Modern physics

3. Wave Packets and the Uncertainty Principle

Outline

3.1. Free electron in one dimension

AGH

Free particle (free electron) is a particle that is not subject to any forces.

V(x)=0 in the Schrödinger equation

the energy of electron

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi(x,t) = E\psi(x,t)$$

hamiltonian   wave function   wave function

Such particles should exhibit all the classical properties: they carry momentum and energy and appear to be localized, i.e. when charged, they leave well-defined tracks in a hydrogen bubble chamber
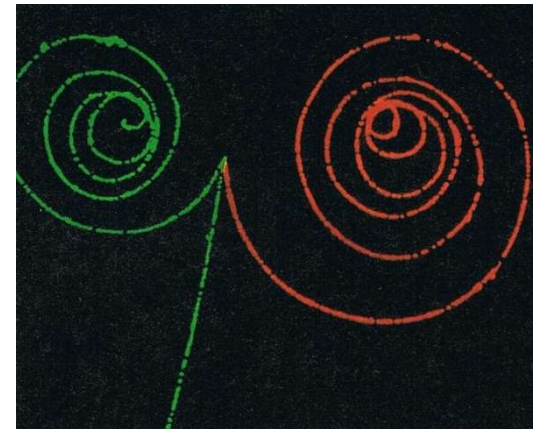
3.1. Free electron in one dimension

How can solution of the Schrödinger wave equation look like a particle?

Heisenberg uncertainty relations place limits on how well we can apply our classical intuitions about position and momentum to quantum phenomena

3.1. Free electron in one dimension

Schrödinger equation for a free electron: Proposed solution:

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t) = i\hbar\frac{\partial}{\partial t}\psi(x,t)$$ ⬅ $$\psi(x,t) = u(x)\exp\left(-\frac{iEt}{\hbar}\right)$$

Hamiltonian includes the kinetic energy E, only

SE takes the simple form:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}u(x) = Eu(x)$$

We introduce the parameter k, the wave number, defined by:

$$k^2 = \frac{2mE}{\hbar^2}$$ ➡ $$\frac{d^2}{dx^2}u(x) + k^2u(x) = 0$$

Solutions are:

$$u(x) = \exp(-ikx)$$ electron is traveling in negative x direction

$$u(x) = \exp(+ikx)$$ electron is traveling in positive x direction

From $k^2 = \dfrac{2mE}{\hbar^2}$ combined with $E = \dfrac{p^2}{2m}$ we get:

$$p = \pm\hbar k$$ eigenvalues of momentum operator $\quad \hat{p} = -i\hbar\dfrac{d}{dx}$

Simple cos(kx) or sin(kx) are not the eigenfunctions of the momentum operator but their combination exp(±ikx) is its eigenfunction. Therefore, the momentum of electron will have a definite value of momentum. Can such a particle be localized in space?

Time-dependent and space-dependent solutions combined give:

plane wave
$$\psi(x,t) = A \exp\left[\frac{i(px - Et)}{\hbar}\right]$$

Wave function of a free electron moving in one direction of x-axis; electron has <u>well-defined momentum p</u> and <u>energy E</u>

Note that for $\exp(ipx/\hbar)$ there is a periodicity in space

$$x \rightarrow x + \lambda \quad \text{wavelength}$$

$$\lambda = \frac{2\pi\hbar}{p} = \frac{h}{p} \quad \text{de Broglie relation}$$

Consequences of solution in a form of plane wave:

$$\psi(x,t) = A \exp\left[\frac{i(px - Et)}{\hbar}\right]$$

1. This solution does not describe a localized particle. The probability of finding a particle is the same at all points in space.

$$\left|\psi(x,t)\right|^2 = \left|A\right|^2$$

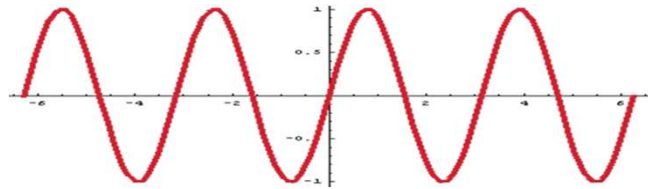2. The proposed function cannot be normalized. The constant A has to be infinitely small!

$$\int_{-\infty}^{+\infty}\left|\psi(x,t)\right|^2 dx = \left|A\right|^2 \int_{-\infty}^{+\infty} dx = 1$$

the integral is infinitely large

3.2. Wave packets

Wave
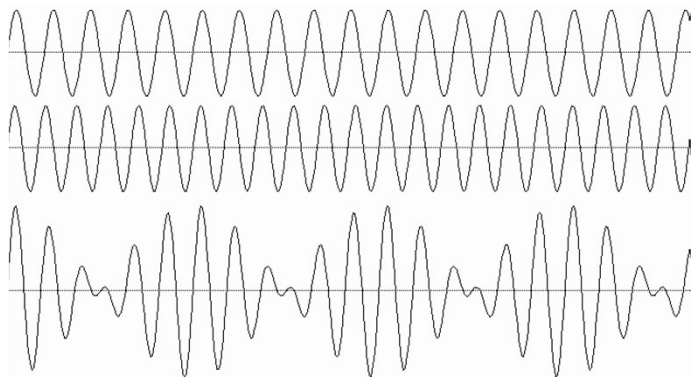
Our traditional understanding of a wave…
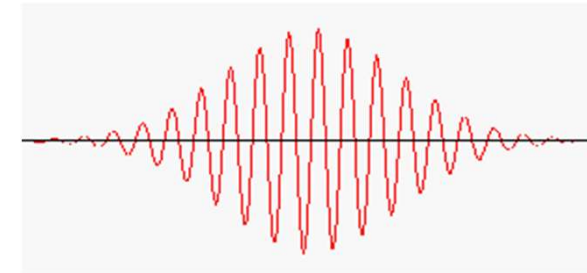
"de-localized" – spread out in space and time

Wave packet

How to construct a wave packet?

If several waves of different wavelengths (frequencies) and phases are superposed together, one would get a localized wave packet

3.2. Wave packets

A wave packet is a group of waves with slightly different wavelengths interfering with one another in a way that the amplitude of the group (envelope) is non-zero only in the neighbourhood of the particle

A wave packet is localized – a good representation for a particle!

$$\psi(x,t) = \int_{-\infty}^{+\infty} A(p) \exp\left(-\frac{i(px - Et)}{\hbar}\right) dp$$

momentum weight

This wave function is a superposition of plane waves with different momenta *p* and describes a free particle localized in the space

3.2. Wave packets

$|A(p)|^2 dp$ is proportional to the probability that the momentum will be found in a window of width *dp* around the value *p*

There are different types of momentum distribution. The type important for us is when *A(p)* is centered about some particular value p_o of momentum and falls off as we depart from p_o (e.g. Gaussian distribution.)
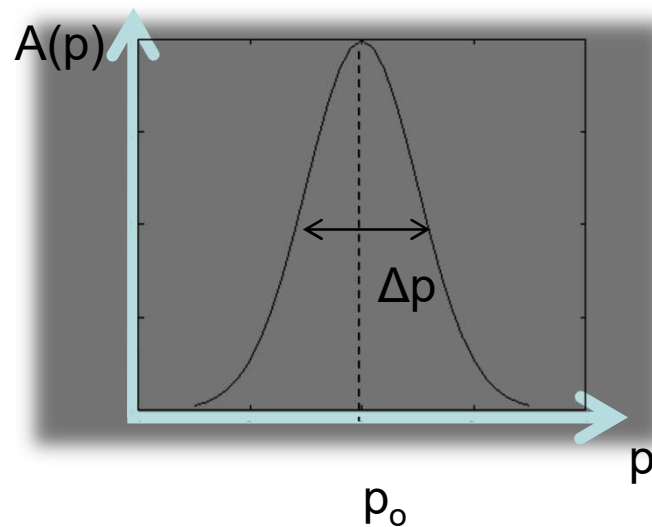
$$A(p) = C \, exp\left[-\frac{a^2(p-p_0)^2}{4\hbar^2}\right]$$

C – constant

A(p) is localized about a central value p_o

How localized the weights A(p) are, depends on a **width** Δp of momenta about p_o. There is little possibility of finding a momentum value larger than $p+\Delta p/2$ or smaller than $p-\Delta p/2$

3.2. Wave packets

The plane wave can be thought of as a limiting case with a width Δp that is infinitely small $\Delta p = 0$. The particle that has a perfectly definite momentum is highly unlocalized in space $\Delta x \longrightarrow \infty$.

 In order to avoid this, i.e. to have a localized particle with finite Δx we need a _nearly_ definite momentum $\Delta p \neq 0$. The narrower the width described by the weights A(p), the more precisely the momentum is constrained.

The more precise the momentum, the more spread out the pulse is in space. The inverse relationship between Δx and Δp is a _general feature of wave packets_ and is described quantitatively by _Heisenberg uncertainty relations_

3.3. Heisenberg uncertainty relation
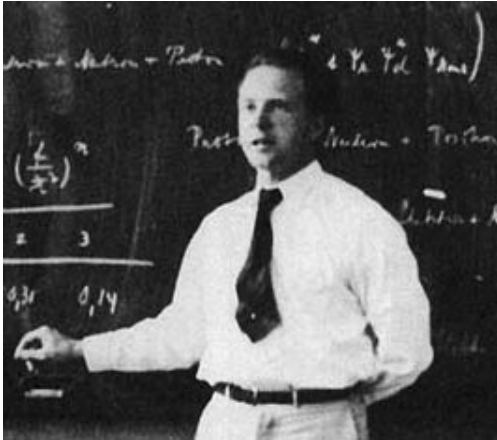
1901-1976

It was discovered in the framework of quantum mechanics by **Werner Heisenberg** in 1927 and plays a critical role in the interpretation of quantum mechanics and in showing that there could be no conflict between quantum and classic physics in their respective domains of applicability.

$$\Delta x \Delta p \geq \hbar/2$$

Position-momentum uncertainty relation

We cannot simultaneously measure the position and the momentum of a particle with arbitrary precision.

Evaluation of width in position and momentum

We define the width in position Δx as the square root of the variance σ²(x) in the space distribution:

$$(\Delta x)^2 = \sigma^2(x) = \left\langle x^2 \right\rangle - \left\langle x \right\rangle^2$$

Similarly, the width in momentum Δp is the square root of variance σ²(p) in the momentum distribution

$$(\Delta p)^2 = \sigma^2(p) = \left\langle p^2 \right\rangle - \left\langle p \right\rangle^2$$

Gaussian wave packet

$$A(p) = C\ exp\left[-\frac{a^2(p-p_0)^2}{4\hbar^2}\right]$$

is one particular example for which the position-momentum Heisenberg relation is realized as an equality.

$$\Delta x \Delta p = \hbar / 2$$

For Gaussian wave packet we have the maximum simultaneous localization in position and momentum, in a sense that the product $\Delta x \Delta p$ is as small as it can be.
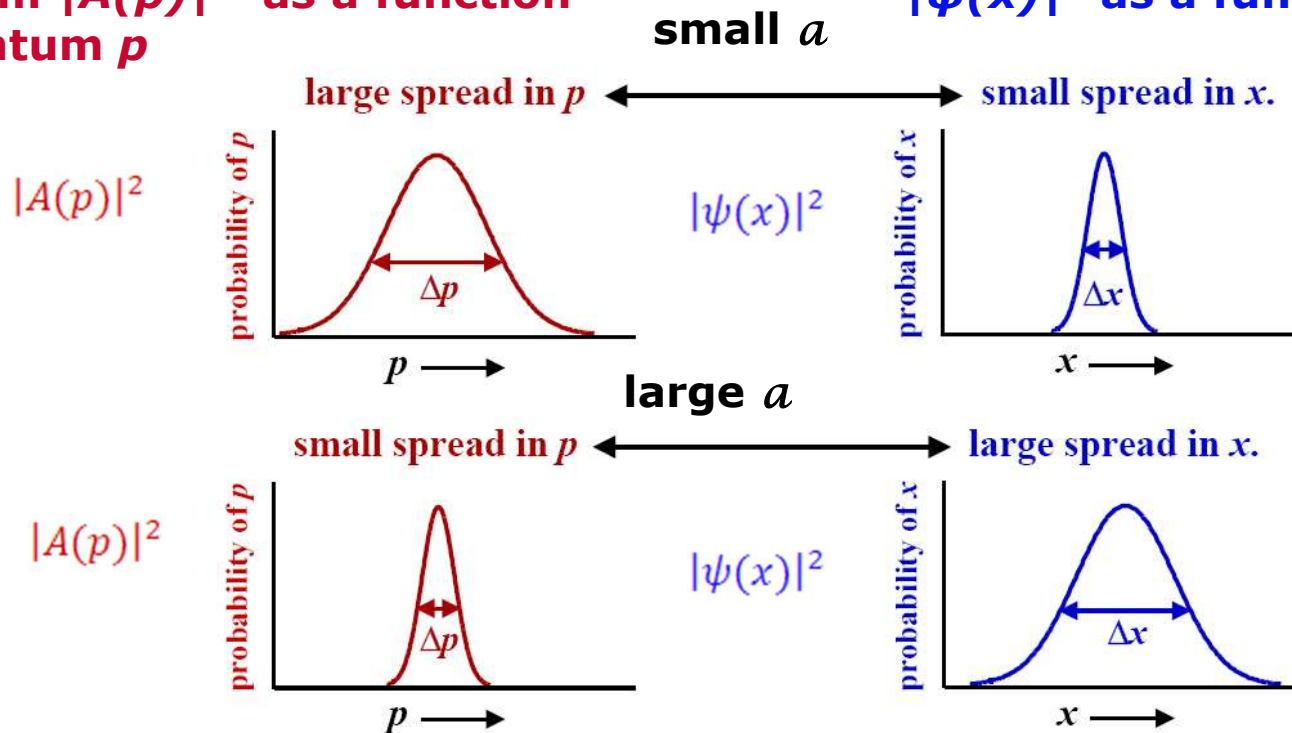
3.3. Uncertainty relation

For the Gaussian wave packet $\quad A(p) = C \, exp\left[-\dfrac{a^2 (p - p_0)^2}{4\,\hbar^2} \right]$

$$\Delta p \propto \hbar/a \qquad\qquad \Delta x \propto a$$

The probability density for momentum $|A(p)|^2$ as a function of momentum p

The probability density $|\psi(x)|^2$ as a function of x

small a

large a

3.3. Uncertainty relation

The Heisenberg uncertainty relation is not restricted to quantum mechanics.

From de Broglie relation: $\Delta p / \hbar = \Delta k$

Heisenberg relation becomes:

$$\Delta k \Delta x \geq 1/2$$

This relation applies equally to pulses of sound!

3.4. The physical meaning of the uncertainty relations

Example: Consider a grain of dust of mass 10^{-7} kg moving with the velocity around 10 m/s. Suppose that measuring instruments available to us leave the velocity uncertain within the range of 10^{-6} m/s (i.e. one part in 10^7). Given the instrumental uncertainty in the velocity, find the intrinsic quantum mechanical uncertainty of a position measurement of the dust of grain.

Solution: The instrumental uncertainty in the momentum is

$$\Delta p = m\Delta v = \left(10^{-7}\, kg\right)\left(10^{-6}\, m/s\right) = 10^{-13}\, kg \cdot m/s$$

Hence, according to the uncertainty relation, the position could be at best be measured to within the window

$$\Delta x \cong \frac{\hbar}{\Delta p} = \frac{1.05 \times 10^{-34}\, J \cdot s}{10^{-13}\, kg \cdot m/s} \cong 10^{-21}\, m$$

This is an extremely small number, of about 10^{11} smaller than the size of one of the approximately 10^{19} atoms that make up the dust particle!

3.4.1. Heisenberg microscope

This „*thought experiment*" was devised by Heinsenberg himself. Imagine a microscope that is designed to measure an electron's x – position and the p_x – the component of the electron's momentum simultaneously.
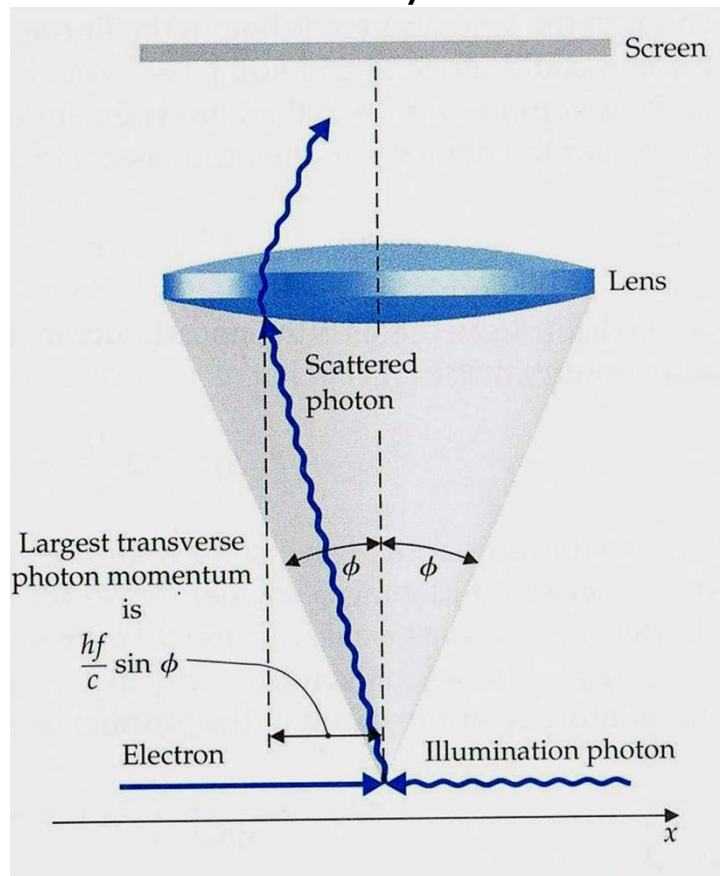

Suppose an electron moves from the left to the right with the well-defined initial momentum p_x. The electron's position is to be observed by shining light on it.

The light comes in the form of a single photon with a precisely known momentum (a precisely known wavelength) coming from the right. The timing of collision between the electron and the photon is arranged so that it takes place under the lens of a microscope. The observation takes place if the photon scatters off the electron and passes through the lens onto a photographic plate.

3.4.1. Heisenberg microscope
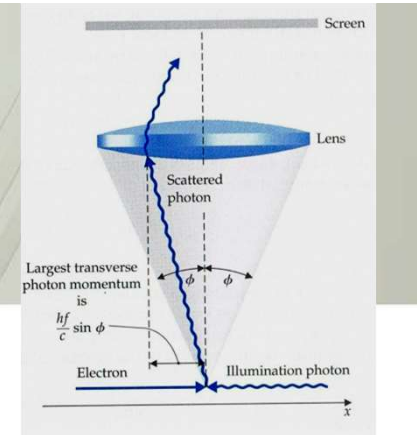
The classical optics gives for the resolution of lens:

$$\Delta x \cong \frac{\lambda}{sin\theta}$$

Not resolved   barely resolved   resolved
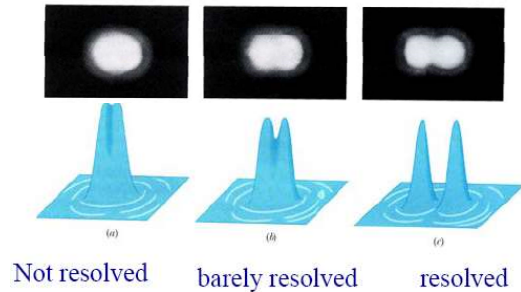
λ-photon wavelength after collision

Δx is simultaneously the ability to locate the electron in space and uncertainty in electron's position; in order to reduce it we need smaller wavelength or larger angle θ

Uncertainty in the electron's momentum (its x-component) Δp_x after collision, when its position is measured, is the same as the uncertainty in the photon's momentum. Photon's momentum after collision is uncertain, because we do not know the exact direction of the photon when it passed through the lens.

$$\Delta p_x \cong 2\frac{hf}{c}sin\theta$$

In contrast to Δx, smaller wavelength (larger frequency f) or larger angle θ raise Δp_x

3.4.1. Heisenberg microscope

The product of Δx and Δp$_x$ is
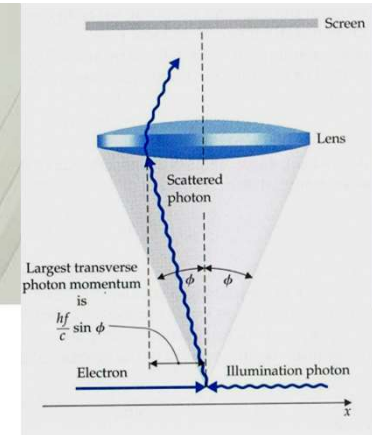
$$\Delta x \Delta p_x \cong \frac{\lambda}{sin\theta} \frac{2hf}{c} sin\theta = 2h = 4\pi\hbar$$

This result is independent of any details of the system and takes the general form of Heisenberg's relation

The complementary wavelike and particlelike properties of radiation can be reconciled only within the limits imposed by the uncertainty principle.

Uncertainty principle always saves us from contradiction.

3.4.2. Two-slit experiment

Electrons passing thought a pair of slits produce an interference pattern even if they pass with such a low intensity that we have only one electron at a time. But it seems that just knowing which slit the electron went through destroys the interference pattern. The uncertainty principle ensures that this is exactly the case!!!

The condition for the constructive interference is

$$a \sin\theta_n = n\lambda \qquad n = 0, \pm 1, \pm 2, ...$$
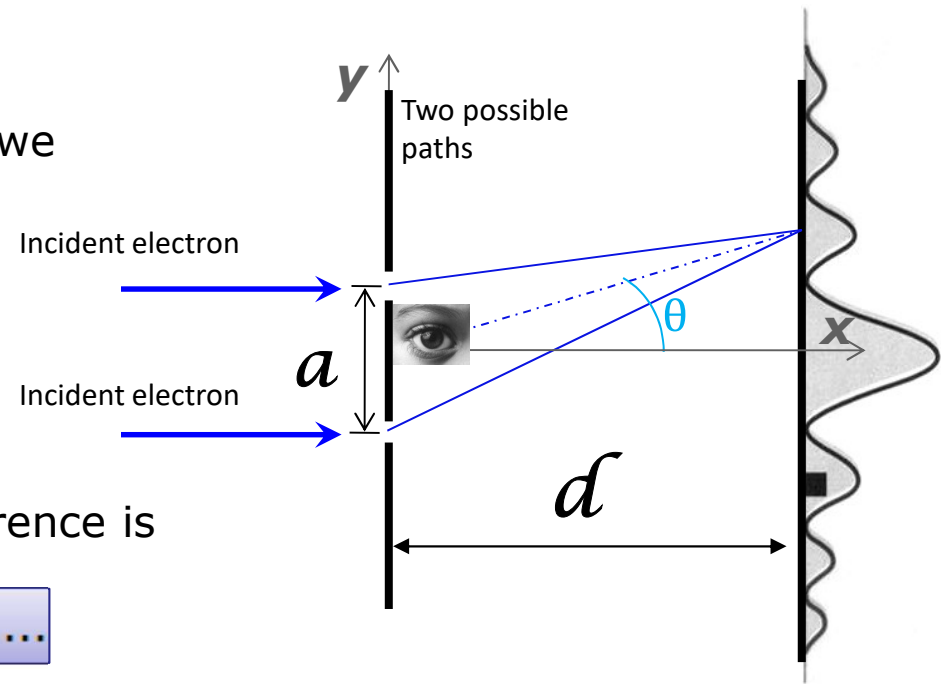
The separation between adjacent maxima on the detection screen is

$$d \sin\theta_{n+1} - d \sin\theta_n = \frac{\lambda d}{a}$$

3.4.2. Two-slit experiment

A monitor (an eye) just behind the slits determines the position of the electron to an accuracy sufficient to tell which slit the electron came through. This is equivalent to a measurement of the y-components of the electron's position with the precision better than the separation between the slits:

$$\Delta y < \frac{a}{2}$$

Any measurement of the position of electron (by scattering a photon at an electron) transfers the photon momentum to the electron and introduces an uncertainty Δp_y in the electron's y momentum. We can estimate the minimum size of the Δp_y by means of the uncertainty principle

$$\Delta p_y > \frac{(\hbar/2)}{(a/2)} = \hbar/a$$

3.4.2. Two-slit experiment

Having introduced an uncertain transverse component of momentum, we have automatically introduced an uncertainty in the arrival spot on the detection screen. If the electron came through carrying a longitudinal momentum p, then the electron moves off the two slits at an angle

$$\Delta\theta = \frac{\Delta p_y}{p} = \frac{\hbar}{ap} = \frac{\lambda}{2\pi a}$$

Finally, the angular uncertainty translates into an uncertainty in the arrival point on the detection screen. The transverse arrival position is uncertain by:

$$\Delta y = d\Delta\theta = \frac{d\lambda}{2\pi a}$$

Comparing this result with the separation between two adjacent maxima:

$$d\Delta\theta = \frac{\lambda d}{a}$$

we see that our monitor has disturbed the electron enough to wipe out the interference pattern

3.5.The time – energy uncertainty relation

There is another uncertainty relation that is quite useful – one involving time and energy. We can find it by using the momentum – position Heisenberg's relation

For $E = p^2/2m$ we have:
$$\Delta E = \frac{(2p\Delta p)}{2m} = \frac{p\Delta p}{m} = \upsilon\Delta p$$

then
$$\Delta E = \upsilon\Delta p \geq \upsilon\frac{\hbar/2}{\Delta x} = \frac{\hbar/2}{(\Delta x/\upsilon)} = \frac{\hbar/2}{\Delta t}$$

$$\Delta E\,\Delta t \geq \hbar/2$$

Time-energy uncertainty relation

It asserts that a state of finite duration Δt cannot have a precisely defined energy, but we deal with the uncertainly in E.

3.5.The time – energy uncertainty relation

If an excited atomic state has a lifetime τ, the excited state does not have a precise energy E_1; rather its energy is uncertain by an amount
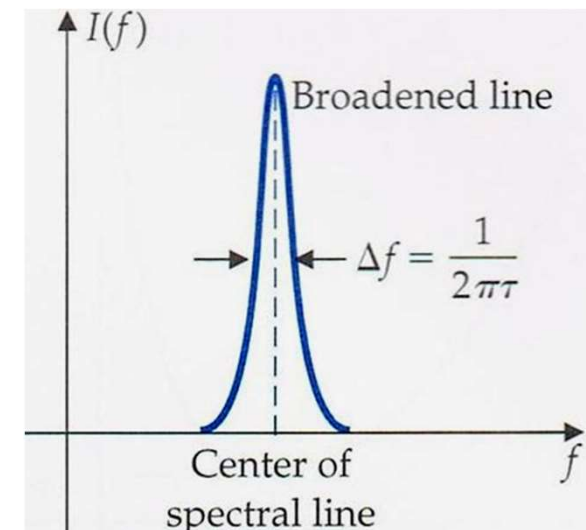
$$\Delta E_1 = \frac{\hbar}{\tau}$$

This uncertainty manifests itself when the state decays to the ground state with energy E_0; the frequency of the radiation emitted in the decay:

$$f = \frac{E_1 - E_o}{h}$$

will be spread by an amount

$$\Delta f = \frac{\Delta E_1}{h} \cong \frac{1}{2\pi\tau}$$

Broadening of spectral lines is a quantum mechanical phenomenon

Estimation of ground state energy

Harmonic oscillator with classical energy

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

ω is the angular frequency of harmonic oscillator

Classically, the minimum energy is zero, which occurs when the kinetic energy is zero (p=0) and the particle is at rest at a position corresponding to the bottom of the potential-energy well.

From the uncertainty principle: both momentum and position cannot be known precisely.

If the uncentrainty in position is $\quad \Delta x = a$

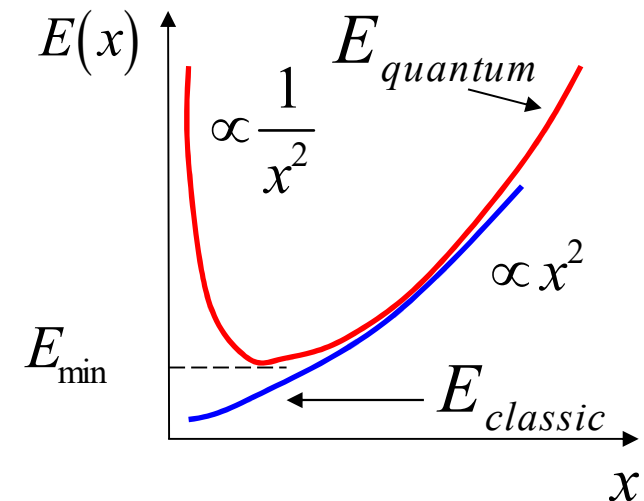then momentum's uncertainty is $\quad \Delta p = \frac{\hbar}{2a}$

Estimation of ground state energy

Near the lowest possible energy, where classically $p=0$

$$\Delta p = p$$

The energy is
$$E(x) = \frac{(\Delta p)^2}{2m} + \frac{1}{2}m\omega^2(\Delta x)^2$$

and
$$E(a) = \frac{\hbar^2}{8ma^2} + \frac{1}{2}m\omega^2 a^2$$

The minimum value of energy can be calculated and the result is

$$E_{min} = \frac{\hbar\omega}{2}$$ **zero-point energy**

The uncertainty principle requires that a little residual motion remain in any physical system

Conclusions

• A free electron in a 1D system can be described by the plane wave resulting from the Schrödinger equation, assuming the potential equal to zero. This solution represents an extreme manifestation of the uncertainty principle ($\Delta p = 0$, $\Delta x \rightarrow \infty$)

• Simultaneous uncertainty in both position and momentum requires construction of wave packets. Then there is a significant probability of finding the particle only in limited regions of space – particle is localized

• The magnitude of the position-momentum and energy-time effects is proportional to Planck's constant, and the restriction would vanish entirely if that constant were equal to zero. Thus Planck's constant once again determines the magnitude of quantum mechanical effects