)|^2 dx \quad \text{and similarly} \quad (\Delta k)^2 = \int_{\mathbb{R}} (k-k_0)^2 |\hat{f}(k)|^2 dk$$

if these integrals exist.

Then the inequality $\boxed{\Delta x \cdot \Delta k \geq \frac{1}{2}}$ holds.

Why? Here, check only case $x_0 = 0, k_0 = 0$ for simplicity.

$$(\Delta k)^2 = \int_{\mathbb{R}} |k\hat{f}(k)|^2 dk \underset{\text{Plancherel}}{=} \int_{\mathbb{R}} |\underbrace{\tfrac{d}{dx} f(x)}_{f'(x)}|^2 dx$$

$$(\Delta x)^2 (\Delta k)^2 = \int_{\mathbb{R}} |x f(x)|^2 dx \int_{\mathbb{R}} |f'(x)|^2 dx \underset{\substack{\text{Schwartz} \\ \text{Inequality}}}{\geq} \left| \int_{\mathbb{R}} (x f(x))^* f'(x)\, dx \right|^2 \underset{(*)}{\geq} \left| \frac{1}{2} \int_{\mathbb{R}} x \frac{d}{dx} |f(x)|^2 dx \right|^2$$

For (*): $\operatorname{Re} f^* f' = (\operatorname{Re} f)(\operatorname{Re} f') + (\operatorname{Im} f)(\operatorname{Im} f') = \frac{1}{2} \frac{d}{dx} |f|^2$

$$\Rightarrow \operatorname{Re} \int x f^* f' dx = \frac{1}{2} \int x \frac{d}{dx} |f|^2 dx$$

$$\Rightarrow \left| \int x f^* f' dx \right|^2 \geq \left| \operatorname{Re} \int x f^* f' dx \right|^2 = \left| \frac{1}{2} \int x \frac{d}{dx} |f|^2 dx \right|^2$$

Hence $(\Delta x)^2 (\Delta k)^2 \underset{\substack{\text{partial} \\ \text{integration}}}{\geq} \frac{1}{4} \left| \int_{\mathbb{R}} |f(x)|^2 dx \right|^2 = \frac{1}{4}$

q.e.d.

*

* In particular: if ψ is a wave packet around x_0 and ϕ its FT centered around k_0 then Δx and Δk measure the widths of the wave packets and $\Delta x \cdot \Delta k \geq \frac{1}{2}$

The uncertainty relation is a fundamental property of waves.

* ~~Ex)~~ The Gauss function $\sim e^{-\frac{x^2}{4\sigma^2}}$ is the (only) example for which precisely $\Delta x \, \Delta k = \frac{1}{2}$. I.e. Gaussian wave packets have the smallest possible uncertainty.

Why? Homework!

* For momentum and position: $\Delta x \, \Delta p \geq \frac{\hbar}{2}$ since $p = \hbar k$

* Generalization to more than one dimension is straightforward:

$$\Delta x \Delta p_x \geq \frac{\hbar}{2} \quad , \quad \Delta y \, \Delta p_y \geq \frac{\hbar}{2} \quad \text{etc.}$$

I.4.3 Time Dependence of Wave Packets

* Return to the general superposition for free particles on p. 17:

$$\psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \int \phi(\vec{k})\, e^{i(\vec{k}\cdot\vec{r} - \omega(\vec{k})t)}\, d^3k$$

Let $\phi(\vec{k})$ again be a packet centered around wave vector $\vec{k_0}$, $\vec{k} = \vec{k_0} + \vec{u}$

Use a Taylor expansion $\omega(\vec{k}) = \omega(\vec{k_0}) + \sum_{i=1}^{3} \frac{\partial \omega}{\partial k_i}\Big|_{\vec{k_0}} u_i + \frac{1}{2}\sum_{i,j} \frac{\partial^2 \omega}{\partial k_i \partial k_j}\Big|_{\vec{k_0}} u_i u_j + \ldots$

For free particles $\omega = \frac{\hbar k^2}{2m}$ and the series terminates after the 2^{nd} order.

Let us assume we don't know that yet:

$$\psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}} \underbrace{e^{i\vec{k_0}\cdot\left(\vec{r} - \frac{\omega(k_0)}{k_0}\hat{k}_0 t\right)}}_{\substack{\text{carrier wave with} \\ \text{phase velocity } \vec{v}_{ph} \\ \frac{\omega(k_0)}{k_0} \text{ in direction of } \vec{k_0} \\ (\hat{k}_0 = \text{unit vector})}} \underbrace{\int \phi(\vec{u})\, e^{i\vec{u}\cdot(\vec{r} - \nabla_k \omega\, t)}}_{\substack{\text{wave packet envelope} \\ \text{as before, propagating} \\ \text{with a group velocity} \\ \vec{v}_{gr} = \nabla_k \omega}} \underbrace{e^{i\frac{1}{2}\sum_{ij} \frac{\partial^2 \omega}{\partial k_i \partial k_j} u_i u_j}}_{\text{correction term}}$$

* If a wave packet is to describe a <u>localized</u> propagating particle we must identify the group velocity of the wave packet with the particle velocity, i.e.

$$\nabla_k \omega = \vec{v} = \frac{\vec{p}}{m} = \frac{\hbar}{m}\vec{k}$$

This is a differential equation for ω. The solution is $\omega = \frac{\hbar k^2}{2m}$ as before.

There could be a constant potential as a const. of integration which we've set to zero.

This is a more physical "derivation" of the dispersion relation for matter waves.

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* Hence $\vec{v}_{ph} = \frac{\omega(k_0)}{k_0}\,\hat{k}_0 = \frac{E}{p}\,\hat{p}$ where $E, \vec{p}$ are particle energy and momentum

$$\vec{v}_{gr} = \nabla\omega\Big|_{\vec{k}_0} = \frac{\vec{p}}{m}$$

and $$\psi(\vec{r},t) = \frac{1}{(2\pi)^{3/2}}\, e^{i\vec{k}_0(\vec{r}-\vec{v}_{ph}t)} \int \phi(\vec{u})\, e^{i\vec{u}(\vec{r}-\vec{v}_{gr}t)}\, e^{i\frac{1}{2}\frac{\hbar}{m}u^2 t}$$

Correction term ~ 1 as long as $\frac{\hbar}{2m}u^2|t| \ll 1$, i.e. for $|t| \ll \frac{2m}{\hbar(\Delta k)^2}$ the wave packet propagates undisturbed.

Correction term oscillating for $\frac{\hbar}{2m}u^2|t| \gtrsim 1$, i.e. for $|t| > \frac{2m}{\hbar(\Delta k)^2}$ the wave packet starts to change shape. You can convince yourself that the wave packet is spreading for $t \to \pm\infty$

Examples: HW