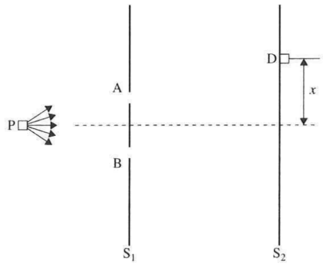
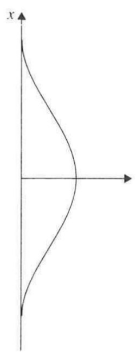
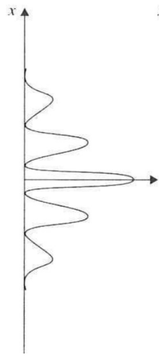
H2: the wave function and the uncertainty principle

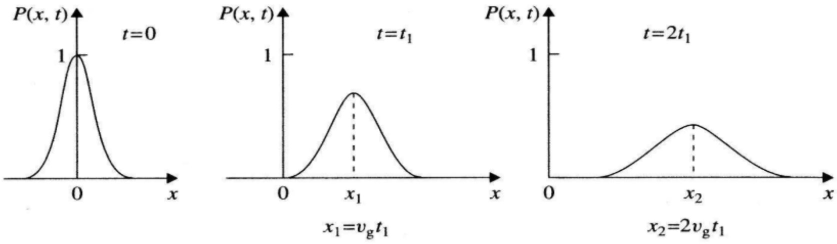
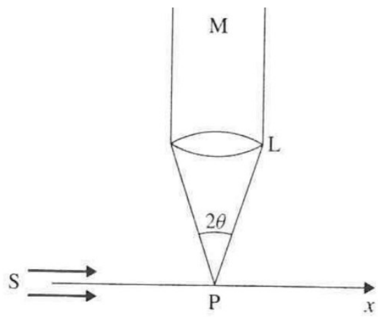
2.1 wave particle duality	
wave-particle: experiment	Source emits monoenergetic particles, ex: electrons > screen S_1 contains two slits A and B > detector screen S_2 behind S_1 
wave-particle: result	expectation:  reality: 
wave-particle: explanation	When the particle goes through the slit, it behaves like a wave > interference with itself When the particle is detected it behaves like a particle > in one experiment we have both wave and particle behaviour
properties of wave particle	- if we put a detector at slit A, there is no diffraction pattern > the place of detection determines the outcome - when we only shoot one e^- at a time, there is still diffraction > the particles interfere with themselves - there is only wave or only particle behaviour at a certain time > states are complementary - we cannot predict the outcome, since the place of detection changes the outcome > we can predict the probability > wave-particle is fundamentally statistical - we can define a wave function for which: $$P(x, y, z, t) \propto \|\Psi(x, y, z, t)\|^2.$$
superposition	let Ψ_A be the wavefunction for slit A, Ψ_B for slit B > then: $P_A \propto \|\Psi_A\|^2, \quad P_B \propto \|\Psi_B\|^2.$ and if both slits are open we find a wavefunction: $$\Psi = \Psi_A + \Psi_B.$$ corresponding to a distribution: $$P \propto \|\Psi_A + \Psi_B\|^2$$

2.2 interpretation of the wave function	
position probability density	Consider an open space with particles > all identical, independent systems with an external force working on them > each particle can be described using a wave function Ψ for that particle > the probability of finding a particle within a volume d**r** = dxdydz: $$P(\mathbf{r},t)\mathrm{d}\mathbf{r} = \|\Psi(\mathbf{r},t)\|^2\mathrm{d}\mathbf{r}$$ so that: $$P(\mathbf{r},t) = \|\Psi(\mathbf{r},t)\|^2 = \Psi^*(\mathbf{r},t)\Psi(\mathbf{r},t)$$ the *position probability density* (since $\Psi \in \mathbb{C}$, Ψ^* is the complex toegevoegde)
normalisation of the probability	the total probability should be 1: $$\int \|\Psi(\mathbf{r},t)\|^2\mathrm{d}\mathbf{r} = 1$$
2.2.1 the superposition principle	
superposition principle	If there are multiple states then: $$\Psi = c_1\Psi_1 + c_2\Psi_2$$ where c_1 and c_2 are complex numbers We also find: Let us write the (complex) wave functions Ψ_1 and Ψ_2 in the form $$\Psi_1 = \|\Psi_1\|\mathrm{e}^{\mathrm{i}\alpha_1}, \qquad \Psi_2 = \|\Psi_2\|\mathrm{e}^{\mathrm{i}\alpha_2}.$$ Using (2.8), we find that the square of the modulus of Ψ is given by $$\|\Psi\|^2 = \|c_1\Psi_1\|^2 + \|c_2\Psi_2\|^2 + 2\mathrm{Re}\{c_1c_2^*\|\Psi_1\|\|\Psi_2\| \exp[\mathrm{i}(\alpha_1 - \alpha_2)]\}$$ so in general: $$\|\Psi\|^2 \neq \|c_1\Psi_1\|^2 + \|c_2\Psi_2\|^2$$
2.3 wave functions for particles having a definite momentum	
the wave function	consider a free particle with mass m moving along the x-axis with momentum $\mathbf{p} = p_x\mathbf{e_x}$ > we can describe it with a regular plane wave: $$\Psi(x,t) = A\exp\{\mathrm{i}[kx - \omega(k)t]\}$$ however we know the relations: $$E = h\nu, \qquad p = \frac{h}{\lambda}.$$ which can be rewritten as: $$E = \hbar\omega, \qquad p = \hbar k.$$ thus the wave function: $$\Psi(x,t) = A\exp\{\mathrm{i}[p_x x - E(p_x)t]/\hbar\},$$
differential wave equation	We note that the wave function (2.13) satisfies the two relations $$-\mathrm{i}\hbar\frac{\partial}{\partial x}\Psi = p_x\Psi$$ and $$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi = E\Psi$$

3D wavefunction	Same, extended to 3D: $$\Psi(\mathbf{r},t) = A\exp\{i[\mathbf{k}.\mathbf{r} - \omega(k)t]\} = A\exp\{i[\mathbf{p}.\mathbf{r} - E(p)t]/\hbar\}$$ With the differential equation: $$-i\hbar\nabla\Psi = \mathbf{p}\Psi$$
normalisation of the wave function	We need to satisfy: $$\int_{-\infty}^{+\infty} \lvert\Psi(x,t)\rvert^2 dx = 1.$$ however, plane waves cannot satisfy this expression, since: $$\int_{-\infty}^{+\infty} \lvert\Psi(x,t)\rvert^2 dx = \lvert A\rvert^2 \int_{-\infty}^{+\infty} dx$$ which cant be 1 > problem > solution: wave packets
2.4 wave packets	
wave packet	Consider a plane wave: $\Psi(x,t) = A\exp\{i[kx - \omega(k)t]\}$ The most general superposition is given by: $$\Psi(x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i[p_x x - E(p_x)t]/\hbar} \phi(p_x) dp_x$$ - where $(2\pi\hbar)^{-1/2}$ is for later convenience - where $\phi(p_x)$ is the amplitude of the wave corresponding to p_x assume $\phi(p_x)$ is sharply peaked around $p_x = p_0$ and falls to zero around $(p_0 - \Delta p_x, p_0 + \Delta p_x)$ > we can rewrite the wave as: $$\Psi(x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i\beta(p_x)/\hbar} \phi(p_x) dp_x$$ where $$\beta(p_x) = p_x x - E(p_x)t$$ now Ψ is largest when $\beta(p_x)$ is constant > $\beta(p_x)$ should be constant at p_0 > thus: $\left[\frac{d\beta(p_x)}{dp_x}\right]_{p_x=p_0} = 0$ is the condition for the *centre of the wave packet*
group velocity of the wave packet	we know: $x = v_g t$ where $$v_g = \left[\frac{dE(p_x)}{dp_x}\right]_{p_x=p_0}.$$ > thus the centre of the wave packet travels at constant speed where the speed can be rewritten as: $$v_g = \left[\frac{d\omega(k)}{dk}\right]_{k=k_0}$$ since: $E = \hbar\omega$, and $p_x = \hbar k$,
phase velocity	= velocity of propagation of the individual plane waves $$v_{ph} = \frac{\omega(k_0)}{k_0} = \frac{E(p_0)}{p_0}.$$

link between v_g and v_{ph}	Due to the correspondence principle, in the limit we know: $v_g = v = \frac{p_0}{m}.$ thus: $\frac{dE(p_x)}{dp_x} = \frac{p_x}{m}$ which gives the relation: $E(p_x) = \frac{p_x^2}{2m}.$ we can therefore find the link: $v_{ph} = \frac{p_0^2/2m}{p_0} = \frac{p_0}{2m} = \frac{v_g}{2}.$
wave packet mathematically	The energy can be written as: $E(p_x) = \frac{p_0^2}{2m} + \frac{p_0}{m}(p_x - p_0) + \frac{(p_x - p_0)^2}{2m} = E(p_0) + v_g(p_x - p_0) + \frac{(p_x - p_0)^2}{2m}.$ but since $\phi(p_x)$ is negligible outside Δp_x, we can neglect the last term: > so for t small enough: $\frac{1}{2m\hbar}(\Delta p_x)^2 t \ll 1.$ We can use this approximation in the wave packet integral: $\Psi(x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i[p_x x - E(p_x)t]/\hbar} \phi(p_x) dp_x$ Which reduces to: $\Psi(x,t) = e^{i[p_0 x - E(p_0)t]/\hbar} F(x,t)$ where $F(x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{i(p_x - p_0)(x - v_g t)/\hbar} \phi(p_x) dp_x.$ > The wave packet (2.37) is the product of a plane wave of wavelength $\lambda_0 = h/\lvert p_0 \rvert$ and angular frequency $\omega_0 = E(p_0)/\hbar$ times a *modulating* amplitude or *envelope* function $F(x,t)$ such that $\lvert\Psi(x,t)\rvert^2 = \lvert F(x,t)\rvert^2$. Since $F(x, t = 0) = F(x + v_g t, t) \quad \textbf{(2.39)}$ this envelope function propagates *without change of shape* with the group velocity v_g (see Fig. 2.4). It should be borne in mind that this is only true for times t satisfying the condition (2.36); at later times the shape of the wave packet will change as it propagates.

2.4.1 Fourier transforms and momentum space wave function	
Wave function in momentum space	Define $\psi(x) \equiv \Psi(x, t=0)$ We find mathematically: $\psi(x) = (2\pi\hbar)^{-1/2} \int e^{ip_x x/\hbar}\phi(p_x)dp_x$ For which the Fourier-coefficients are: $\phi(p_x) = (2\pi\hbar)^{-1/2} \int e^{-ip_x x/\hbar}\psi(x)dx$ >> if we include time this concludes: $\Psi(x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{ip_x x/\hbar}\Phi(p_x,t)dp_x$ in space and $\Phi(p_x,t) = (2\pi\hbar)^{-1/2} \int_{-\infty}^{+\infty} e^{-ip_x x/\hbar}\Psi(x,t)dx$ in momentum space
normalisation of the wave function	If the wave function $\phi(p_x)$ is normalised to unity: $\int_{-\infty}^{+\infty} \lvert\phi(p_x)\rvert^2 dp_x = 1$ then the wave function $\psi(x)$ is also normalised to unity:
2.4.2 Gaussian wave packet	
properties of Gaussian wave packet	Consider the momentum wave function : $\phi(p_x) = C\exp\left[-\frac{(p_x - p_0)^2}{2(\Delta p_x)^2}\right]$ - peaked around p_0 - Δp_x is the width of the distribution - $\lvert\phi(p_x)\rvert^2$ drops ro 1/e of its maximum at $p_x = p_0$ +- Δp_x
> normalizing the wave function	we know: $\int_{-\infty}^{+\infty} e^{-\alpha u^2}e^{-\beta u}du = \left(\frac{\pi}{\alpha}\right)^{1/2} e^{\beta^2/4\alpha}$ with $u = p_x - p_0$, $\alpha = (\Delta p_x)^{-2}$ and $\beta = 0$, we have $\int_{-\infty}^{+\infty} \lvert\phi(p_x)\rvert^2 dp_x = \lvert C\rvert^2 \pi^{1/2}\Delta p_x.$ The normalisation condition (2.44) is therefore fulfilled by taking $\lvert C\rvert^2 = \pi^{-1/2}(\Delta p_x)^{-1}.$ thus: $\mathrm{C} = \frac{1}{\sqrt{\Delta p_x \sqrt{\pi}}}$ which gives $\phi(p)_x = \frac{1}{\sqrt{\Delta p_x \sqrt{\pi}}} exp(-\frac{(p_x - p_0)^2}{2(\Delta p_x)^2})$
wave function in space	We can find the wave function in space $\psi(x)$ using Fourier analysis > we will find once again a gaussian wave with the properties: - maximum at x=0 - falls to 1/e of its maximum at x=+-Δx - Δx the width of the wave > thus: $\Delta x \Delta p_x = \hbar$

evolution of the wave over time	we can find an expression for the wave and thus the probability density: $P(x,t) = \frac{1}{\sqrt{\pi}} \frac{\Delta p_x/\hbar}{\sqrt{\left[1+(\Delta p_x)^4 t^2/(m^2\hbar^2)\right]}} \exp\left[-\frac{(\Delta p_x/\hbar)^2 (x-v_g t)^2}{1+(\Delta p_x)^4 t^2/(m^2\hbar^2)}\right]$ with $v_g = p_0/m$ We can see that the width Δx of the wave packet changes over time: $\Delta x(t) \equiv \frac{\hbar}{\Delta p_x}\left[1+\frac{(\Delta p_x)^4}{m^2\hbar^2}t^2\right]^{1/2}$ > the wave becomes more delocalised over time 
2.5 The Heisenberg uncertainty principle	
Heisenberg uncertainty principle	the width Δx of the space-distribution is linked to the width Δp_x of the momentum-distr.: $\Delta x\, \Delta p_x \geq \hbar$ > certainty in x-position means uncertainty in x-momentum
2.5.1 the γ-ray microscope	
γ-ray microscope	Consider a microscope that radiates waves with wavelength λ > position of particle can be determined to an error: $\Delta x = \frac{\lambda}{\sin\theta}$ in order to measure the position of a particle, a photon needs to Compton-scatter on the particle and re-enter the microscope > the photon gets recoil-momentum: $p_\gamma = h/\lambda.$ > we can never know the momentum for the particle, since we only know the angle θ at which the photon got scattered > uncertainty in the momentum: $\Delta p_x \simeq \frac{h}{\lambda}\sin\theta$ thus we find: $\Delta x \Delta p_x \simeq h$ 

2.5.2 stability of atoms	
Bohr radius	= radius for which an e^- is in its ground energy state In classical energy the energy of a e^- in orbit with radius r is given by: $$E = \frac{p^2}{2m} - \frac{e^2}{(4\pi\varepsilon_0)r}.$$ > where r can be any radius > e^- can have any energy-level however in quantum, the energy levels are quantised, not continuous > say p is the average momentum of the e^- > momentum is defined within a range Δp of p > this implies there is a smallest value of uncertainty Δr for the radius: $\hbar/p$ > say r is the average radius, we have $rp \simeq \hbar$ and thus: $$E(r)\approx\frac{\hbar^2}{2mr^2} - \frac{e^2}{(4\pi\epsilon_0)\,r}$$ There is a minimum value E_0 for E at r = r_0 such that dE/dr = 0: $$r_0 = \frac{(4\pi\epsilon_0)\,\hbar^2}{me^2} = a_0 \quad : \text{ de Bohr straal}$$ and thus we find: $$E\,(r=r_0) = -\frac{m}{2\hbar^2}\left(\frac{e^2}{(4\pi\epsilon_0)}\right)^2$$ >> lowest value of E compatible with the uncertainty principle
2.5.3 the uncertainty relation for time and energy	
time-energy uncertainty	let $\psi(t) = \psi(r=r_0, t)$ be the time-wave function for a fixed $r=r_0$ > can be expressed with superposition of waves with different angular frequencies: $$\Psi(t) \;=\; \frac{1}{\sqrt{2\pi}}\int G(\omega)e^{-i\omega t}d\omega$$ Where the G(ω) can be found with Fourier-analysis: $$G(\omega) \;=\; \frac{1}{\sqrt{2\pi}}\int \Psi(t)e^{i\omega t}dt$$ we thus find the relation: $$\Delta\omega\Delta t \gtrsim 1.$$ and since $E=\hbar\omega$ we find: $$\Delta E\,\Delta t \gtrsim \hbar.$$
interpretation of t-E uncertainty	Since t is a parameter, not a variable, we cannot use the same interpretation as x-p unc. However ΔEΔt implies that if a state exists for only a time Δt > then the energy can only be defined to a precision $\hbar/\Delta t$
2.5.4 Energy width and natural lifetime of excited states of atoms	
energy an lifetime of a state	consider an excited state in an atom with energy E_b > define the lifetime τ_b of the state as the average duration of the state ie: after a time τ_b, half of the atoms have emitted a photon > the energy of the state can be found in the interval: $$\Delta E_b = \frac{\hbar}{\tau_b}$$ the natural energy width of state b
energy of ground state	The ground state should be stable > $\tau_a = \infty$ and thus the energy is sharply defined, $\Delta E_a = 0$

natural linewidth of a frequency	there is a uncertainty in energy > energy emitted between states a and b is not sharply defined ie: there is an interval of energies: $$\Delta E_{ab} = \Delta E_a + \Delta E_b = \hbar\left(\frac{1}{\tau_a} + \frac{1}{\tau_b}\right)$$ the natural linewidth is defined as *the interval of frequencies of emitted photons*: $$\Delta \nu_{ab} = \Delta E_{ab}/h.$$