CHM 305: The Quantum World
Lecture 1

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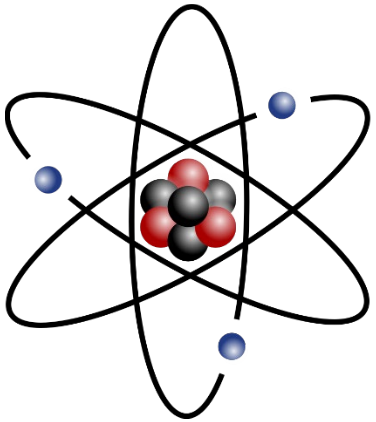
Introducing quantum mechanics

The development of quantum mechanics was a revolution in physics that occurred in the early 20^{th} century

- QM is necessary evil to reproduce experiments!
- Matter is not a smooth continuum
- Tiny fundamental units of matter and light (photons, electrons, protons, atoms, molecules) behave according to new laws
- Trajectories are probabilistic, not deterministic
- Classical mechanics falls out of quantum theory in certain limits (high energy, heavy masses)

classical

- Meter scale
- Kilogram scale
- Typical kinetic energy ~ 100 J



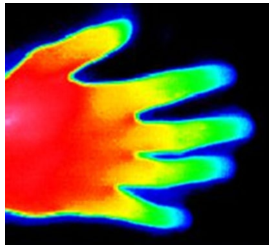
quantum

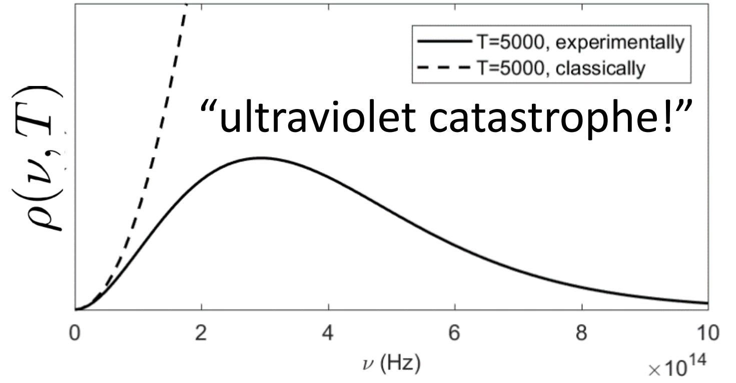
- 10^{-9} m scale
- 10^{-26} kg scale
- Typical atomic energies ~ 10^{-19} J

Not what we are used to experiencing, but hugely important to chemistry!

Famous experiments poked holes in classical physics

blackbody radiation

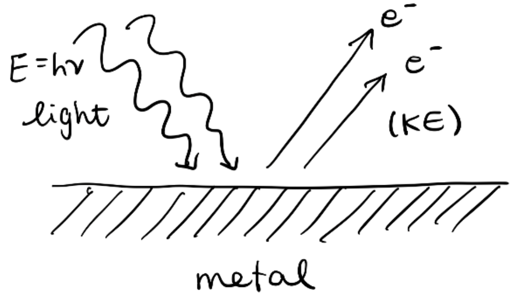


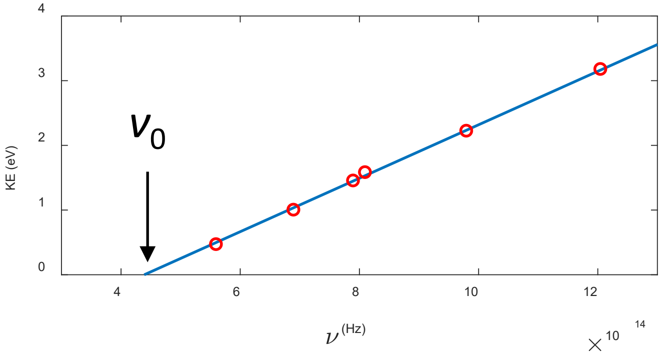


Classical physics fails to predict the frequency spectra of light emitted by hot objects

Max Planck (Nobel Prize 1918)

photoelectric effect

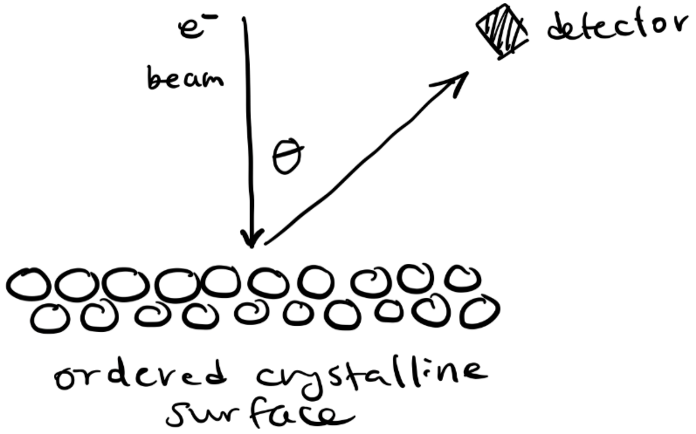




Classical physics fails to predict the emission of electrons from metal surfaces after radiation with light

Albert Einstein (Nobel Prize 1921)

electron diffraction



Classical physics fails to predict the angle-dependence of electrons scattered off ordered surfaces

Davisson and Thomson
(Nobel Prize 1937)

Famous experiments poked holes in classical physics

blackbody radiation

Light seems to carry energy proportional to its frequency, not its intensity

$$E = h\nu$$

Max Planck (Nobel Prize 1918)

photoelectric effect

Waves sometimes act an awful lot like particles!

(e.g. they come in discrete units called photons)

Albert Einstein (Nobel Prize 1921)

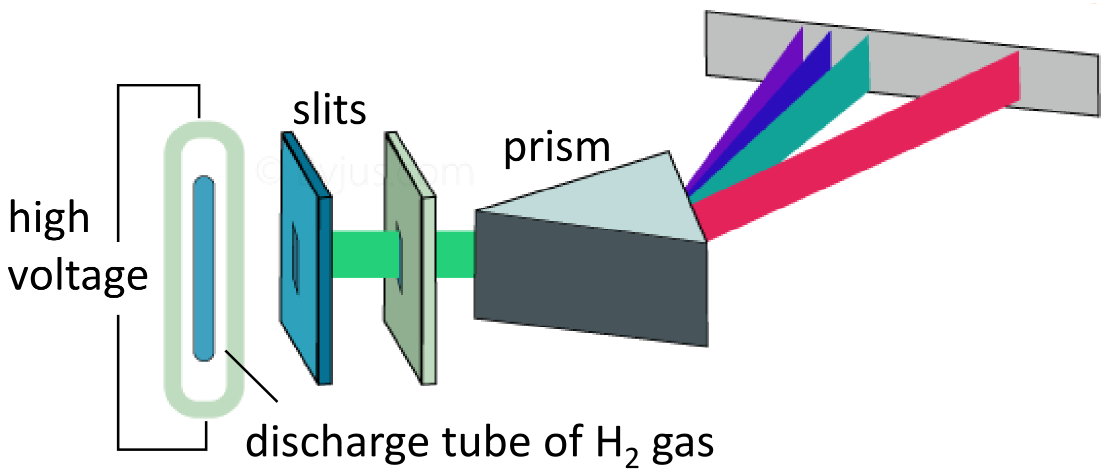
electron diffraction

Particles sometimes act an awful lot like waves!

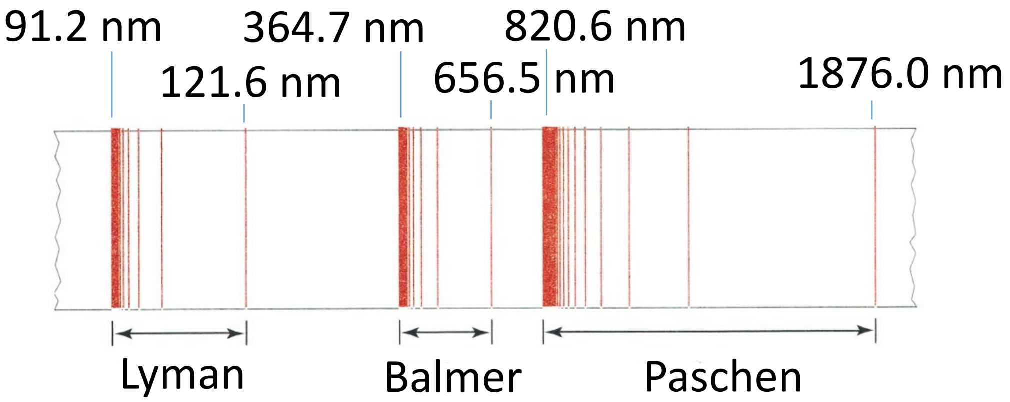
(e.g. they can show interference patterns!)

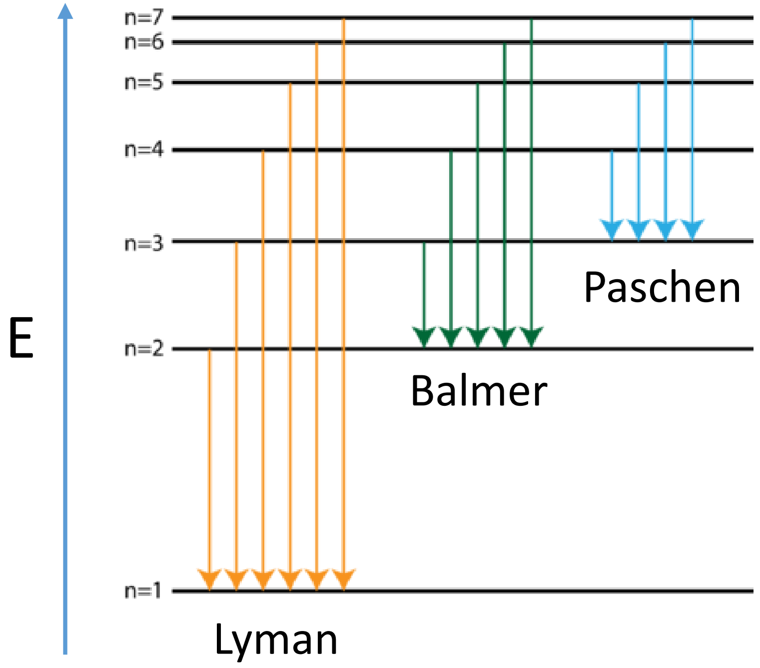
Davisson and Thomson
(Nobel Prize 1937)

Famous experiments poked holes in classical physics



atomic hydrogen emission spectrum





- Highly excited atoms are observed to emit only discrete frequencies of light
- The energy of the system must be quantized!

- **By the midterm, we'll better understand where these discrete energy spectra come from and how to predict them in atoms and molecules**

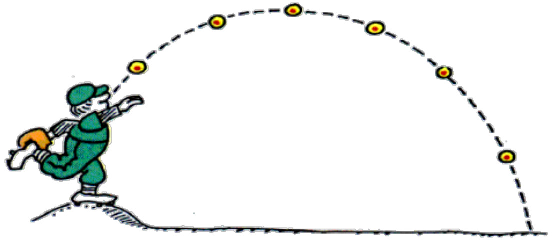
Wave-Particle Duality

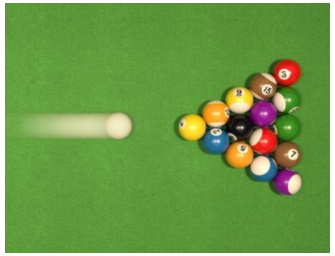
Learning goals:

- Remind ourselves how classical waves behave
- Articulate some ways in which quantum objects behave like particles and also like waves
- Calculate the de Broglie wavelength for a particle, and determine whether or not this wavelength is experimentally meaningful

Classical mechanics

particles





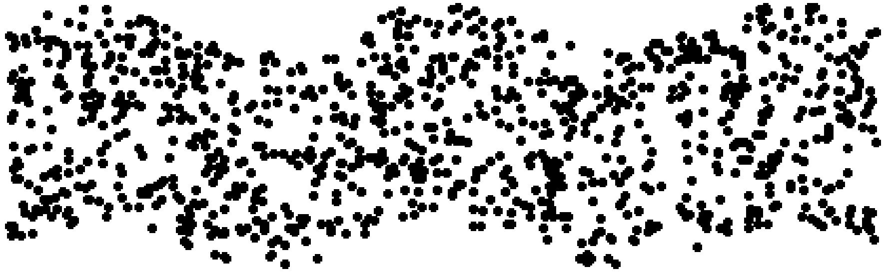
Newton's laws $F = ma = m\ddot{x}$

Can calculate trajectories in time:

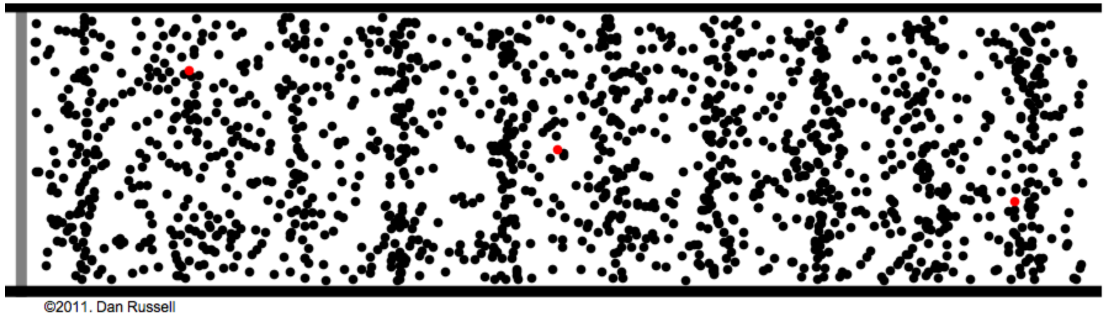
$$x(t),\ \dot{x}(t),\ \ddot{x}(t)$$

waves

transverse



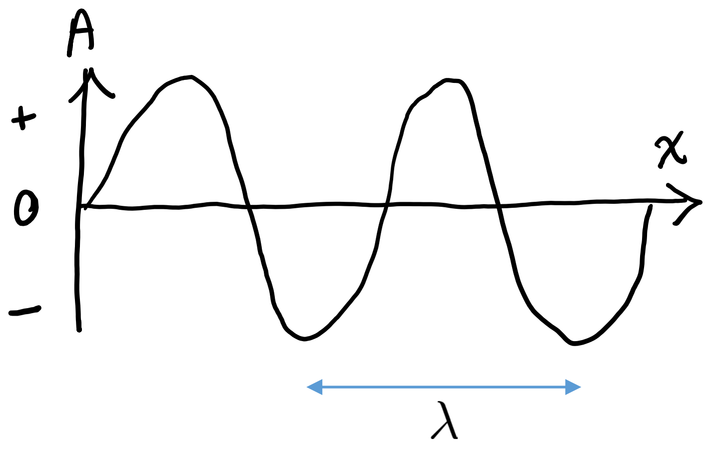
longitudinal or compression



Can calculate displacement as a function of time:

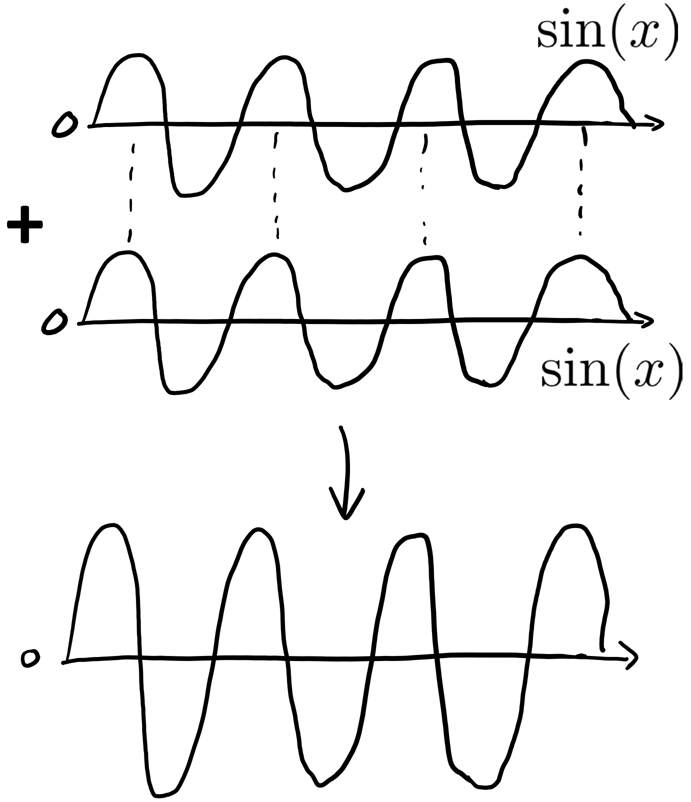
$$\frac{\partial^2 g}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 g}{\partial t^2} \quad \rightarrow \quad g(x,t)$$

Classical wave phenomena

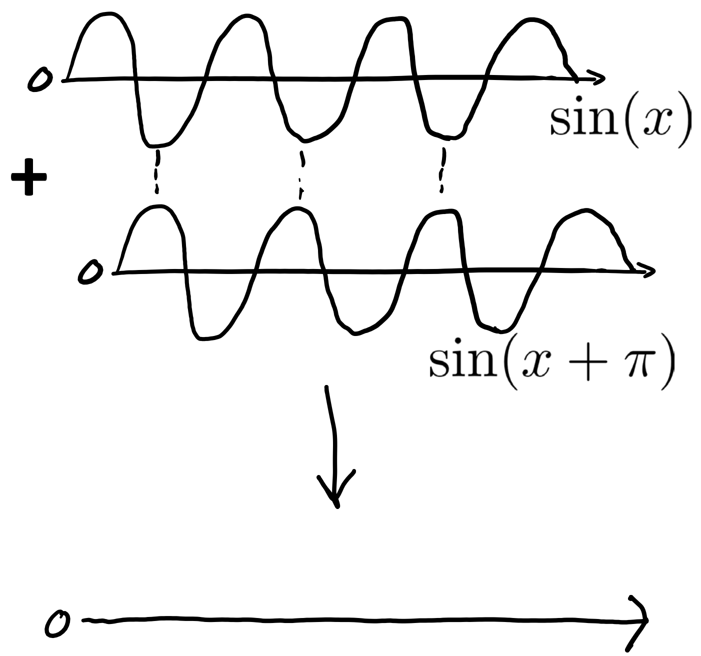


- displacement or oscillation about zero mean
- amplitude has a sign
- interference, diffraction effects depend on relative *phases* of waves

constructive interference
waves *in-phase* (0°)



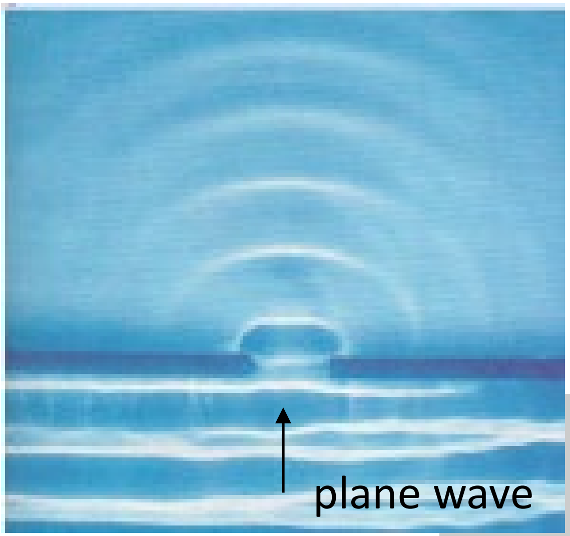
destructive interference
waves *out-of-phase* (180°)



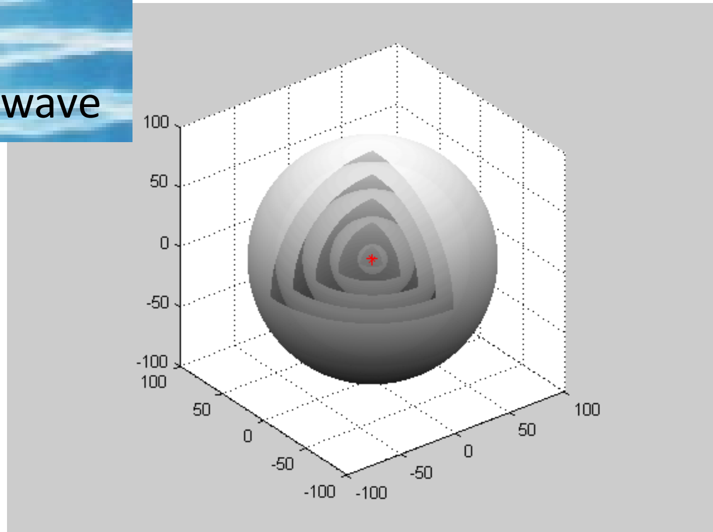
Classical wave phenomena

Waves are delocalized

Wave fronts can be curved

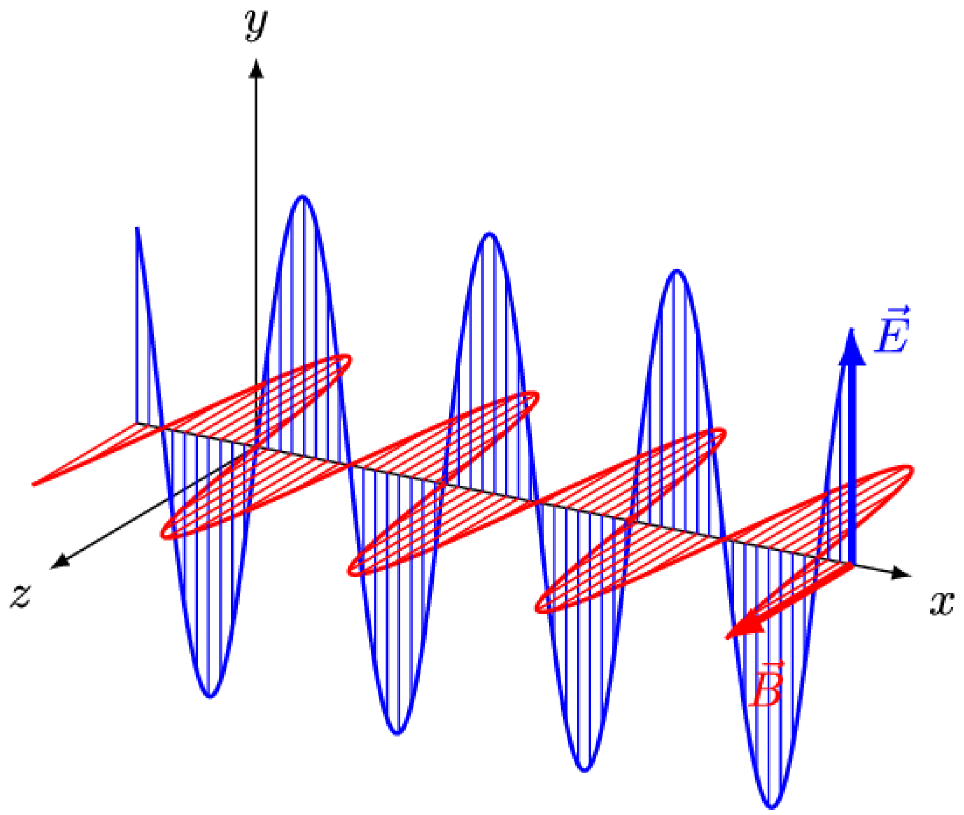


cylindrical wave emitted from a point source in 2D space



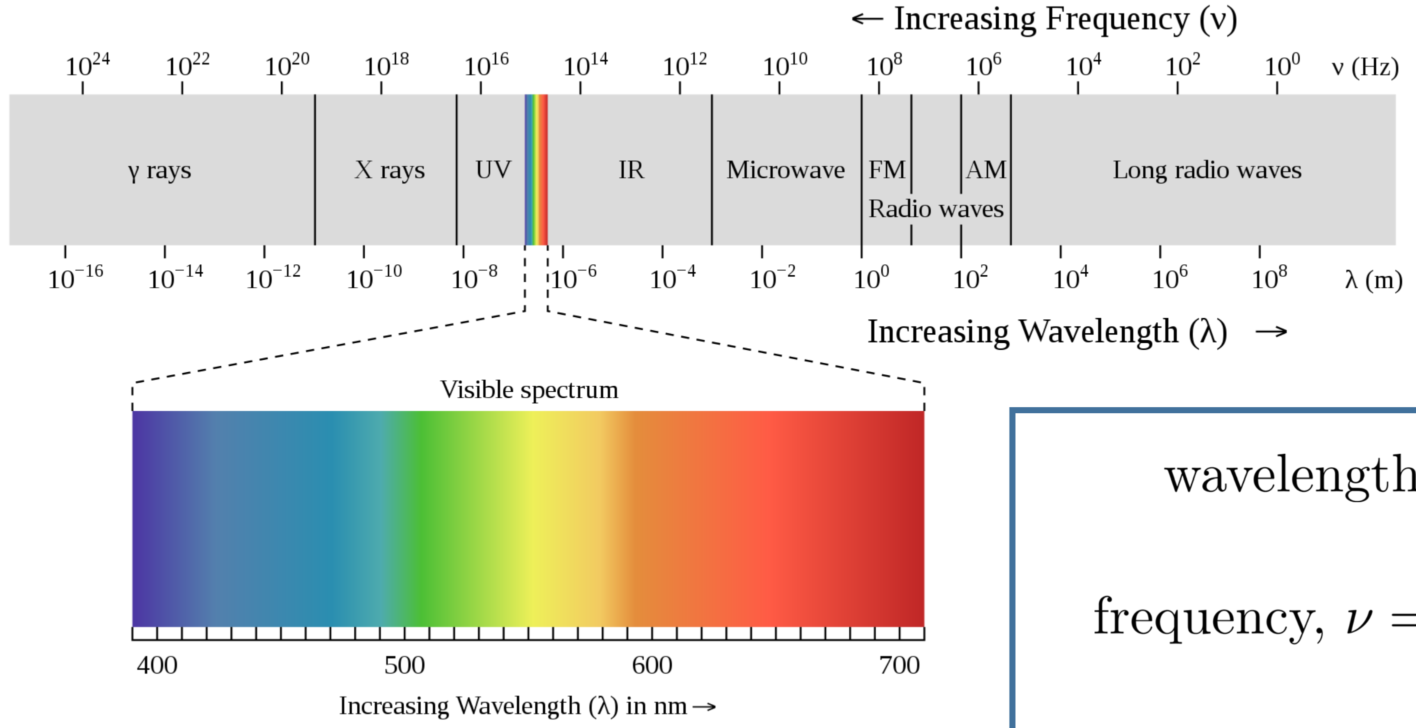
point sources emit spherical waves in 3D space

Light is an electromagnetic wave



A valid solution to Maxwell's equations!

$$E_y(x,t) \sim \sin(kx - \omega t)$$
$$B_z(x,t) \sim \sin(kx - \omega t)$$



wavelength, λ

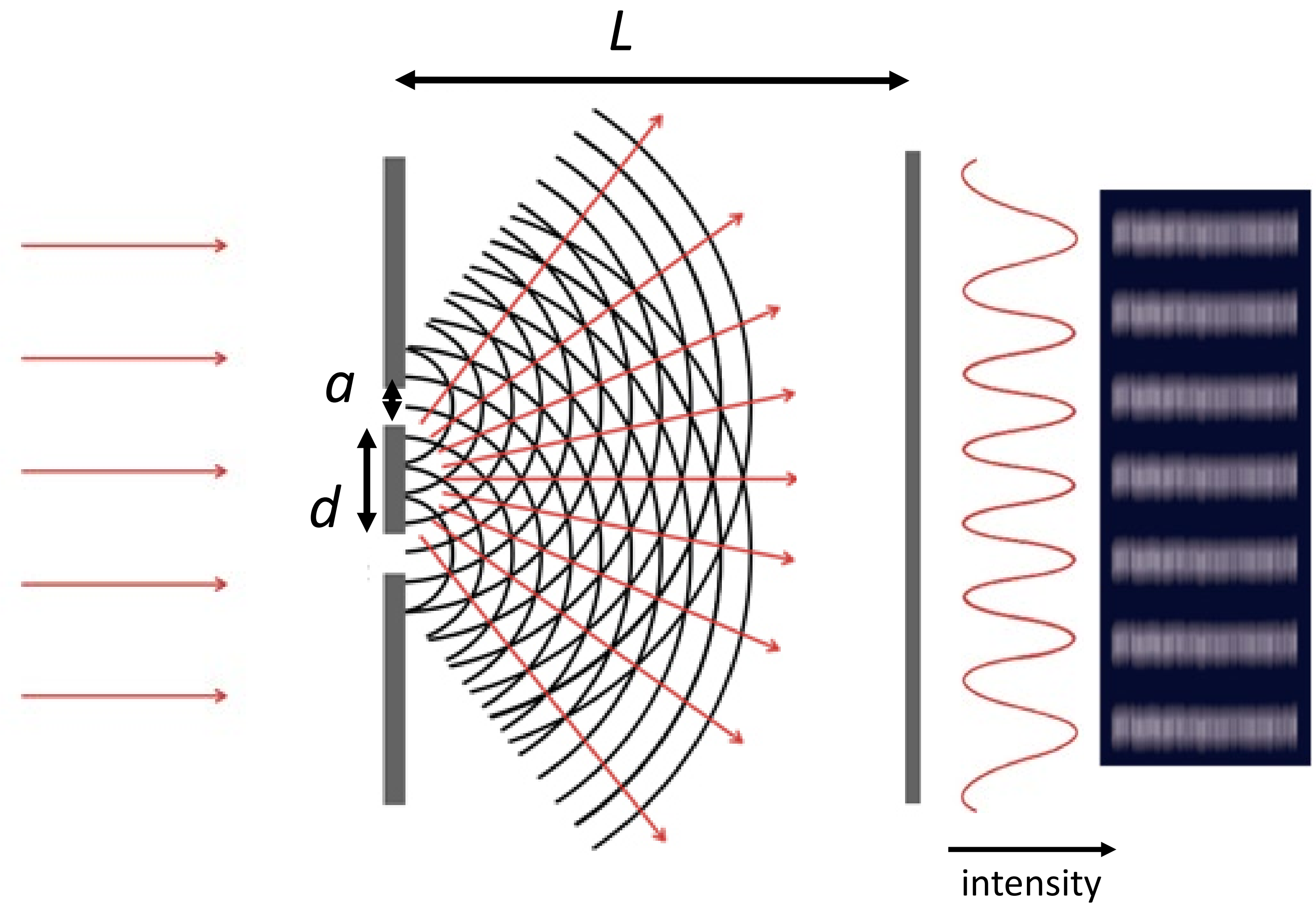
frequency, $\nu = \dfrac{c}{\lambda}$

wavenumber, $\tilde{v} = \dfrac{1}{\lambda}$

$$E = h\nu$$

$$h = 6.626 \times 10^{-34}\,\mathrm{J \cdot s}$$

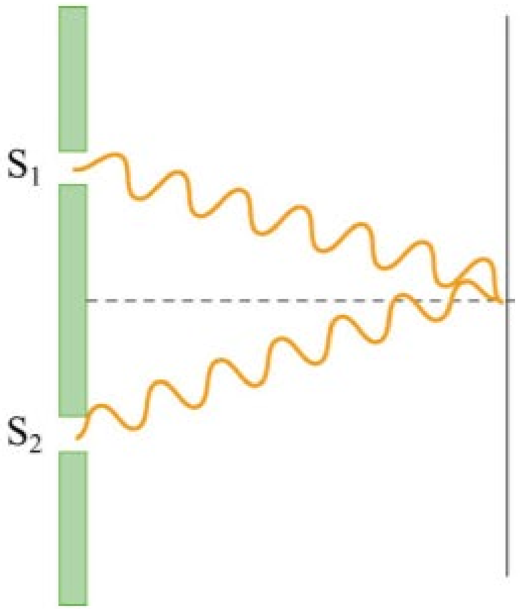
Classical diffraction of light through a double slit



- Each slit becomes a new point source of light
- Two sources interfere with one another
- Destructive interference at minima, constructive at maxima

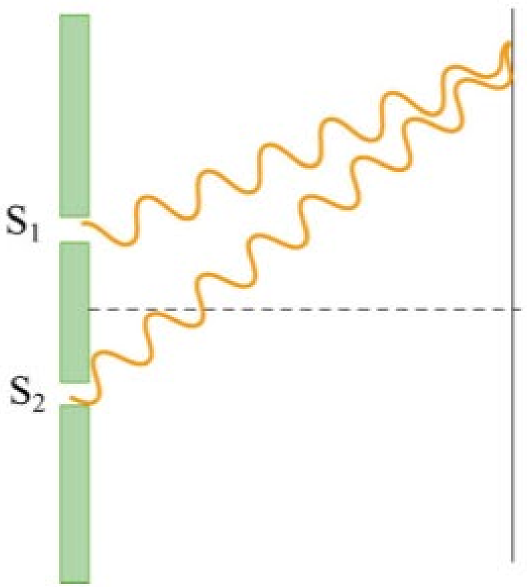
Which positions on the screen are bright or dark?

A



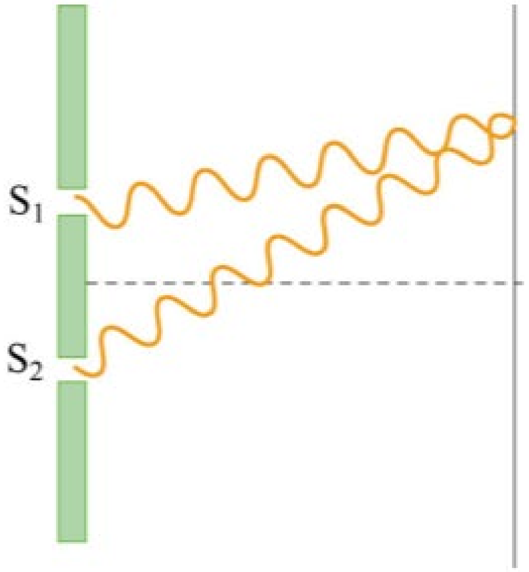
constructive interference
Bright!

B



constructive interference
Bright!

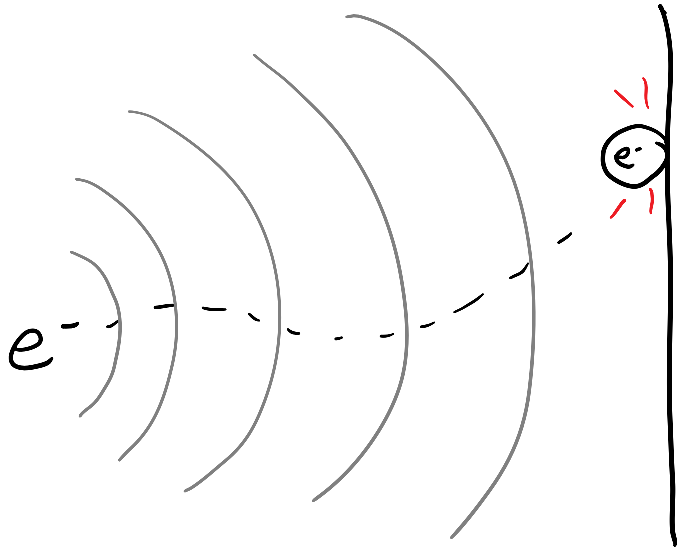
C



destructive interference
Dark

Quantum mechanical wave-particle duality

A small particle (e^-, atom, molecule) shows properties of both waves and particles:

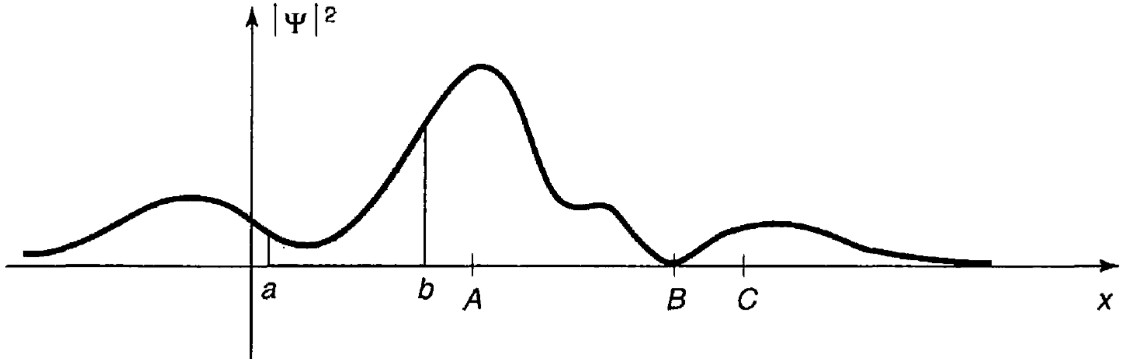


Imagine if sound waves behaved like this!

Quantum particles are governed by a *wavefunction*

$$\psi(x,t)$$

- Describes the probability distribution of where we expect to find the particle



$$\int_a^b |\psi(x,t)|^2 dx \quad = \Bigg\{$$ probability of finding the particle between *a* and *b*, at time *t*

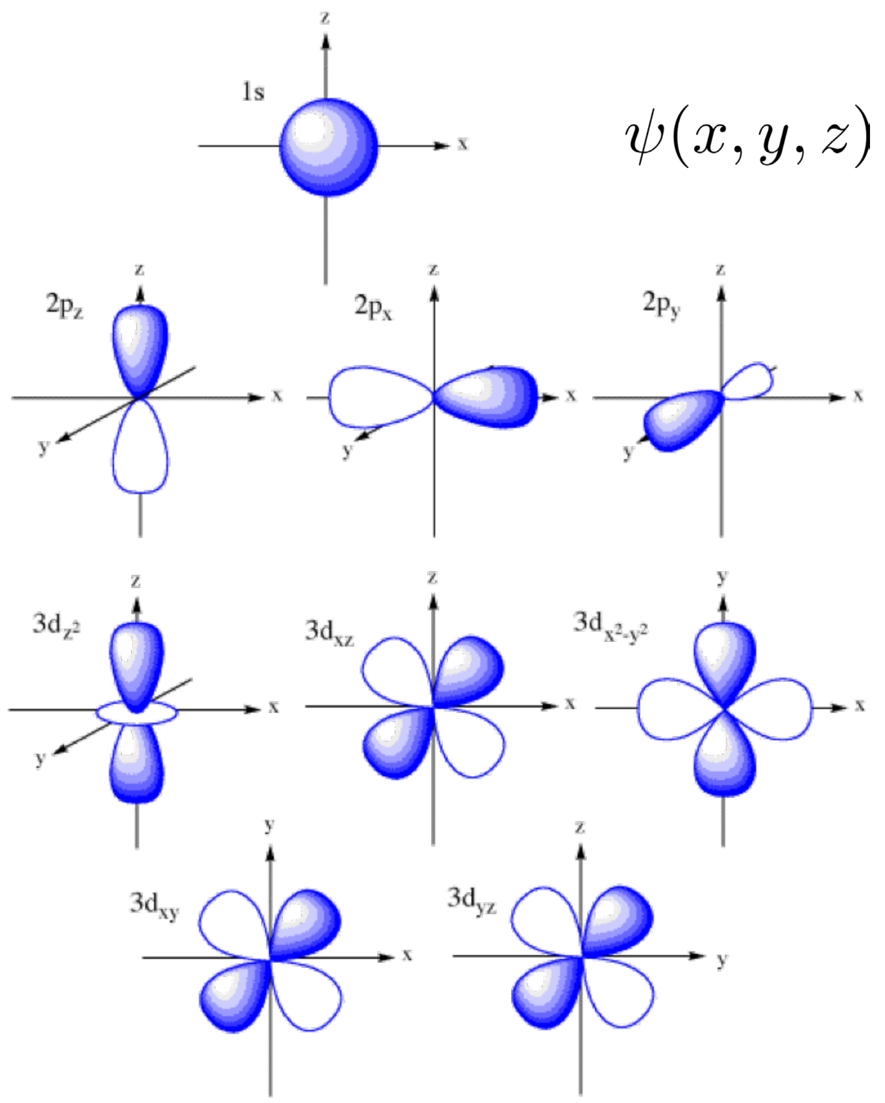
Atomic orbitals are electron wavefunctions

Recall atomic orbitals from general chemistry:

- Diffuse, three-dimensional probability distributions of where you expect to find the electron
- Have lobes with amplitudes of different signs (just like waves)

Probability of finding the electron at (x,y,z) coordinates:

$$P \propto |\psi(x, y, z)|^2$$



What is the wavelength of a particle?

Einstein used special relativity to relate light's wavelength and momentum:

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

In 1924, de Broglie asked, what if the same was true for a particle?

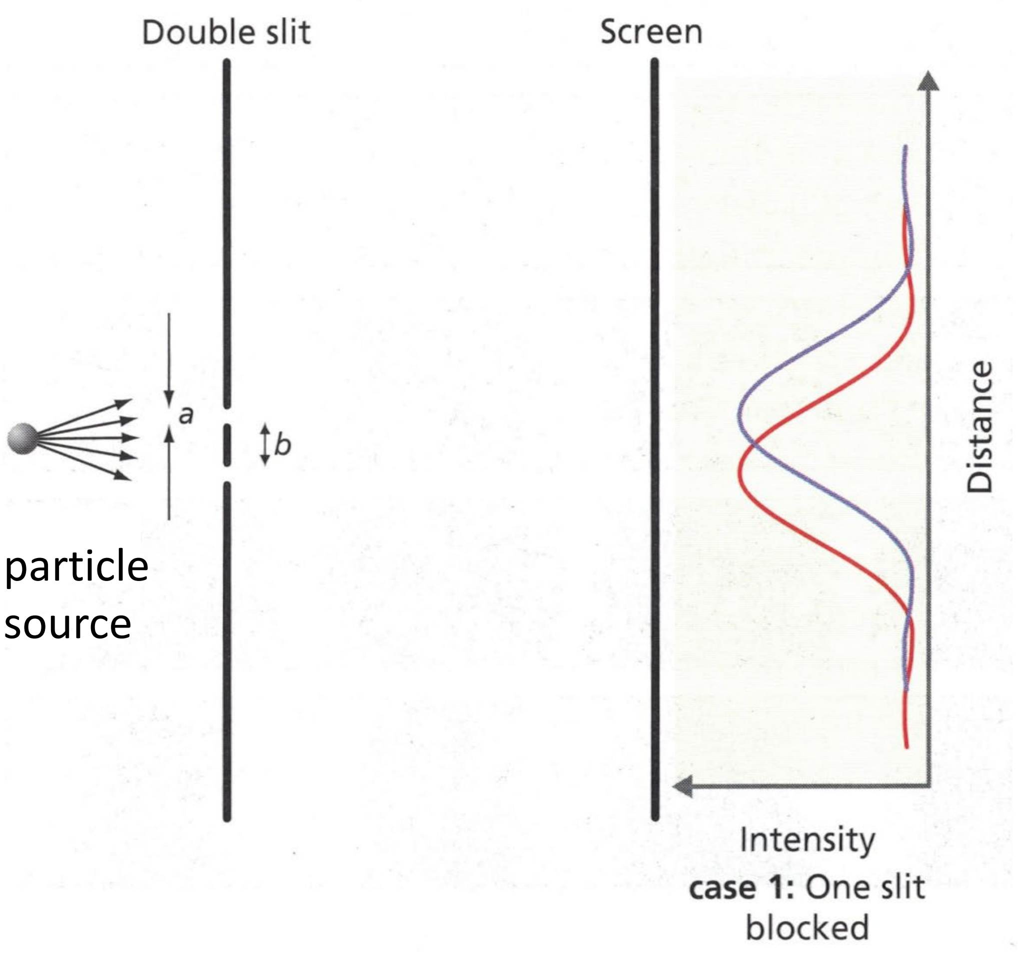
$$\lambda_\mathrm{d} = \frac{h}{p} = \frac{h}{mv}$$

For a sense of scale:

Baseball (150 g) being thrown at 10 m/s	$\lambda_\mathrm{d} \sim 4 \times 10^{-34}\,\mathrm{m}$
N_2 molecule in an ideal gas at 300 K	$\lambda_\mathrm{d} \sim 0.2\,\text{Å}$
Electron accelerated to 10^6 m/s in a 100 V CRT	$\lambda_\mathrm{d} \sim 1\,\text{Å}$

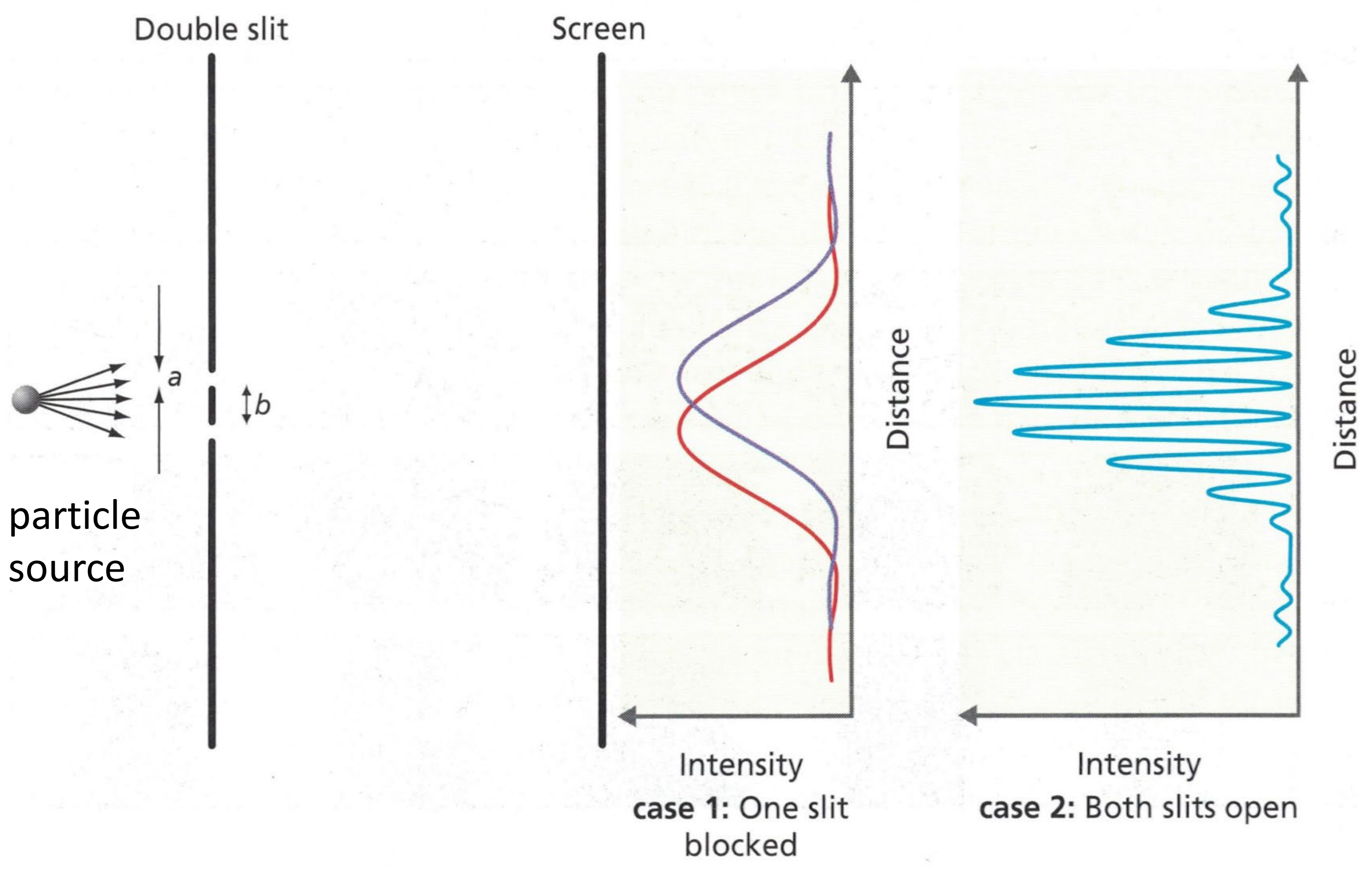
atomic scale! Similar to x-ray wavelengths

Particle diffraction through a double slit



particle source

Particle diffraction through a double slit



A single particle's wavefunction shows interference as it passes through both slits simultaneously

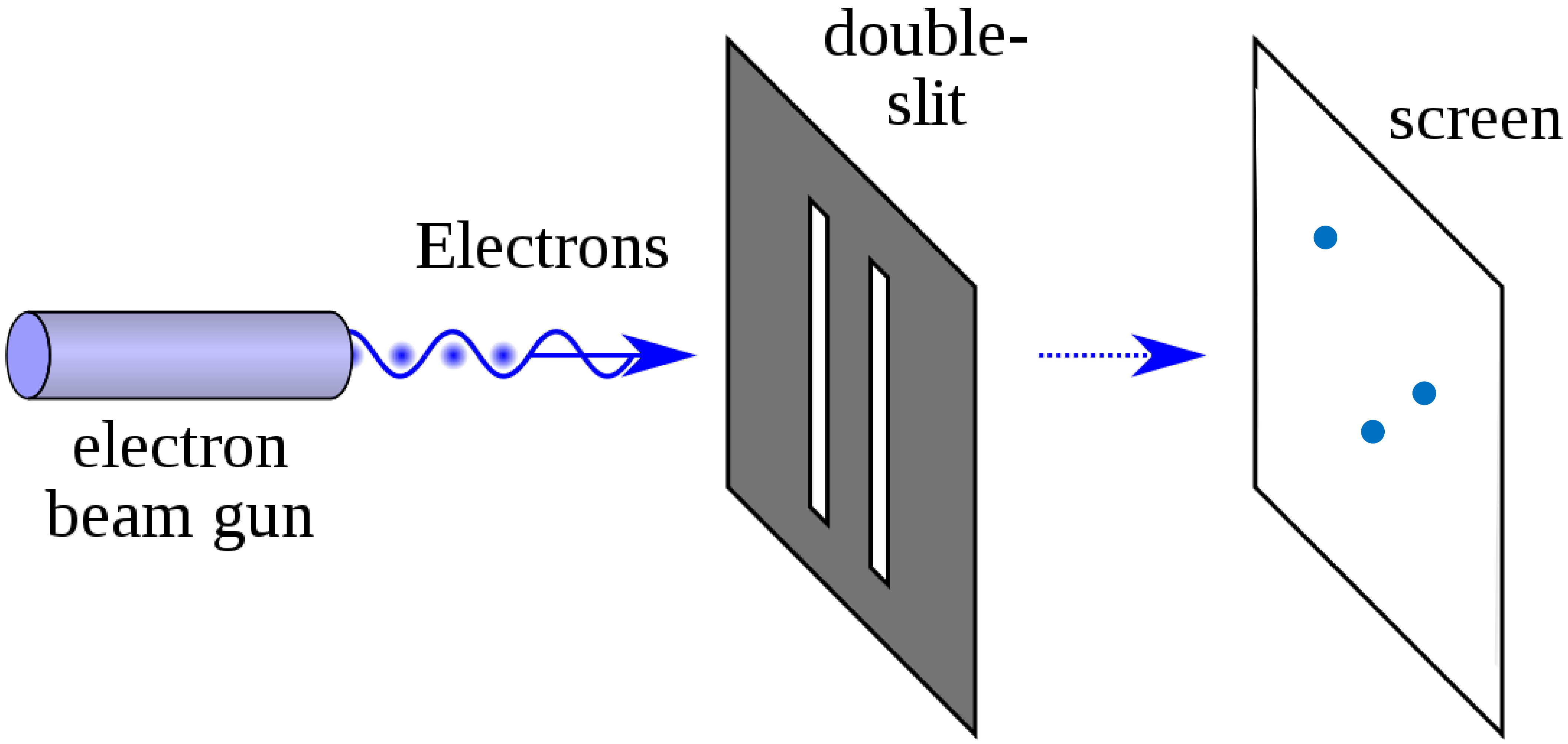
Wave-like

- spatial distribution shows interference

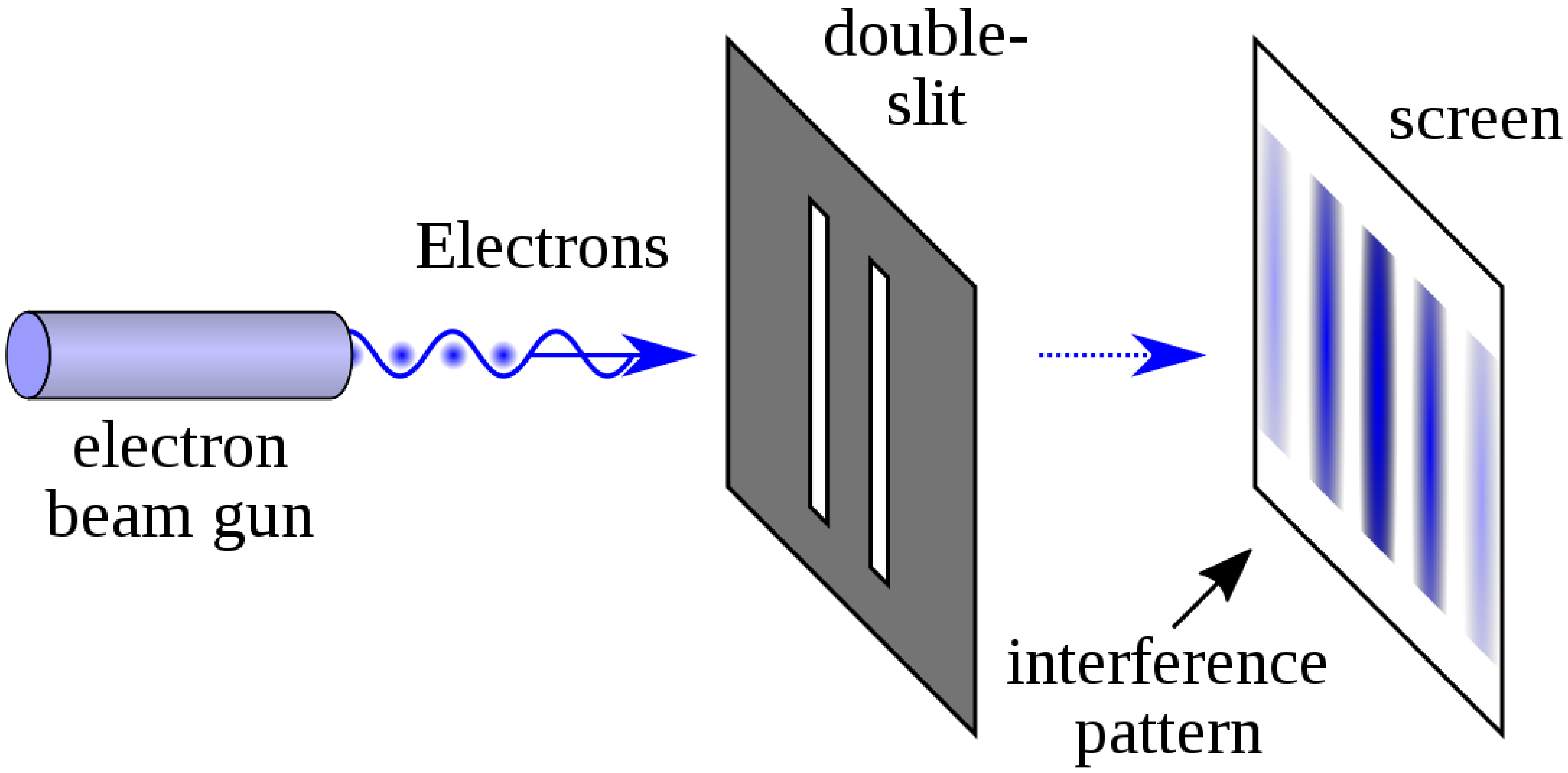
Particle-like

- individual events as e^- hits screen in specific places

Electron diffraction through a double slit



Electron diffraction through a double slit



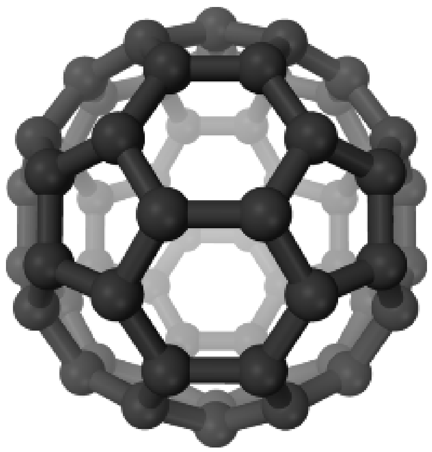
Diffraction of large molecules!

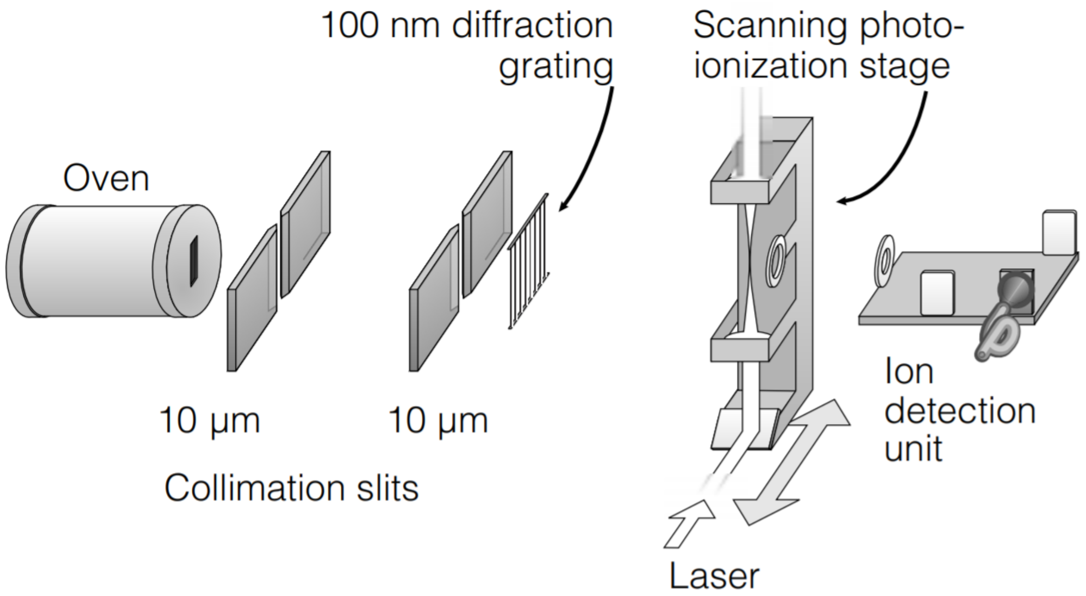
letters to nature

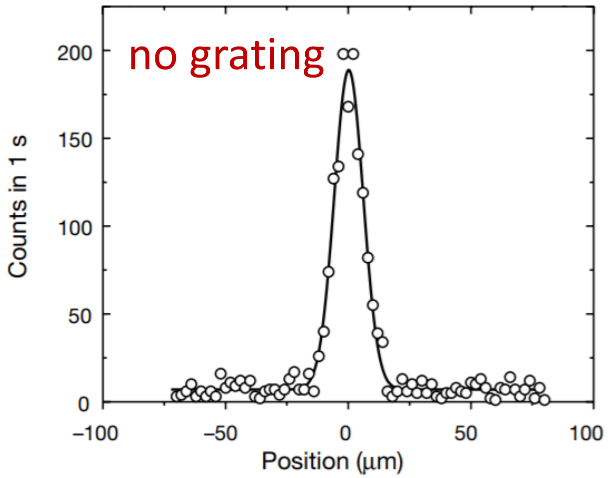
Wave–particle duality of C_{60} molecules

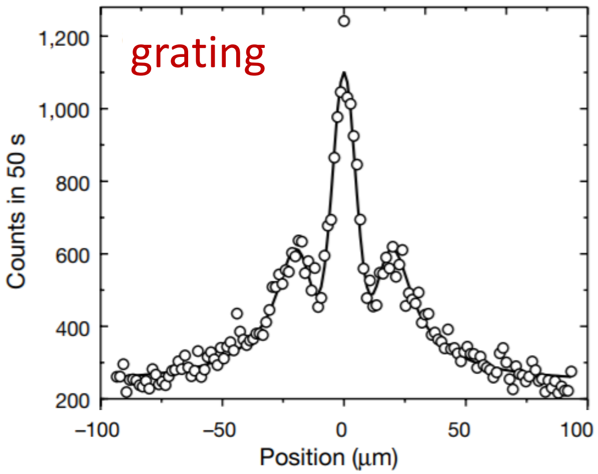
Markus Arndt, Olaf Nairz, Julian Vos-Andreae, Claudia Keller, Gerbrand van der Zouw & Anton Zeilinger

NATURE | VOL 401 | 14 OCTOBER 1999 |

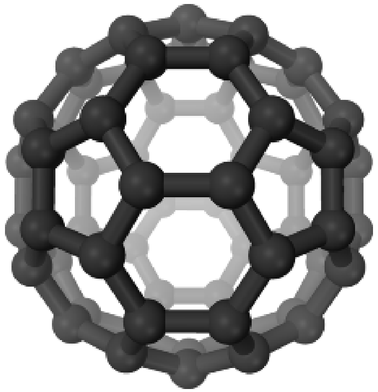








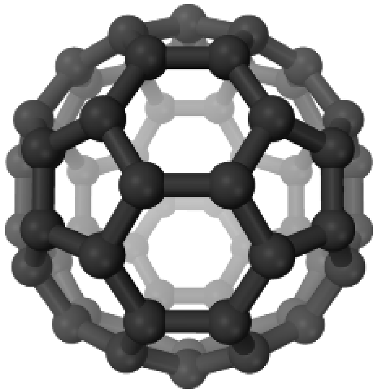
Practice problem: diffraction of C_{60}



The typical velocity of a C_{60} molecule in the original diffraction experiment is 220 m/s.

What is the de Broglie wavelength? How does it compare to the diameter of a C_{60} molecule?

Practice problem: diffraction of C_{60}



The typical velocity of a C_{60} molecule in the original diffraction experiment is 220 m/s.

What is the de Broglie wavelength? How does it compare to the diameter of a C_{60} molecule?

$$\lambda_d = \frac{h}{p} = \frac{h}{mv} = \frac{6.626 \times 10^{-34}\,\mathrm{Js}}{(720 \times 10^{-3}\,\frac{\mathrm{kg}}{\mathrm{mol}}) \cdot (\frac{1\,\mathrm{mol}}{6.022 \times 10^{23}}) \cdot (220\,\mathrm{m/s})} = 2.52 \times 10^{-12}\,\mathrm{m} = \boxed{0.0252\,\mathrm{\AA}}$$

The diameter of a buckyball is ~ 7 Å, much larger than λ_d. Astonishingly, diffraction can still be observed, using a fine grating and a detector with sufficient spatial resolution!

Wave or particle? One more analogy.

- An electron or atom is always simultaneously both a wave and a particle
- It's in the process of us observing it that it appears to be one or the other (depending on how we look)