State of a quantum system - Postulate 1

Lecture 2

CHM 439

Quantum Chemistry

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Lecture Plan

- About waves and their wave function (Courtesy: Prof. M. Weichman)
- Back to the double-slit experiment
- Matter waves and their wave function
- The first postulate of QM

Summary of the double-slit experiment with electrons

- Interference pattern observed at the detector when both slits are open.
- Closing either slit results in "particle-like" distribution at the detector (predominantly one bump).*
- Slowing down the rate of electrons (one electron at a time) still gives the interference pattern.
- If we try to observe which slit the particle goes through we get back the "particle-like" distribution.
- The fate of each electron cannot be predicted but the final interference patten is exactly reproducible (for the same source and same slits).

N.B. Here, "particle-like" actually refers to a single-slit interference pattern!

Interference of matter waves for larger particles

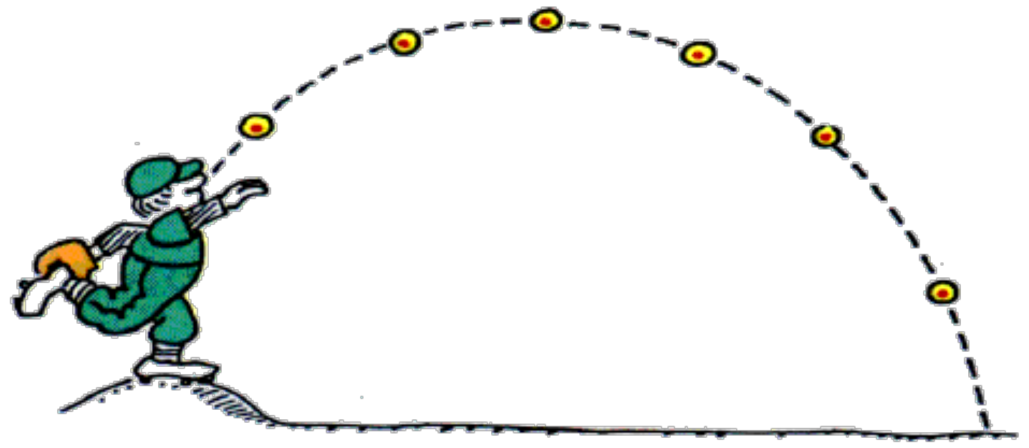
Electron diffraction through multiple slits (*Am. J. Phys.* **42**, 4, 1974)

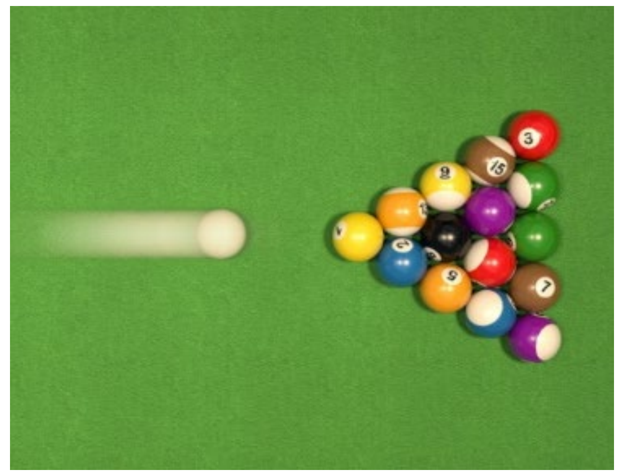
Single slit

Two slits

Classical mechanics

particles





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

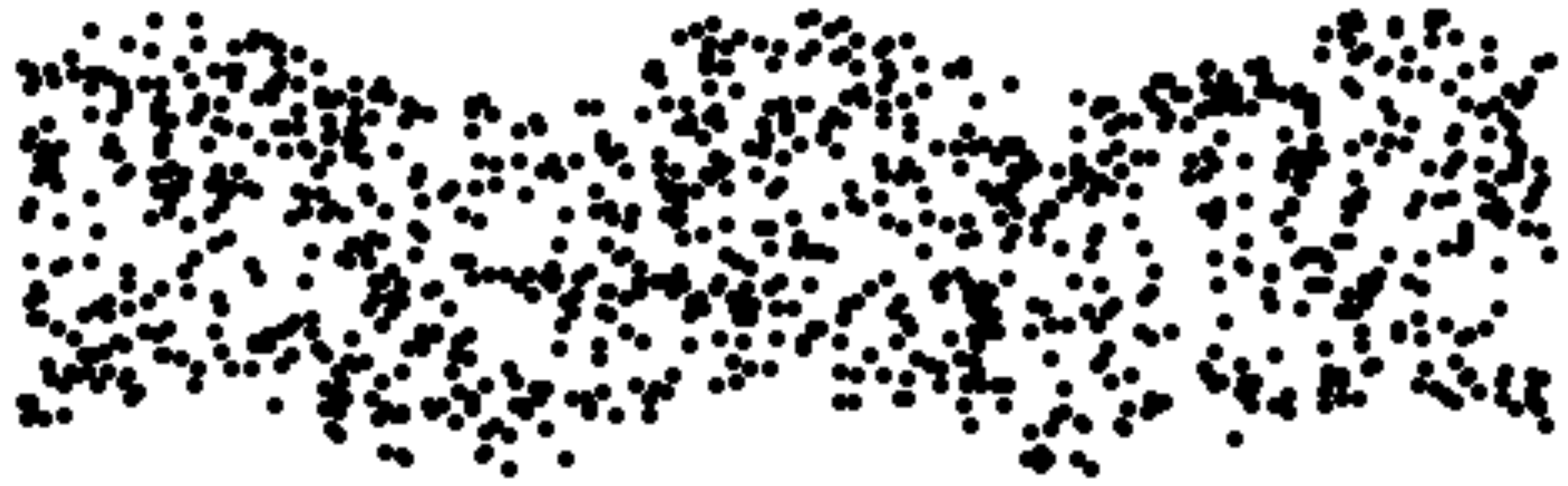
can calculate trajectories in time:

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

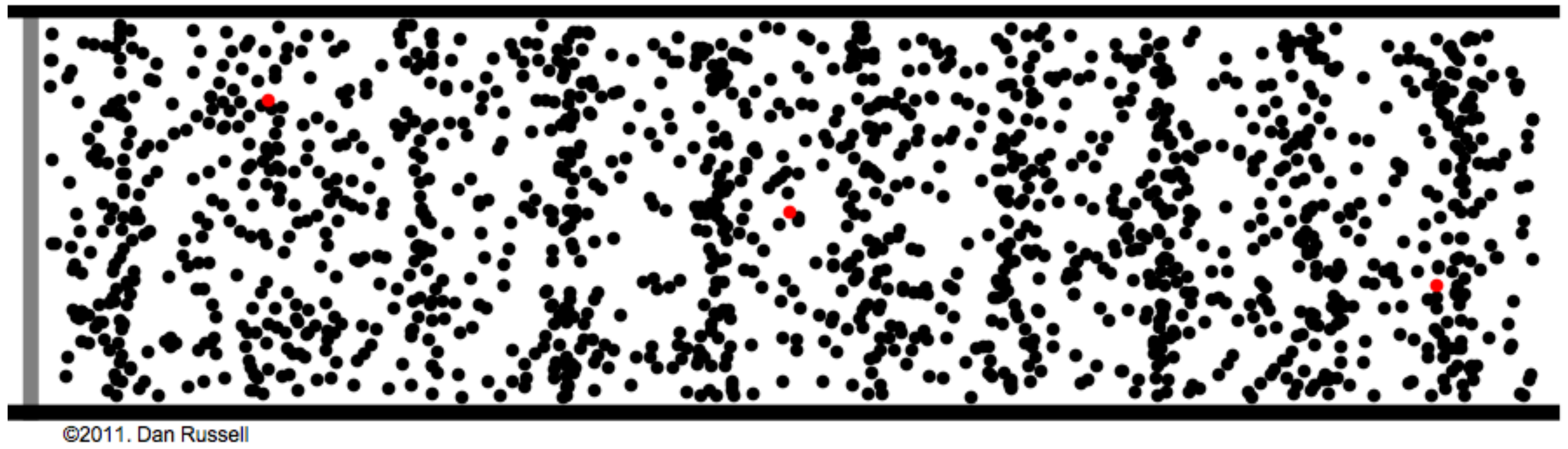
Courtesy: Prof. M. Weichman

waves

transverse waves



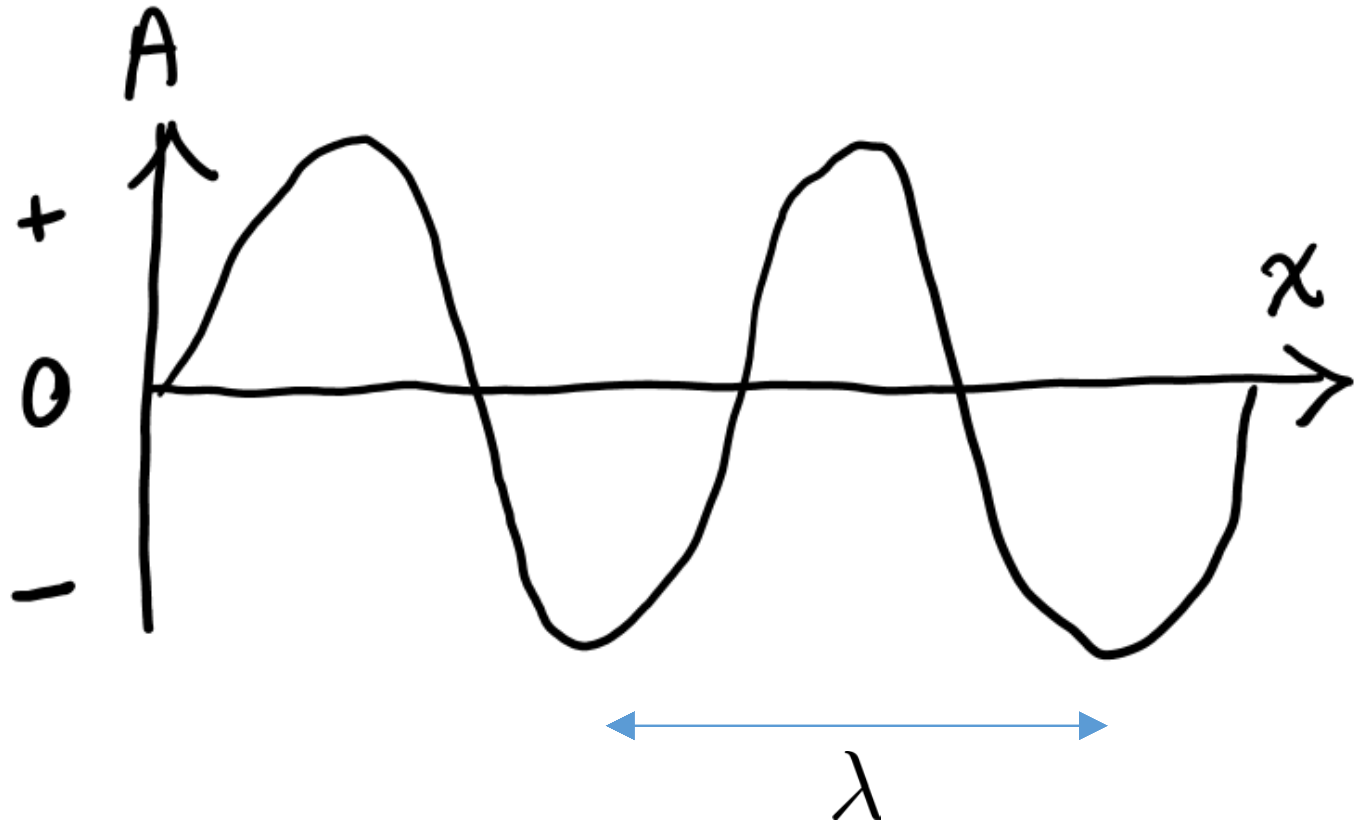
longitudinal or compression waves



can calculate displacement as a function of time:

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

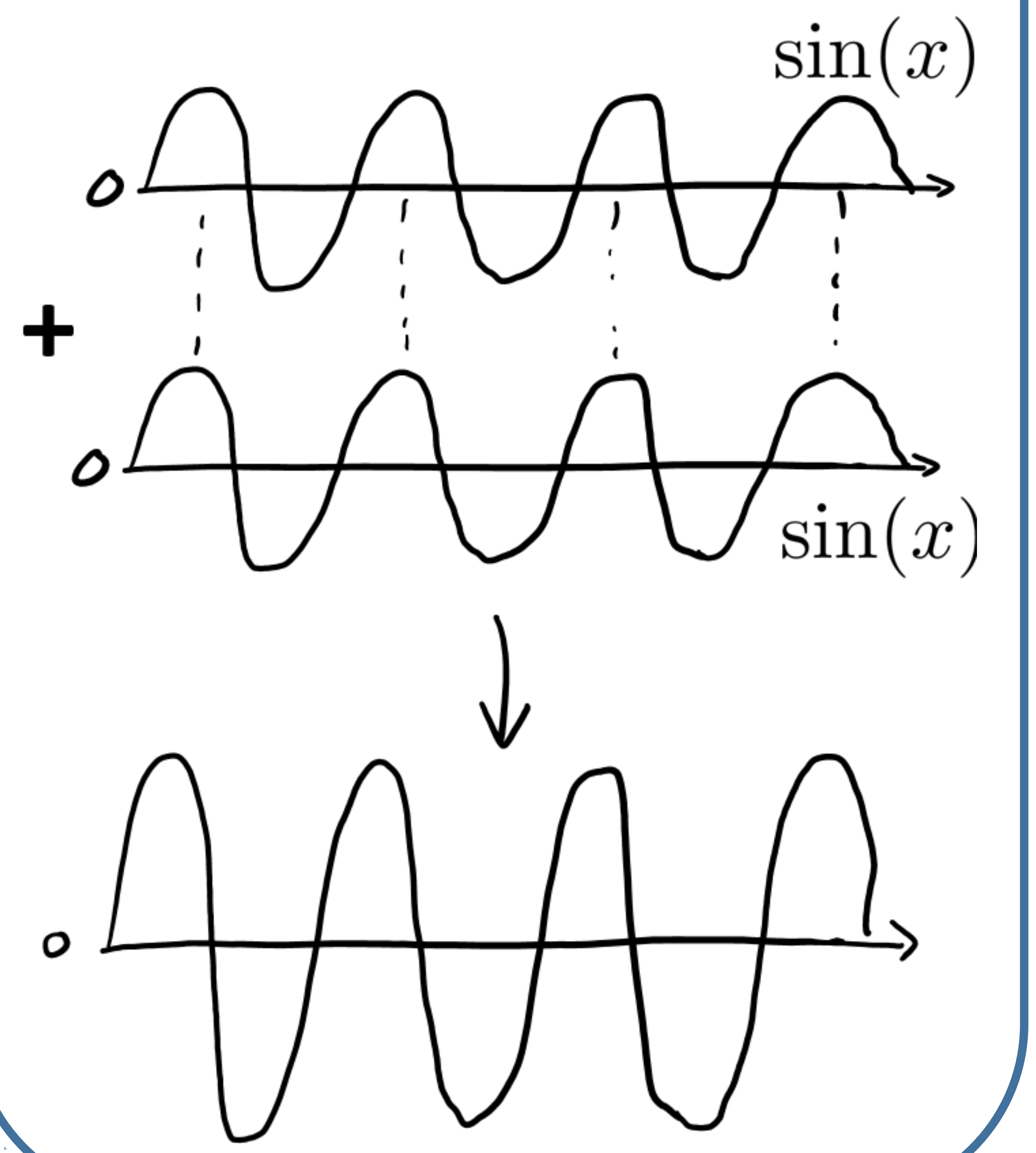
Classical wave phenomena



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

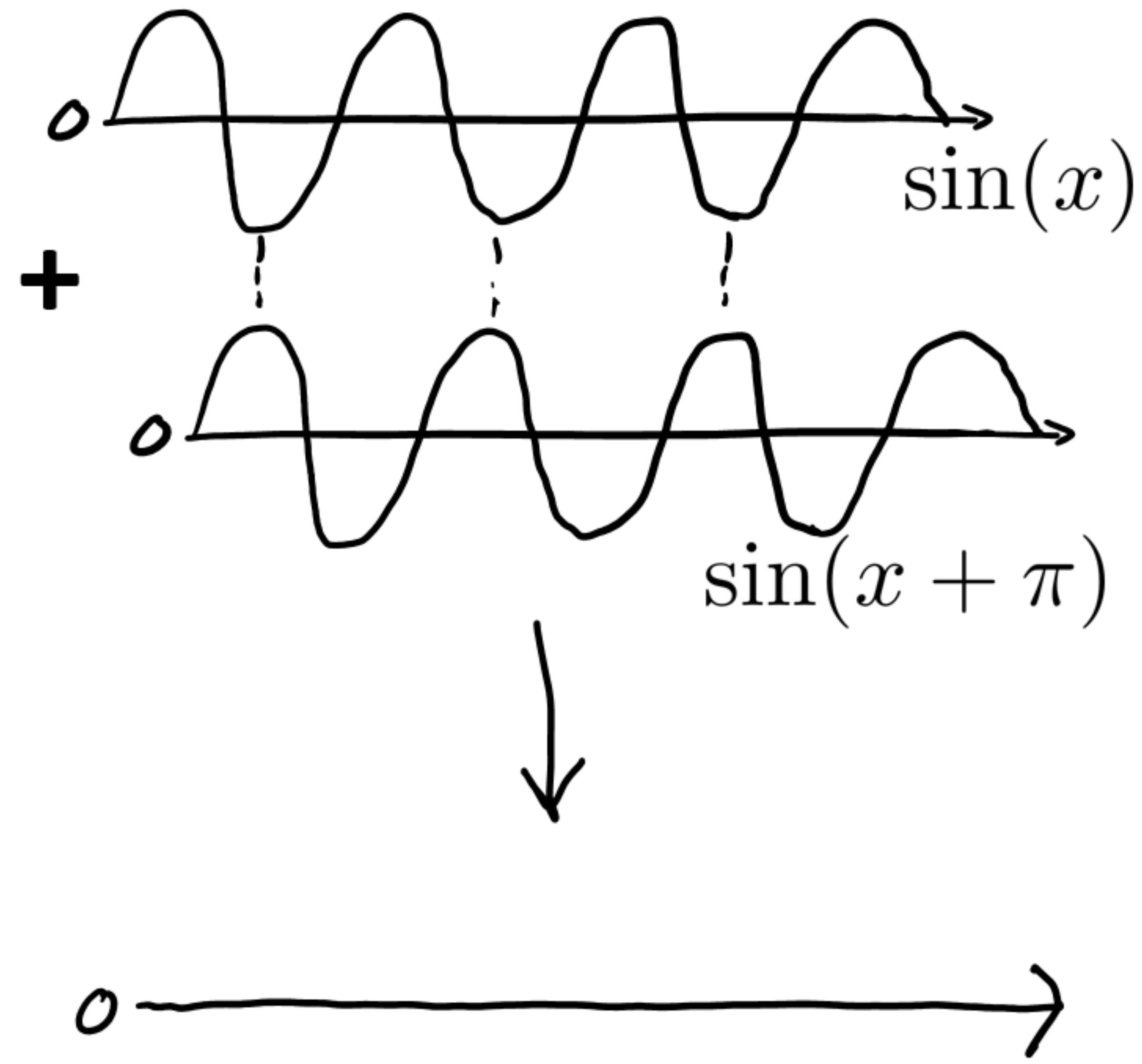
constructive interference

waves *in-phase* (0º)



destructive interference

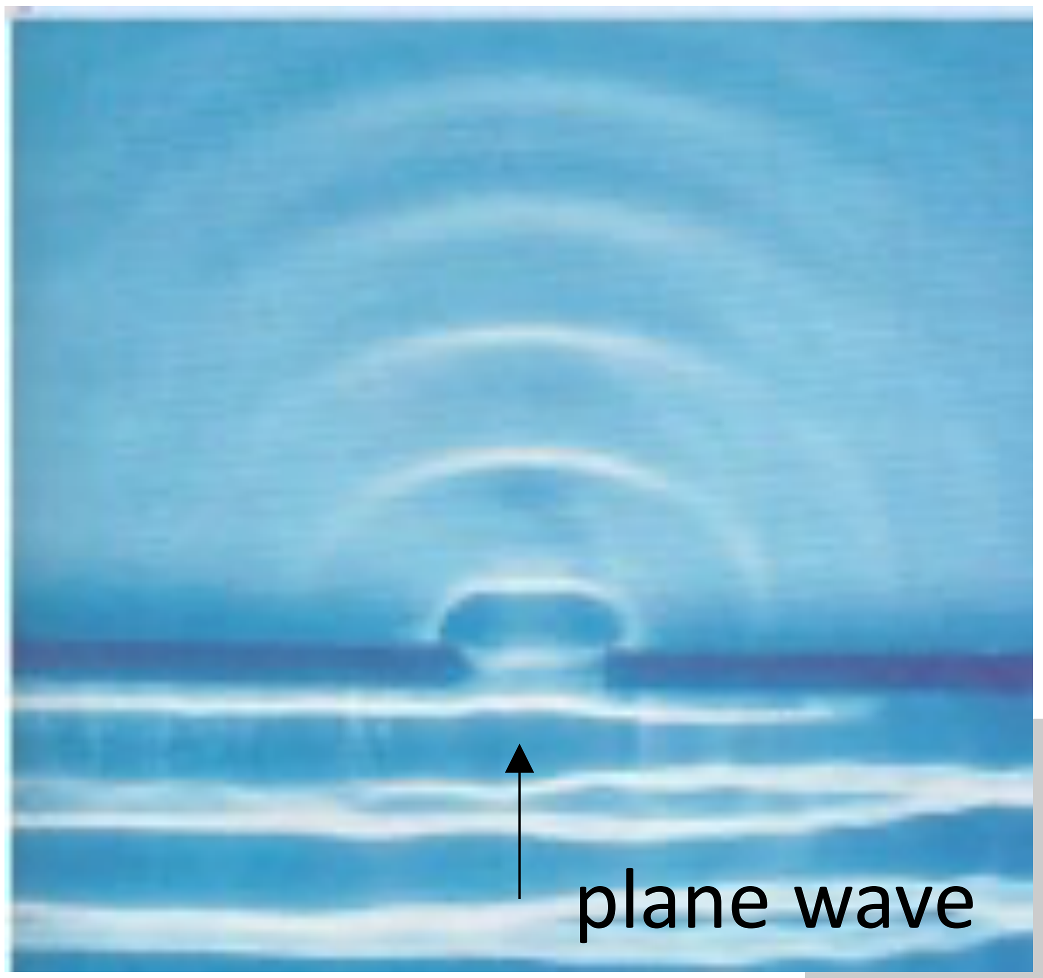
waves *out-of-phase* (180º)



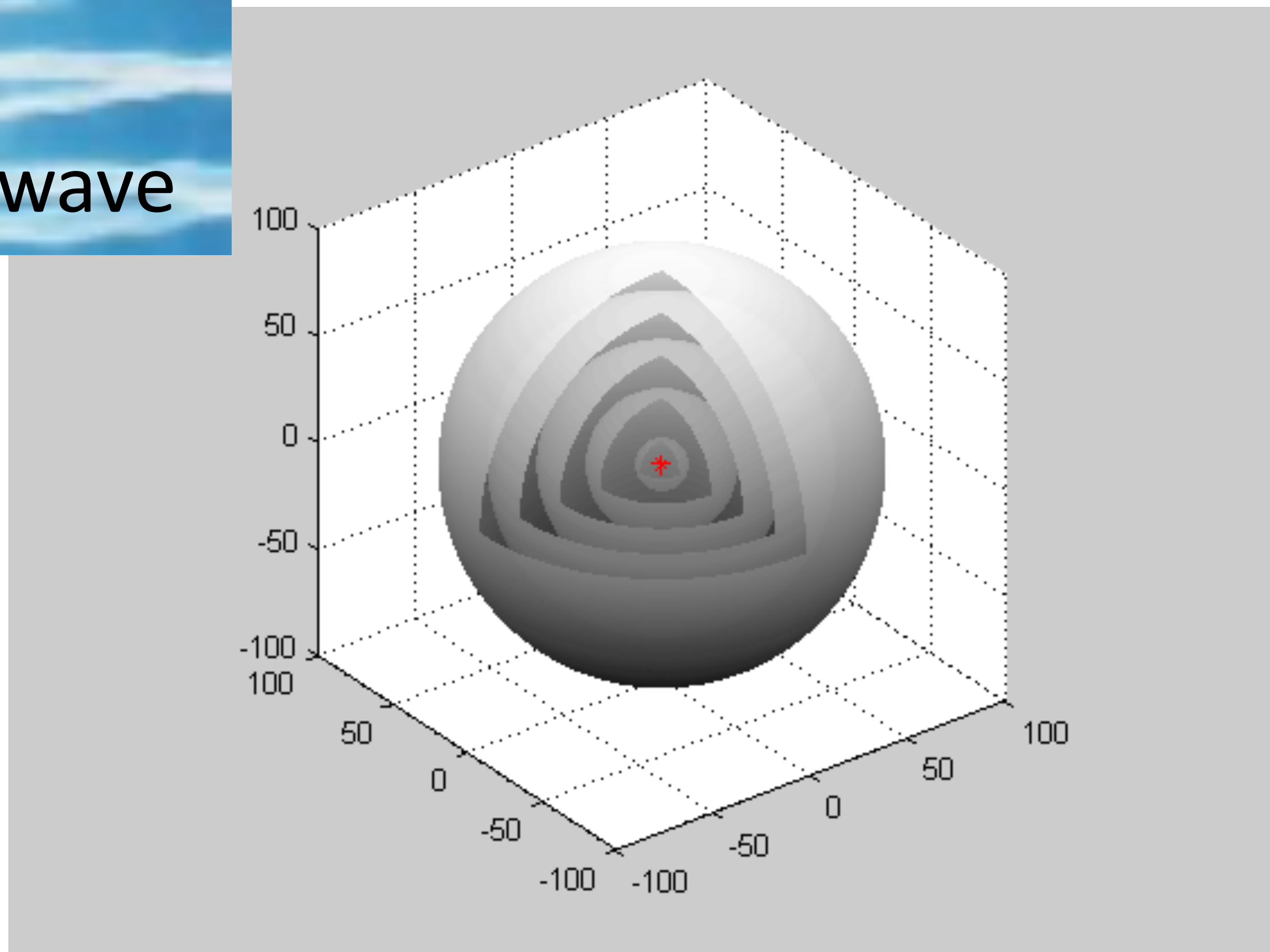
Classical wave phenomena

waves are delocalized

wave fronts can be curved

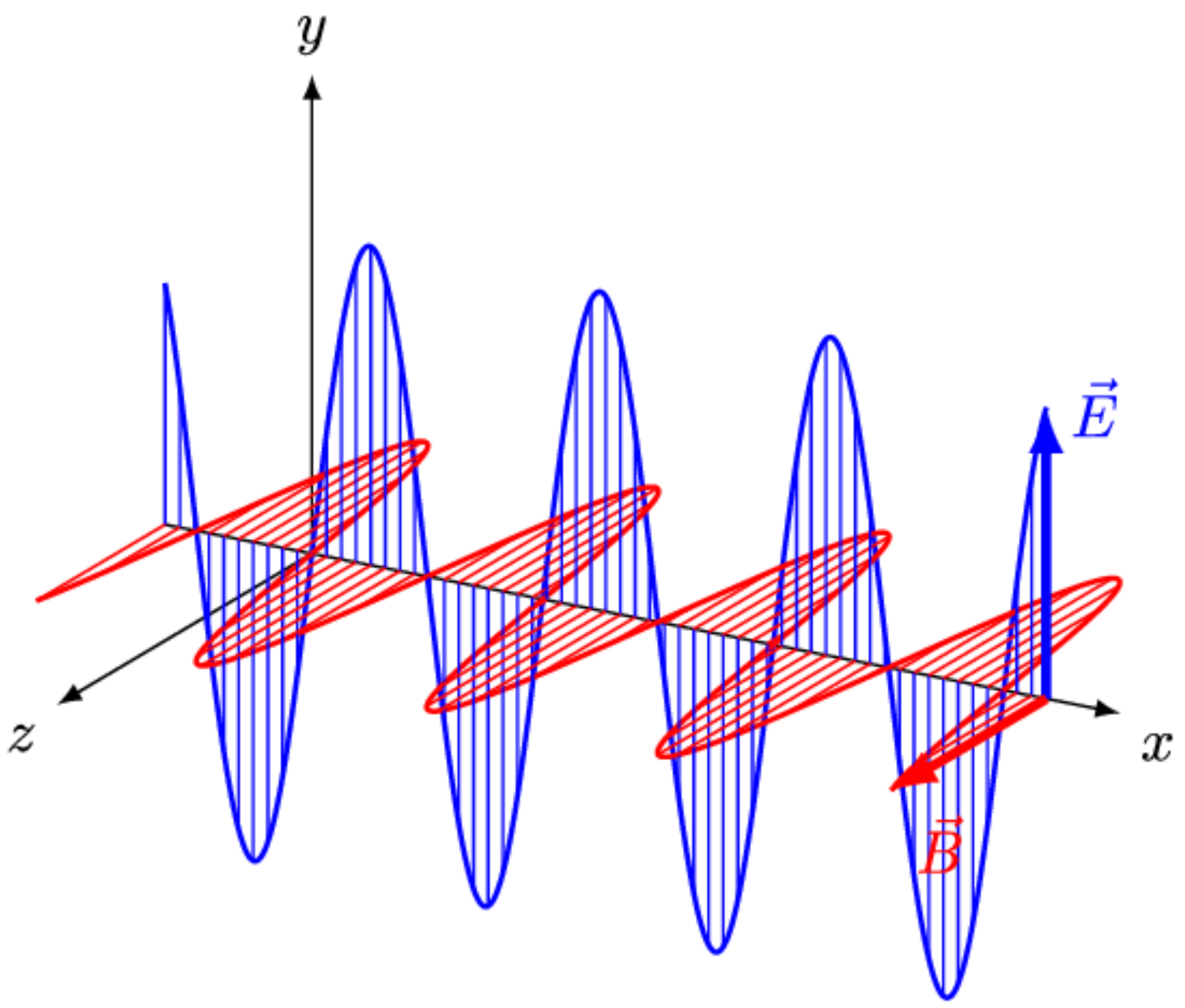


cylindrical wave emitted from a point source in 2D space



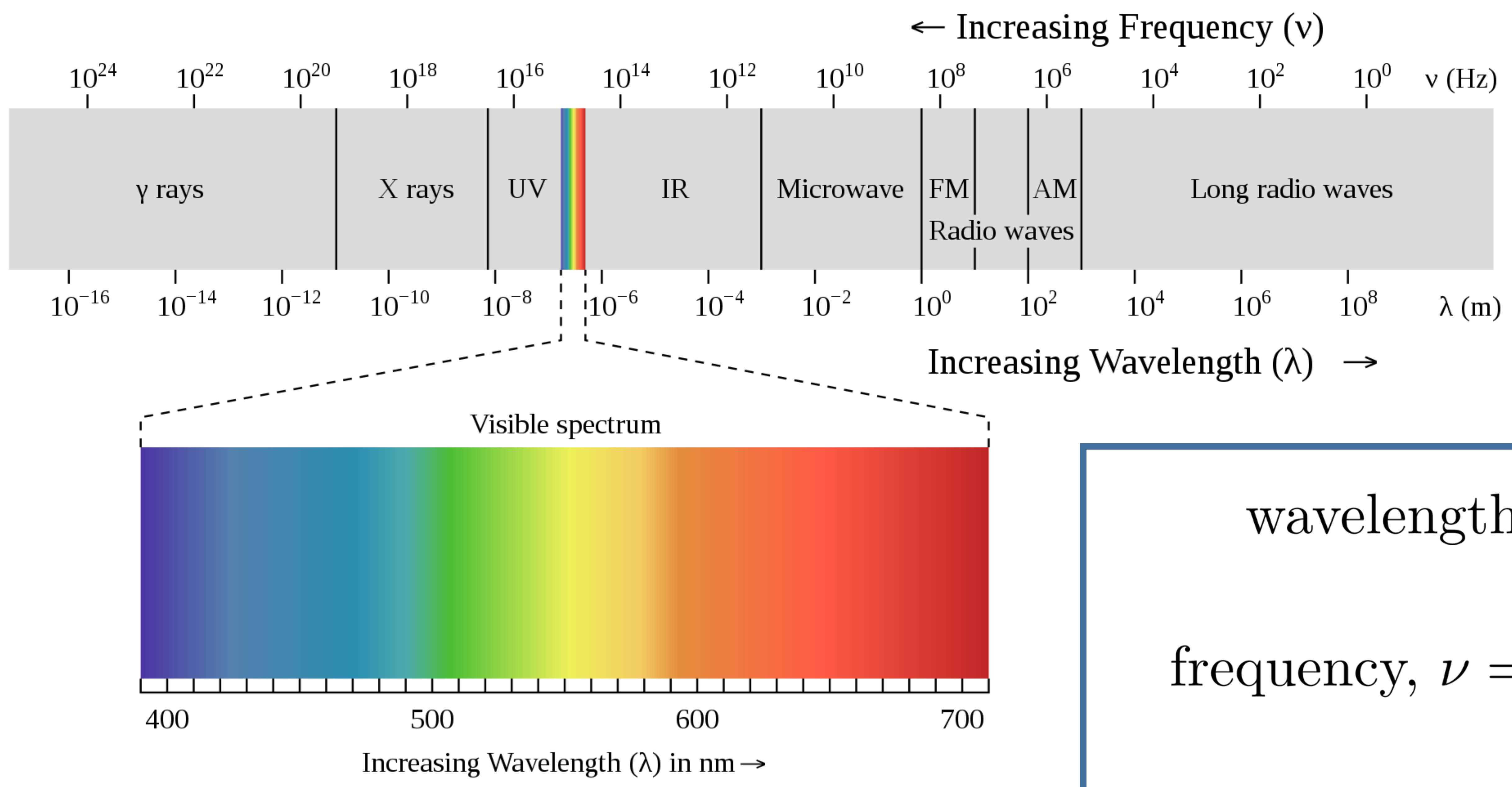
point sources emit spherical waves in 3D space

Light is an electromagnetic wave



a valid solution to Maxwell's equations!

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

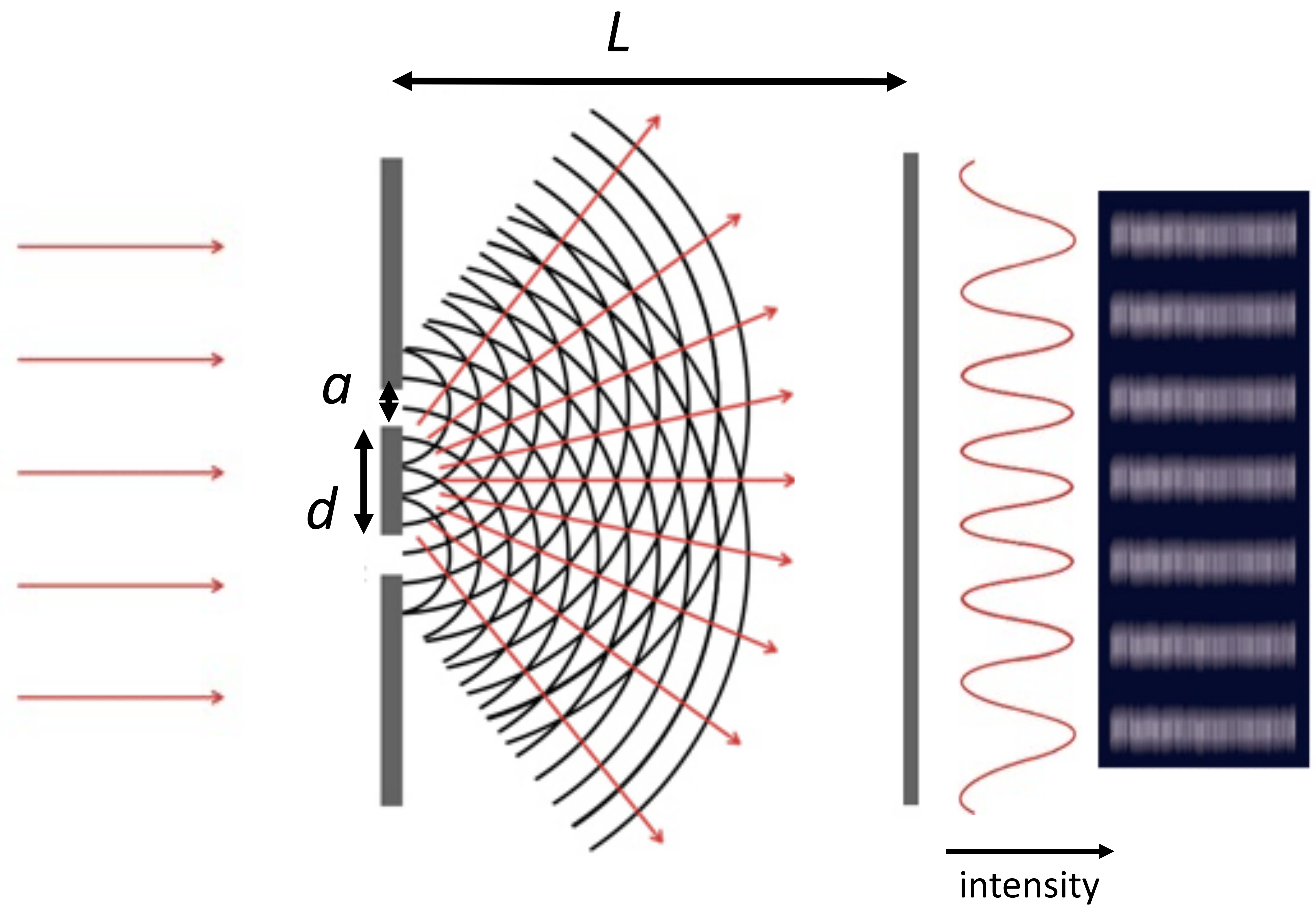


$$\text{wavelength, } \lambda$$
$$\text{frequency, } \nu = \frac{c}{\lambda}$$
$$\text{wavenumber, } \tilde{v} = \frac{1}{\lambda}$$

$$E = h\nu$$

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

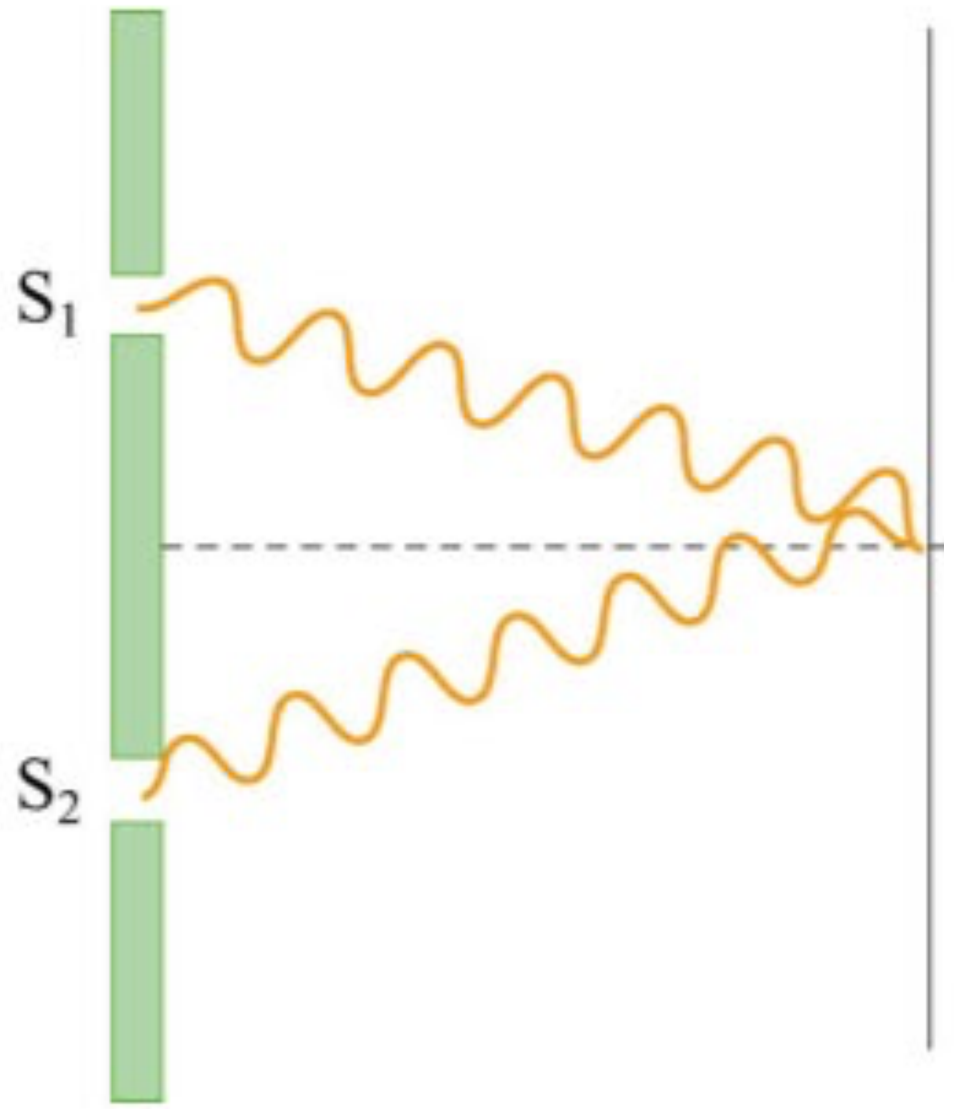
Classical diffraction of light through a double slit



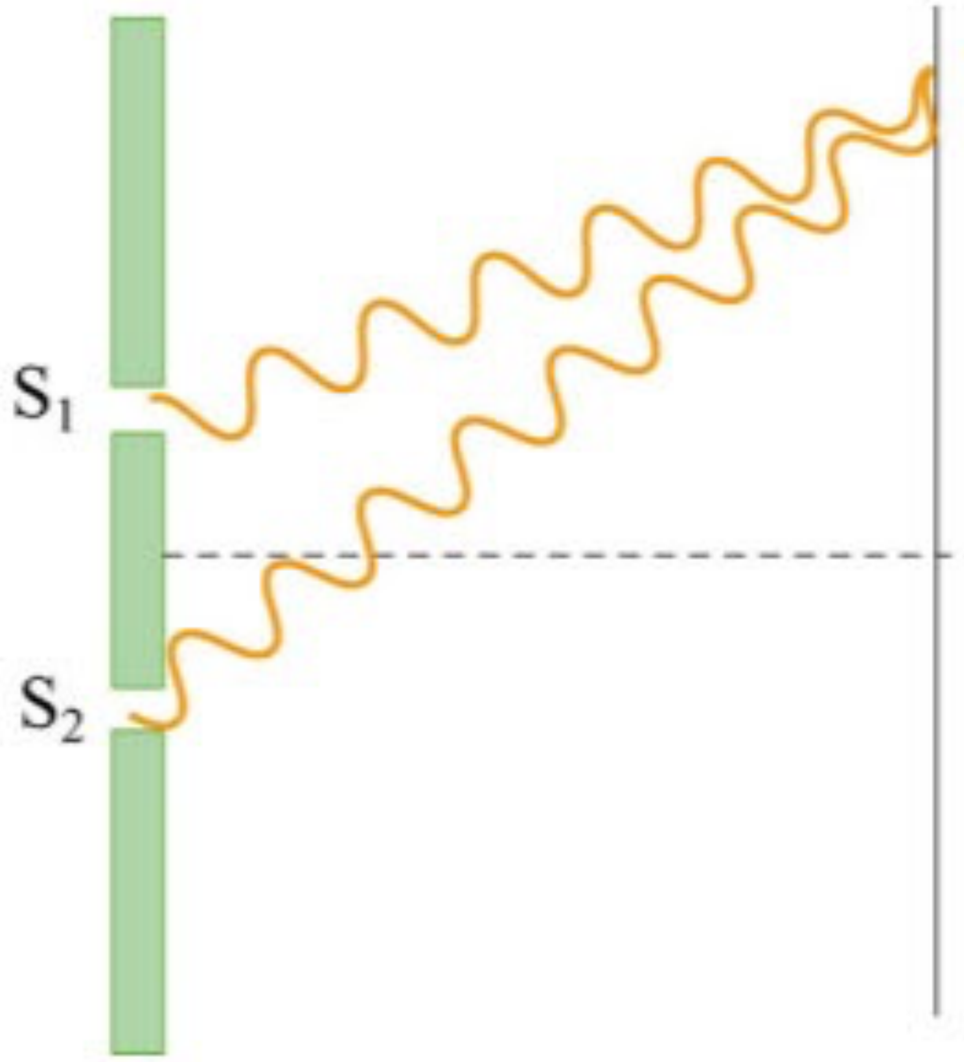
- each slit becomes a new point source of light
- two sources interfere with one another
- destructive interference at minima, constructive at maxima

Which positions on the screen are bright or dark?

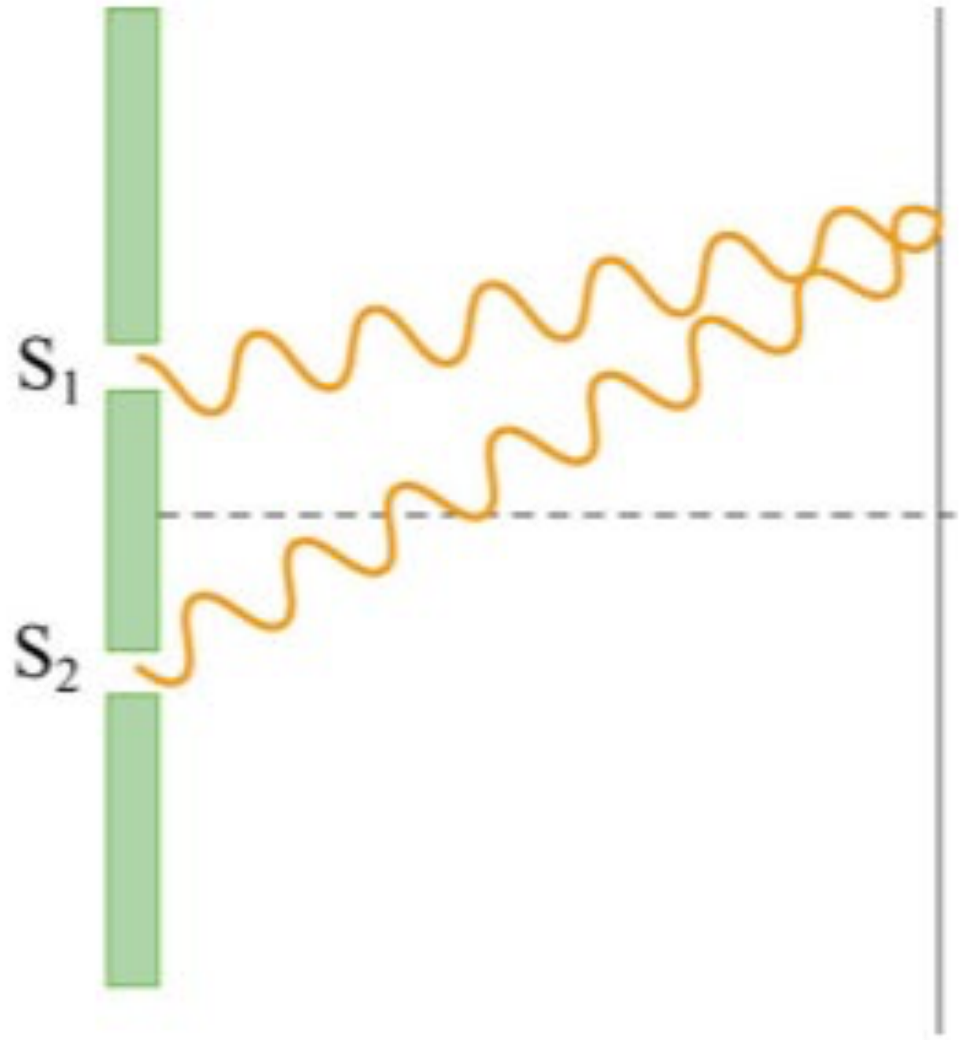
A



B

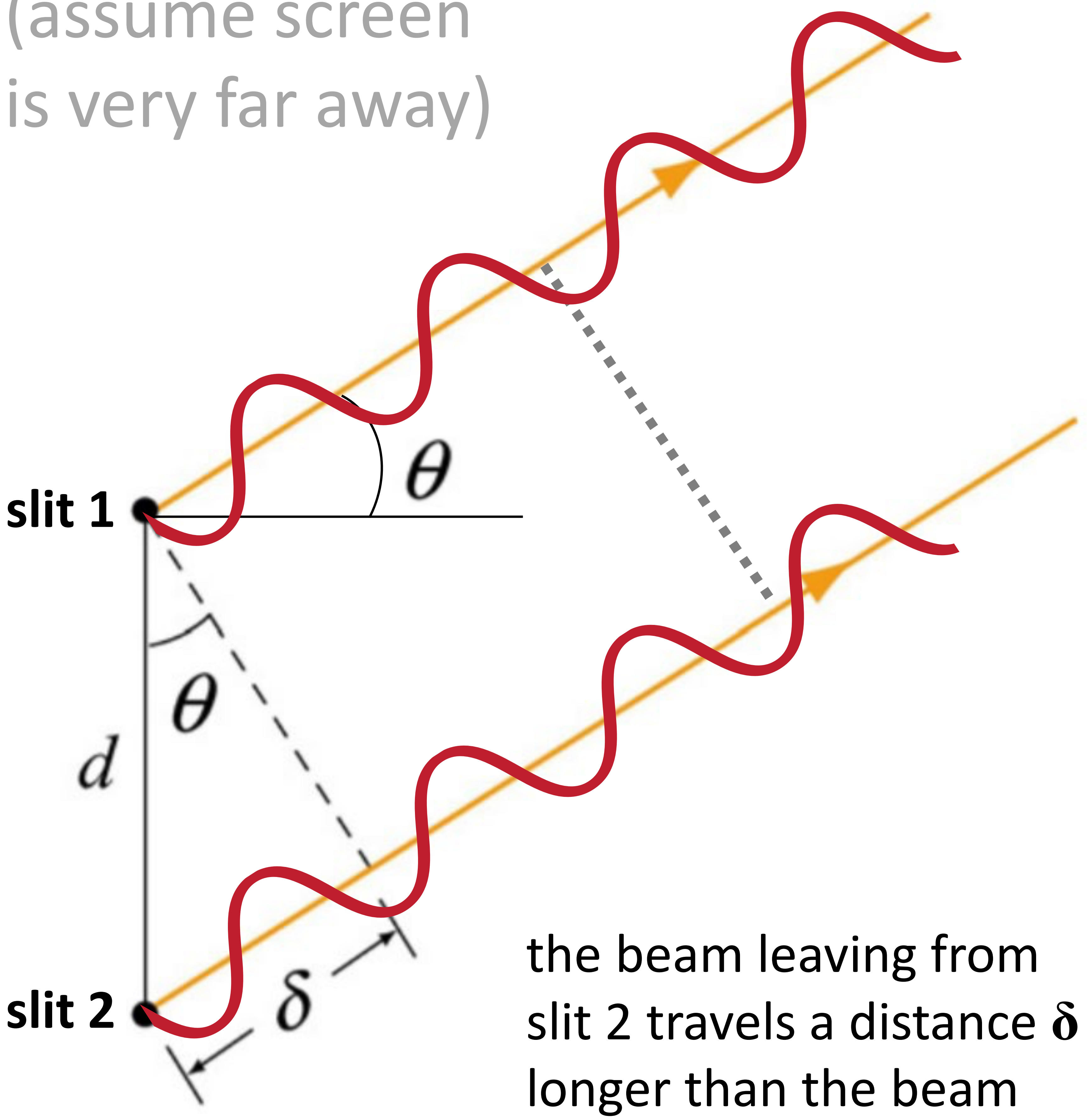


C



Determining the fringe positions mathematically

(assume screen is very far away)



the beam leaving from slit 2 travels a distance **δ** longer than the beam leaving slit 1

waves interfere constructively when difference between the pathlengths traveled from each slit to the screen is a round integer multiple of the wavelength

$$\delta = d\sin\theta = m\lambda, \quad m = 0, \pm 1, \pm 2, \ldots$$

$$\sin\theta = m\lambda/d$$

bright spots appear at angles:

$$\theta_{\text{bright}} = \arcsin(m\lambda/d)$$

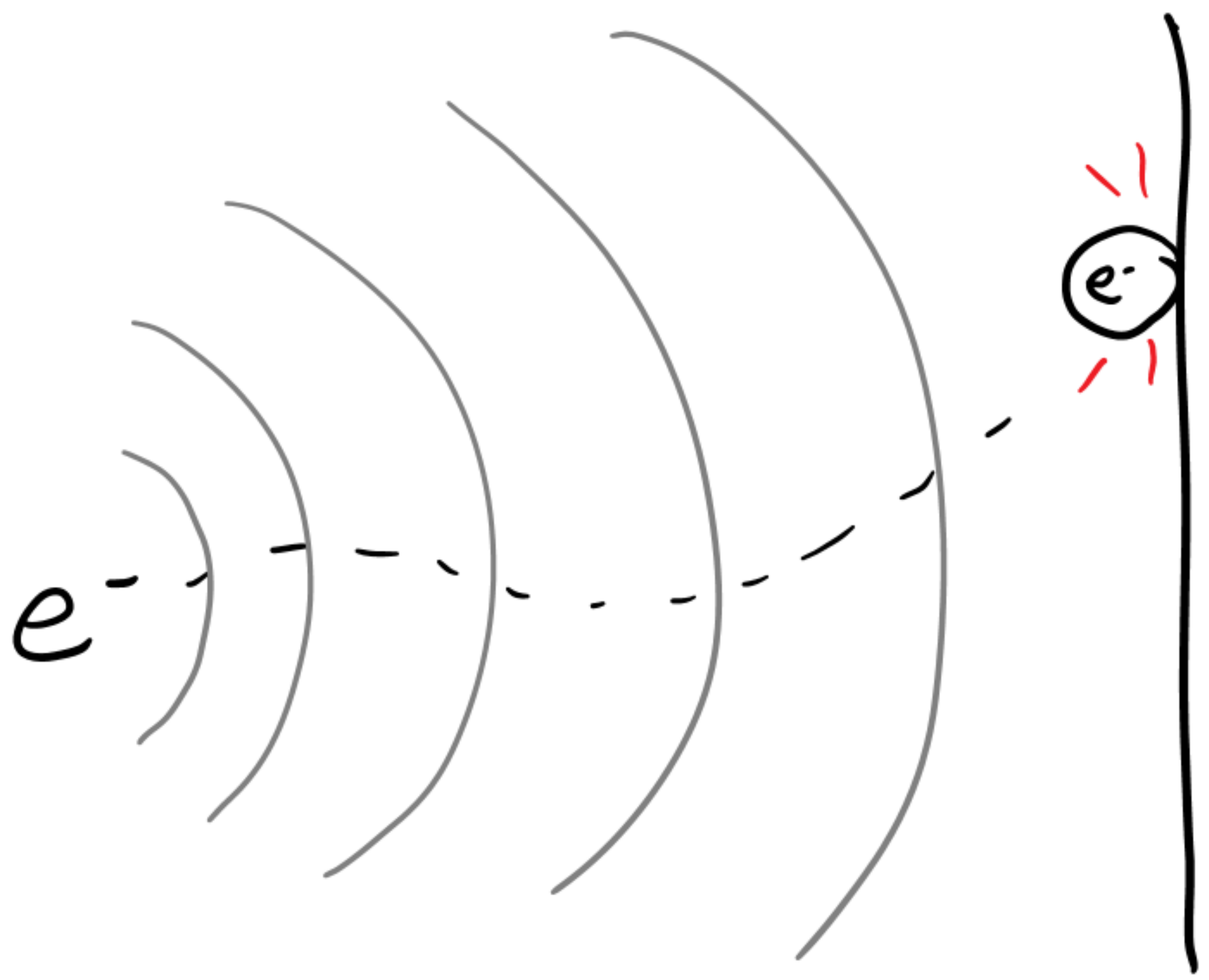
how might we alter this expression to locate the angles where dark spots appear?

$$d\sin\theta = \underline{(m + 1/2)}\lambda, \quad m = 0, \pm 1, \pm 2, \ldots$$

$$\boxed{\theta_{\text{dark}} = \arcsin((m + 1/2)\lambda/d)}$$

Quantum mechanical wave-particle duality

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

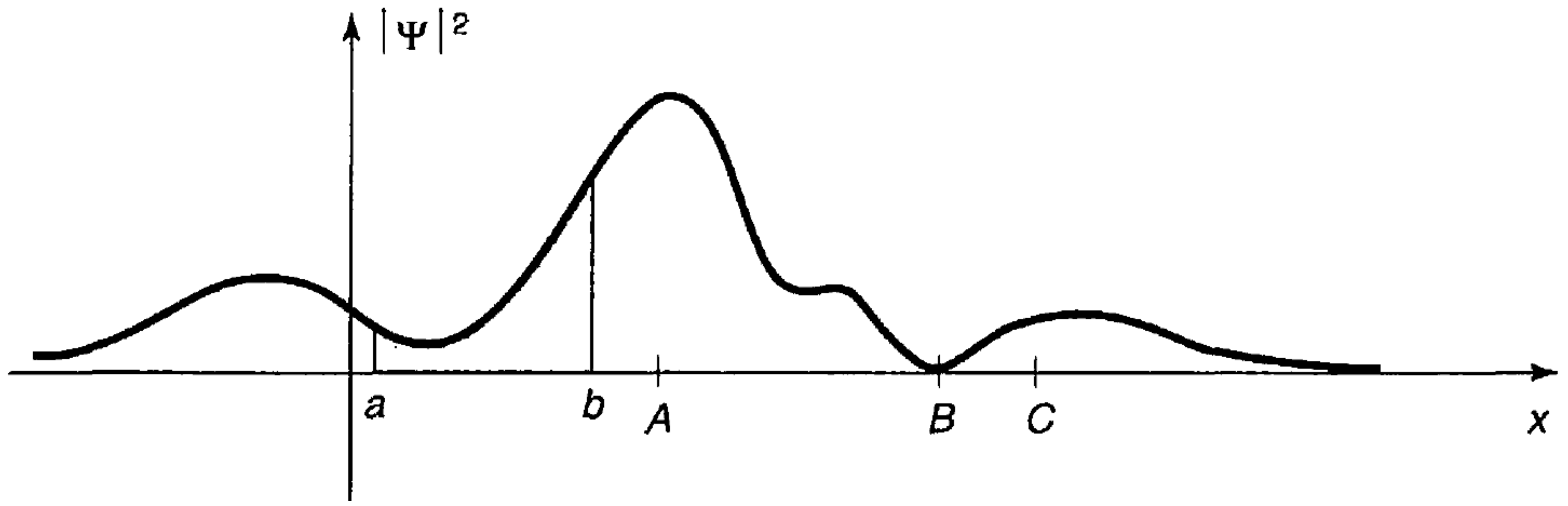


imagine if sound waves behaved like this!

quantum particles are governed by a *wavefunction*

$$\psi(x, t)$$

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



$$\int_a^b |\psi(x,t)|^2 dx \quad = \left\{ \text{probability of finding the particle between } a \text{ and } b\text{, at time } t \right.$$

Summary of the double-slit experiment with electrons

Non-classical result ($P_{12} \neq P_1 + P_2$)

- Interference pattern observed at the detector when both slits are open.
- Closing either slit results in "particle-like" distribution at the detector (predominantly one bump).*

Individual slits also correspond to waves.

- Slowing down the rate of electrons (one electron at a time) still gives the interference pattern.

P_{12} results from individual electron events!

- If we try to observe which slit the particle goes through we get back the "particle-like" distribution.

Emergence of an uncertainty principle.

- The fate of each electron cannot be predicted but the final interference patten is exactly reproducible (for the same source and same slits).

A new definition for the state of a system.

N.B. Here, "particle-like" actually refers to a single-slit interference pattern!

Acknowledgements

Wikipedia commons
Google images
YouTube
The textbooks of the course.
https://weichman.princeton.edu