Chapter 0: Photoelectric effect

the experiment

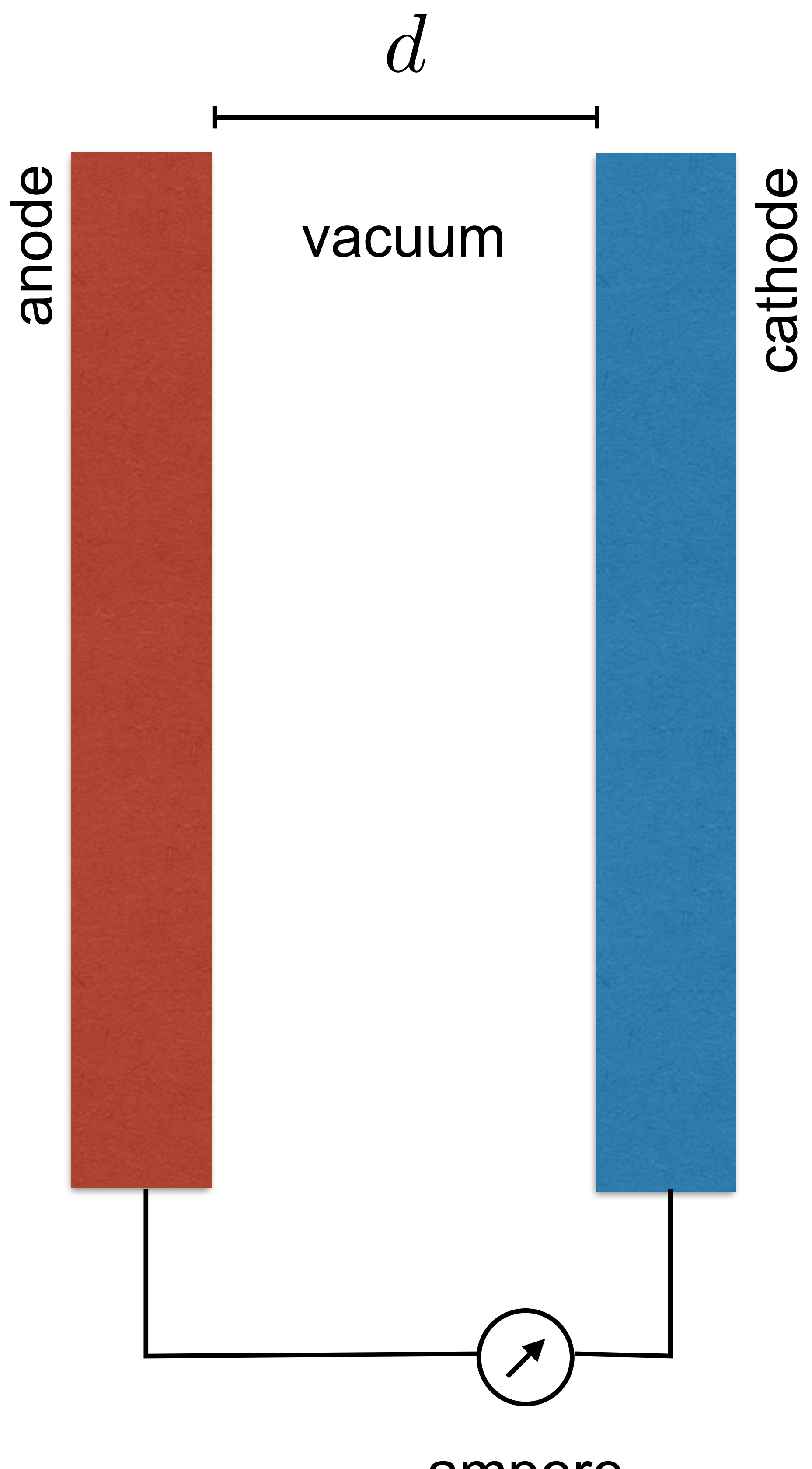
- photocurrent, stopping potential
- four inconsistencies with Maxwell theory of electromagnetic radiation
- Einsteins new suggestion (1905)
  - statistical mechanics considerations about entropy of EM radiation
  - consequences of Einstein's suggestion
- importance of photo-electric effect (extra information)
  - photo-electron spectroscopy: information about electronic structure
  - photon-multipliers: detect light
  - photo-oxidiation of DNA & proteins: cancer, cell death
  - radiation damage in (protein) x-ray crystallography

goals

- become further familiar with concept of quantization
  - wave-particle duality
  - pave the way for quantization of particle energy states: quantum mechanics

Photoelectric effect

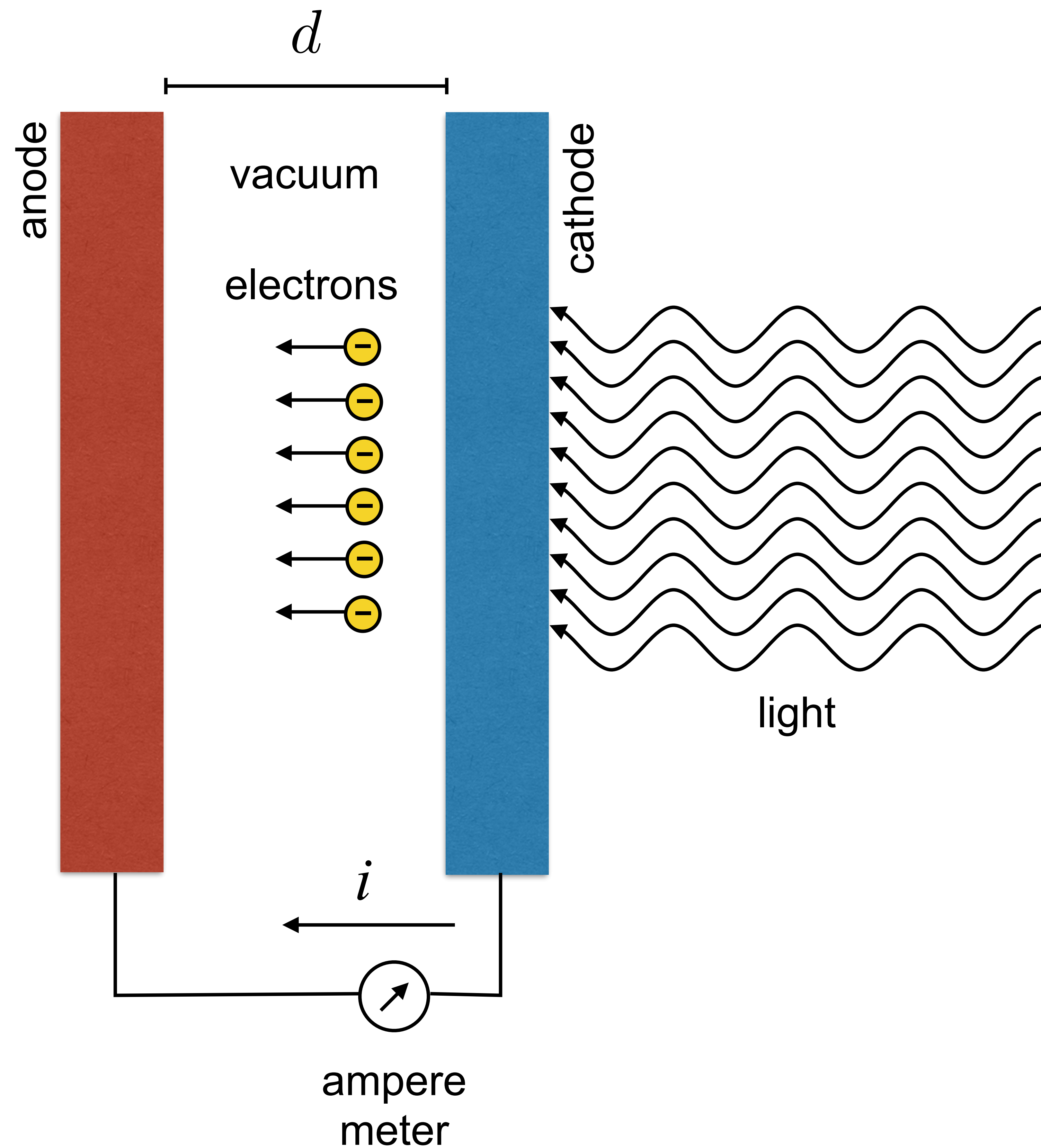
the experiment



Photoelectric effect

the experiment

electrons released by light

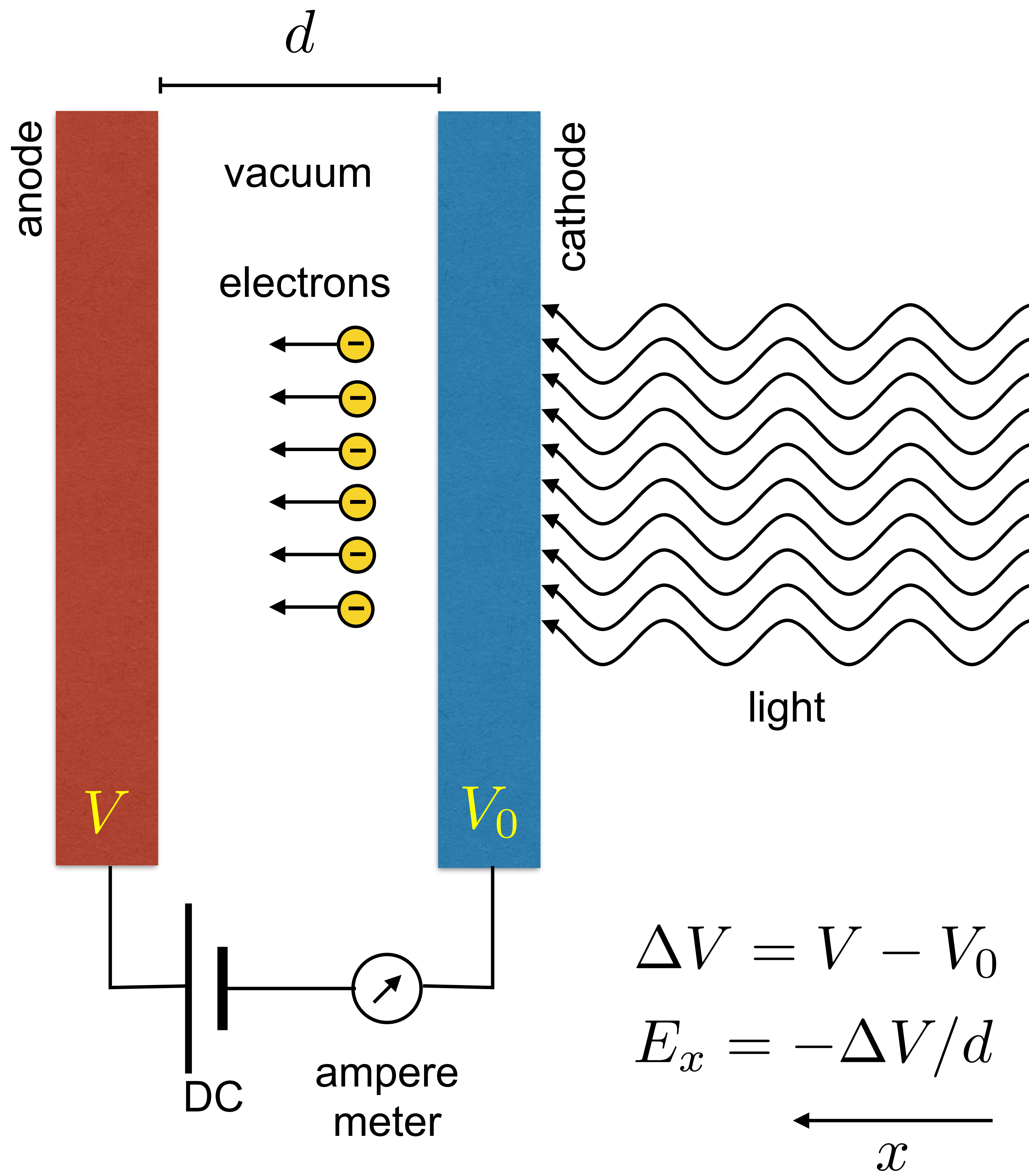


Photoelectric effect

the experiment

electrons released by light

stopping potential

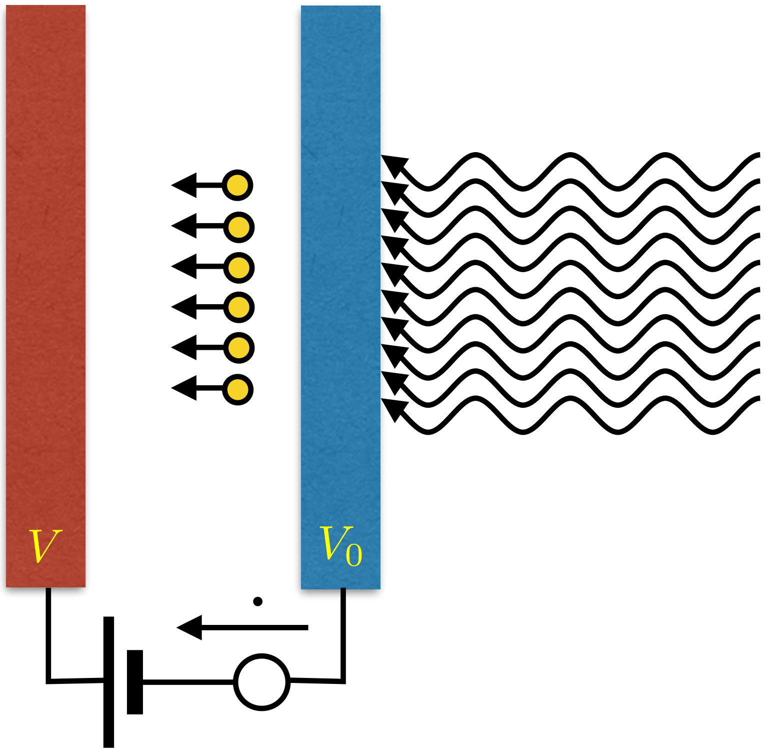


$$\Delta V = V - V_0$$

$$E_x = -\Delta V / d$$

Photoelectric effect

theoretical considerations before 1905



electrons attracted by positive ions

work function w

energy of electro magnetic waves

independent of frequency

$$I = \langle \mathbf{S} \rangle = \langle \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} \rangle$$

energy deposited in volume proportional to time

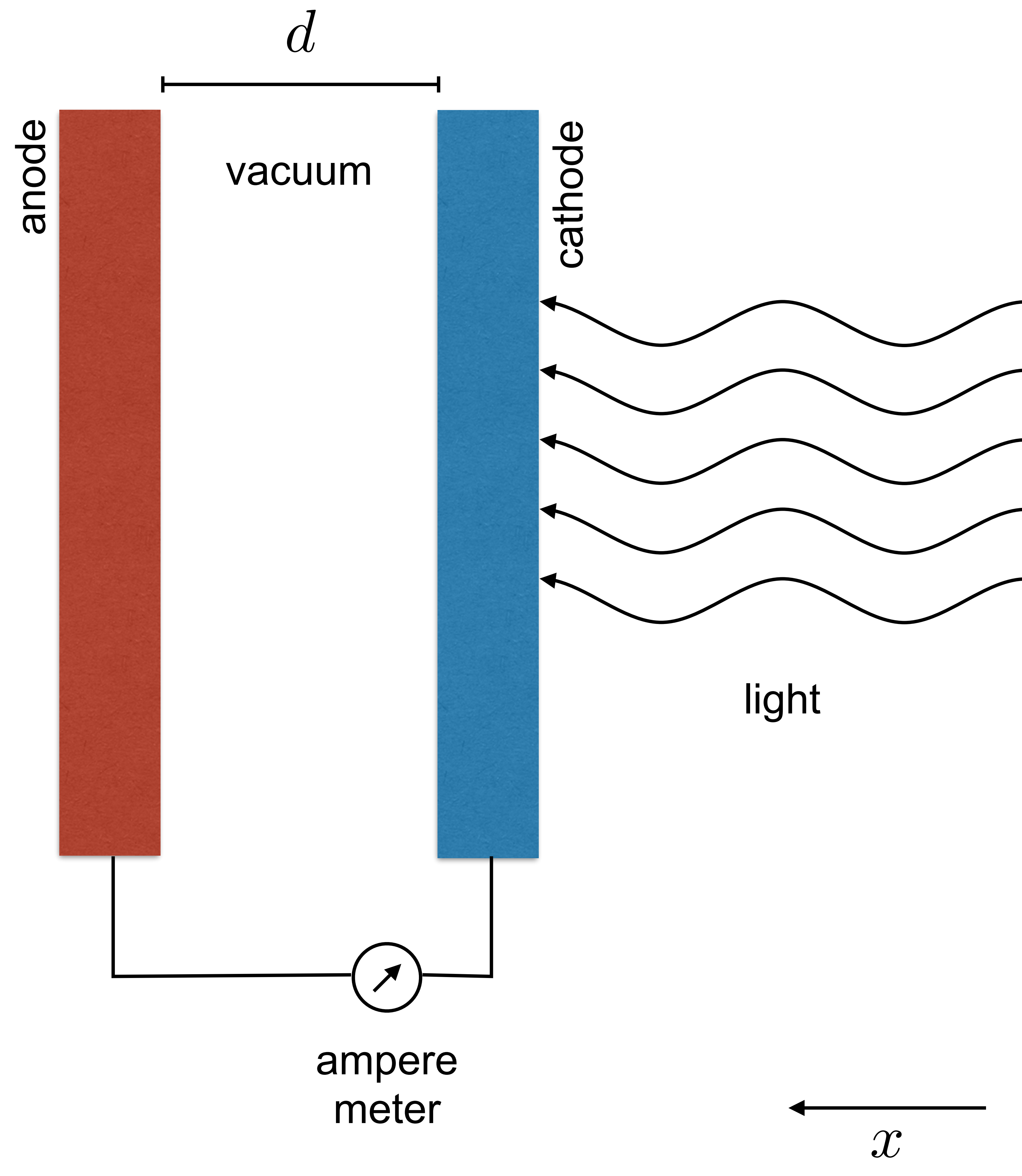
photo-current matter of intensity and/or time

kinetic energy function of intensity

Photoelectric effect

experimental observations

threshold frequency

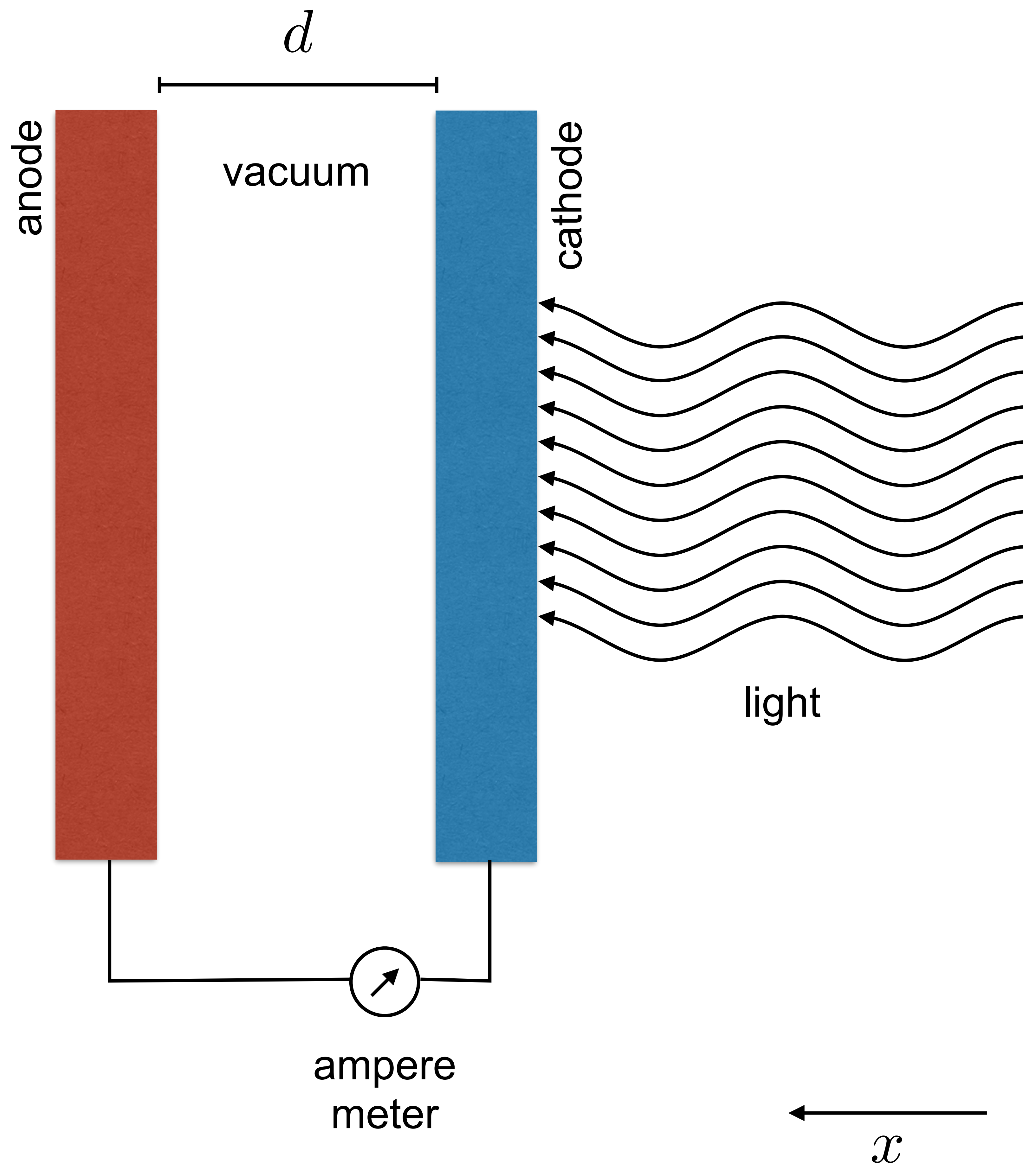


Photoelectric effect

experimental observations

threshold frequency

independent of intensity

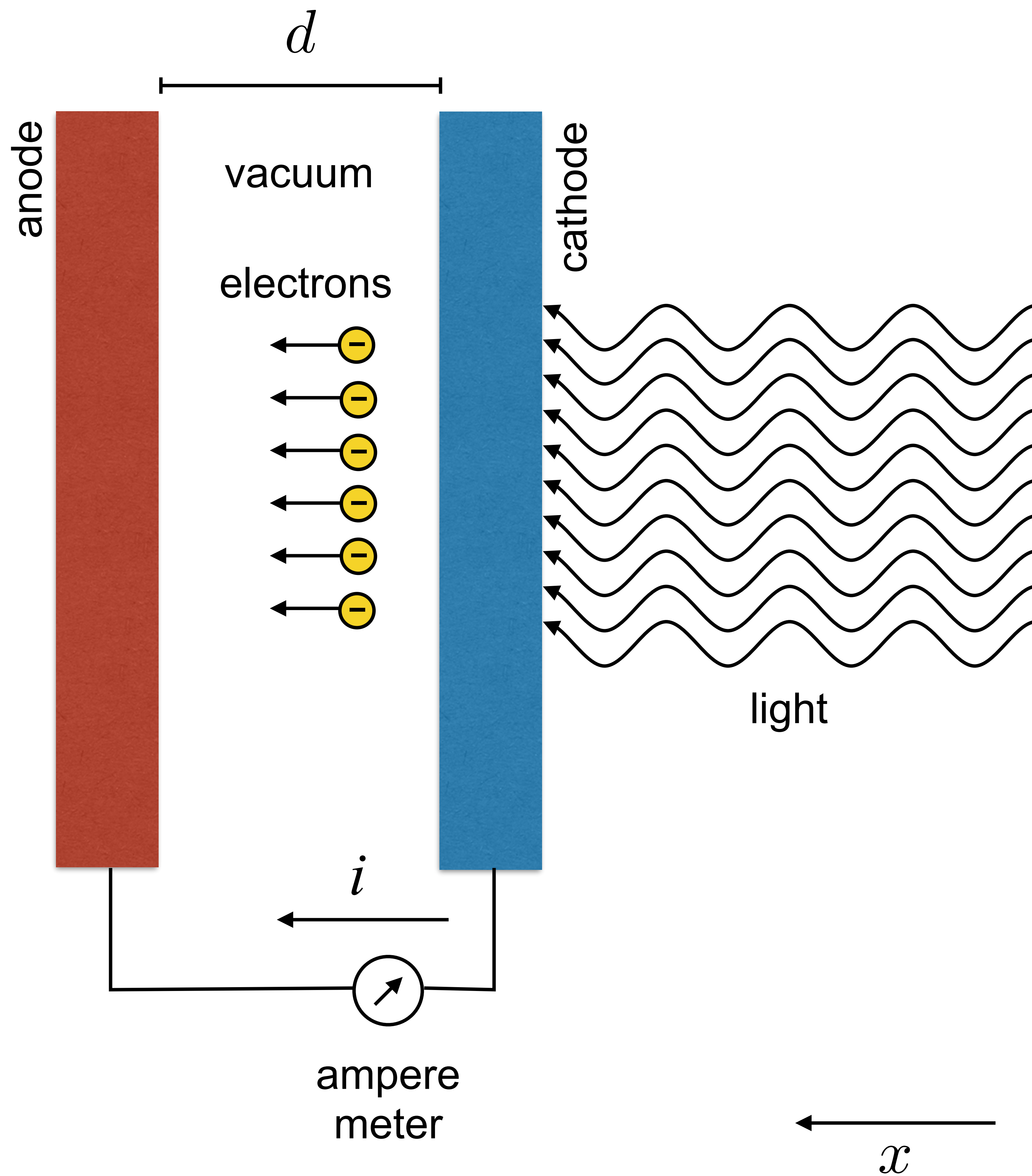


Photoelectric effect

experimental observations

threshold frequency

independent of intensity



Photoelectric effect

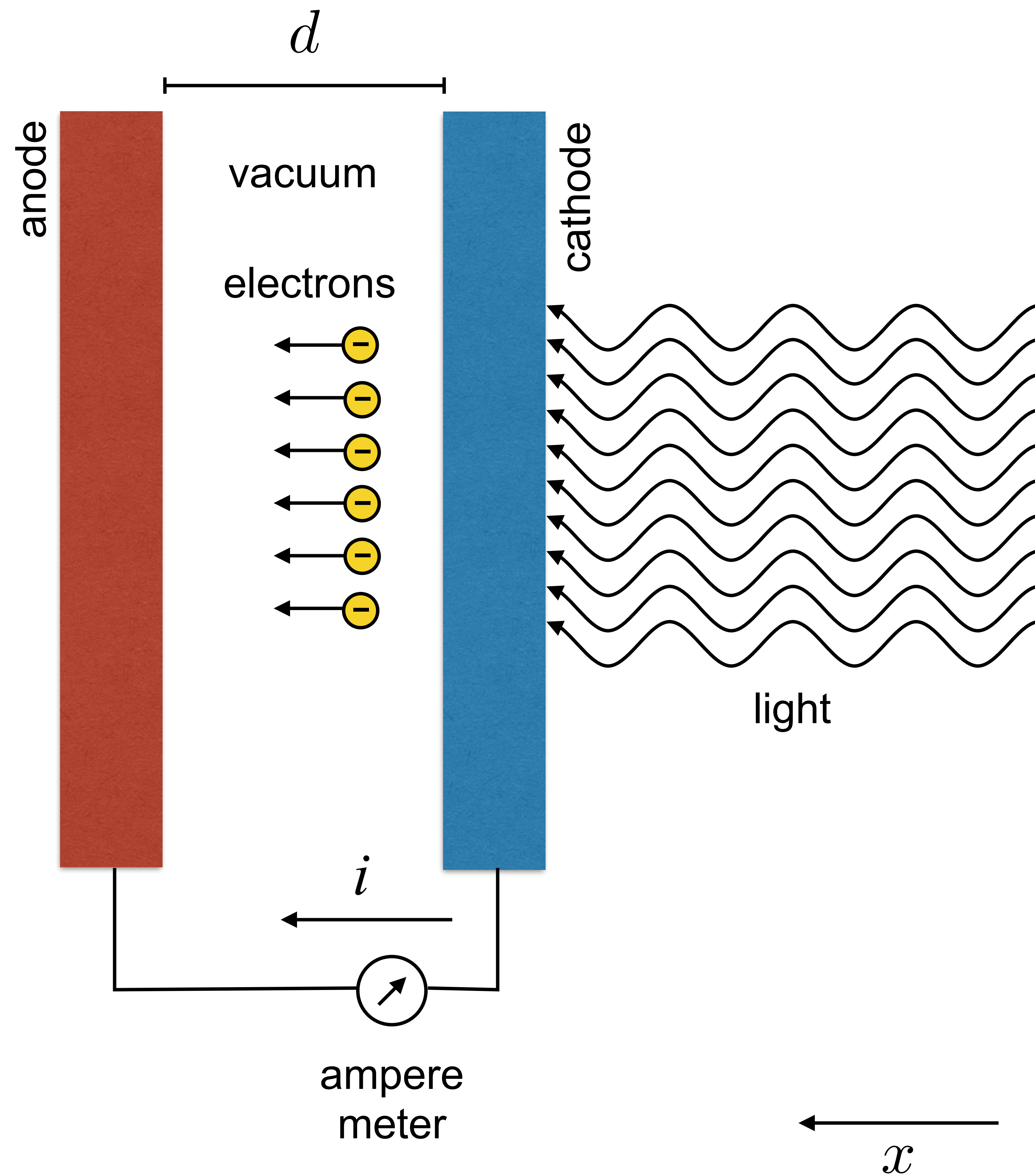
experimental observations

threshold frequency

independent of intensity

maximum photocurrent

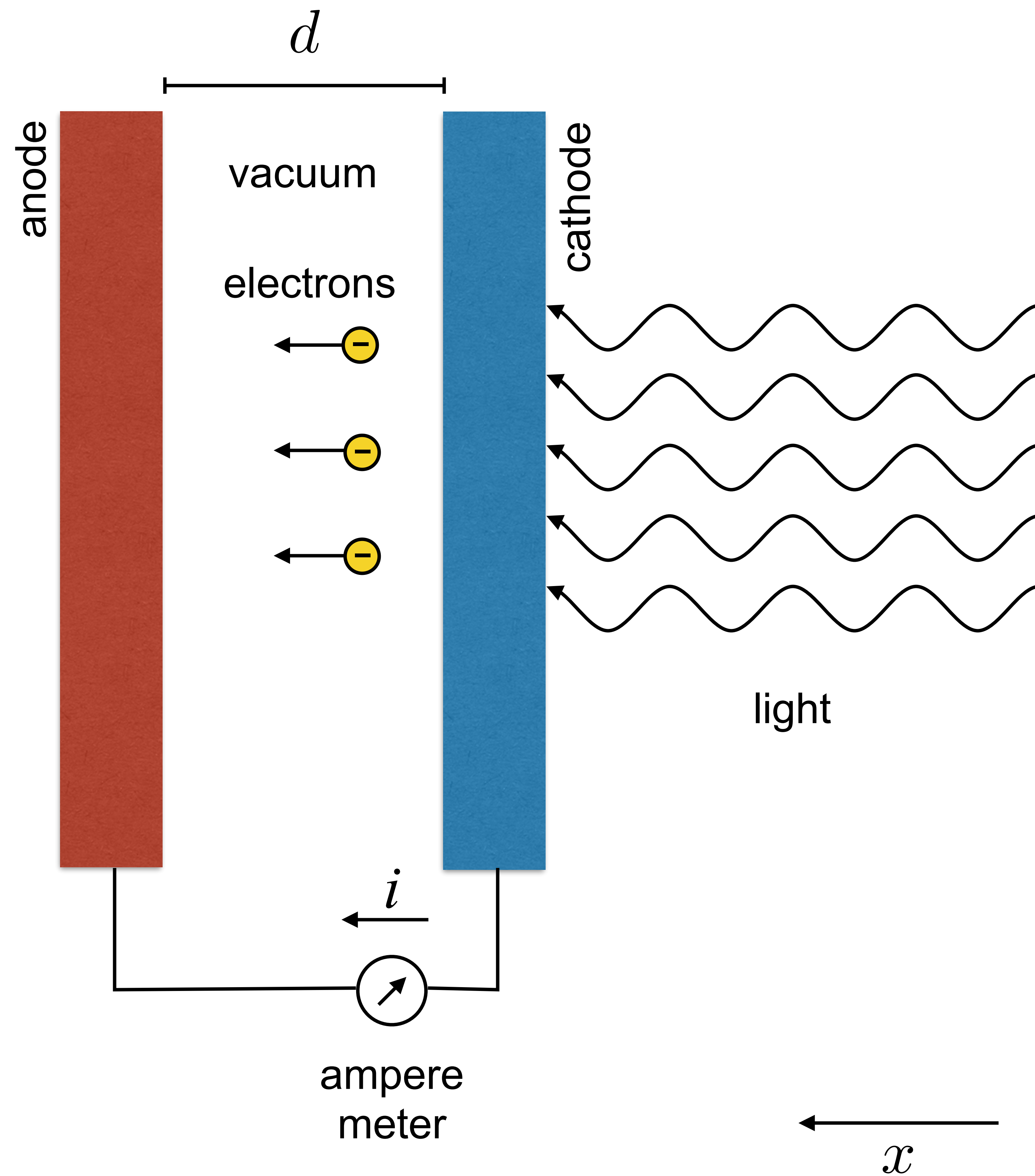
linear in intensity



Photoelectric effect

experimental observations

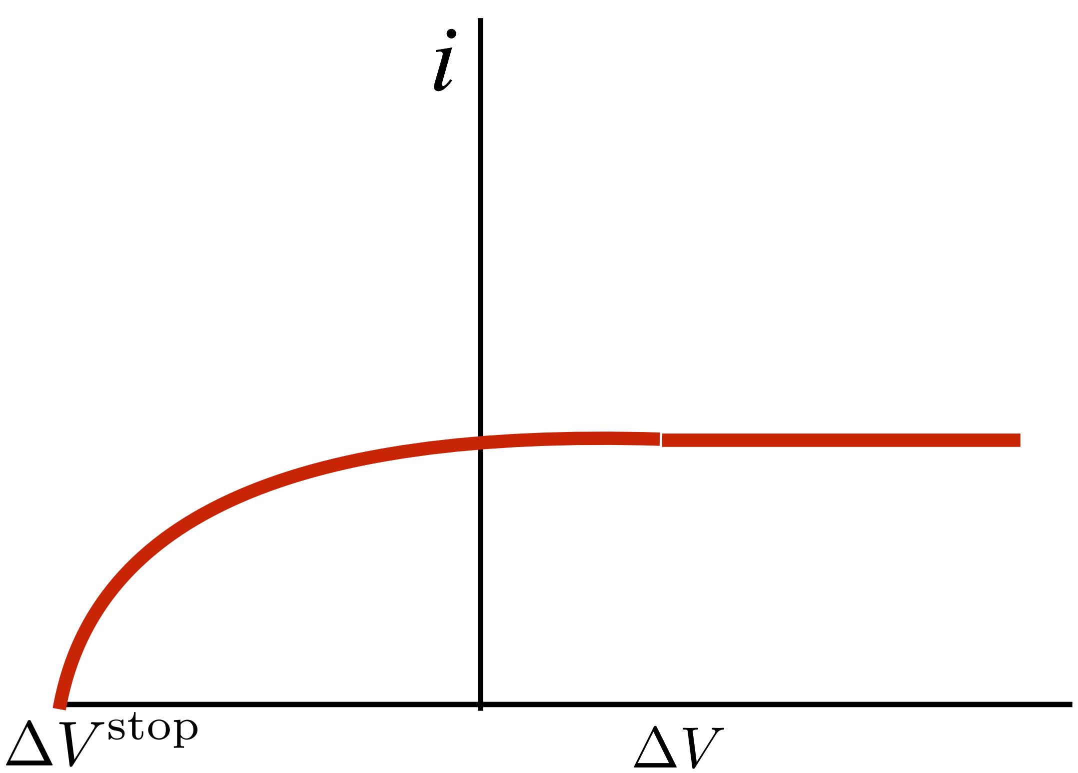
- threshold frequency
  - independent of intensity
- maximum photocurrent
  - linear in intensity

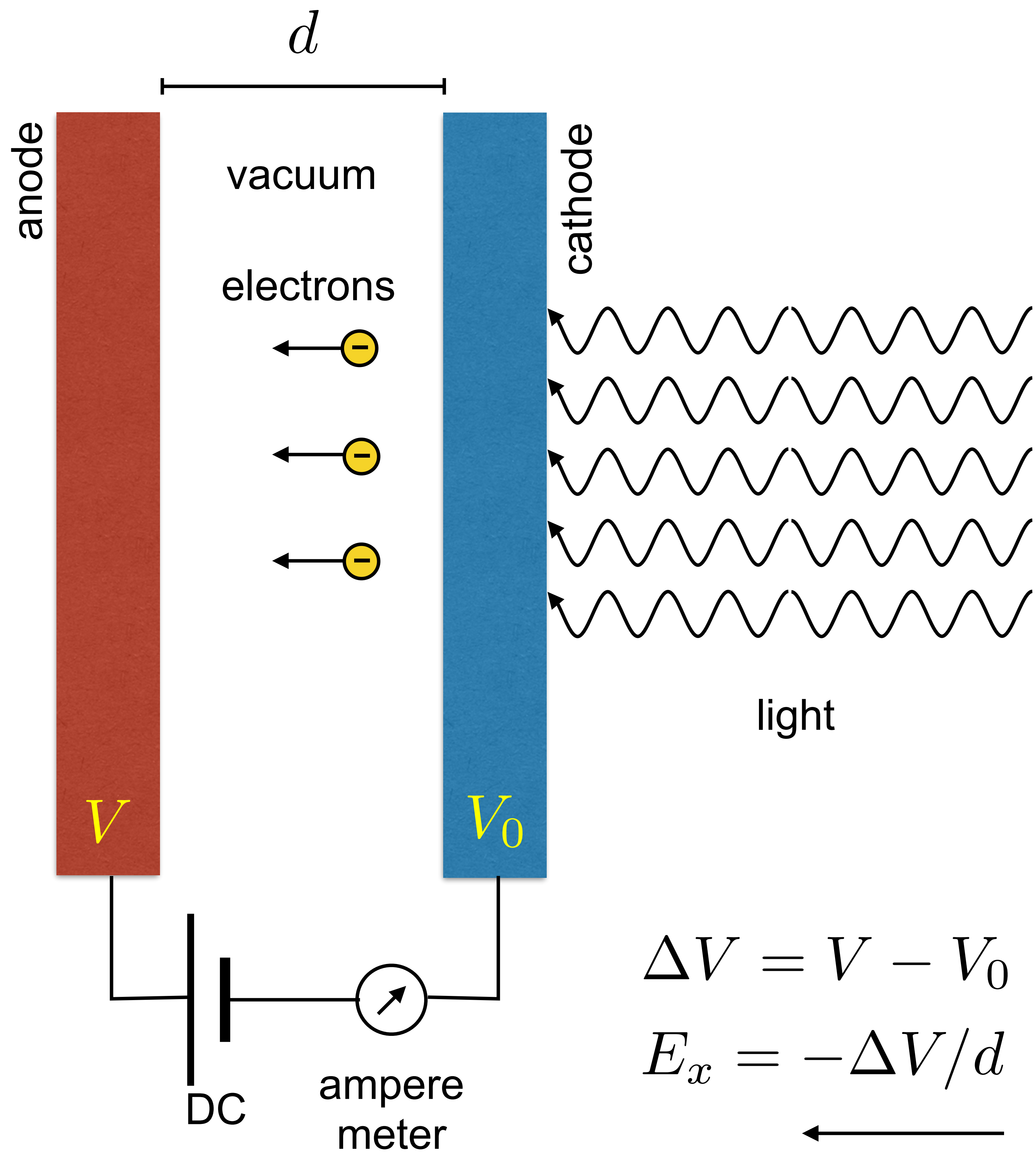


Photoelectric effect

experimental observations

- threshold frequency
  - independent of intensity
- maximum photocurrent
  - linear in intensity
- stopping potential





$$\Delta V = V - V_0$$

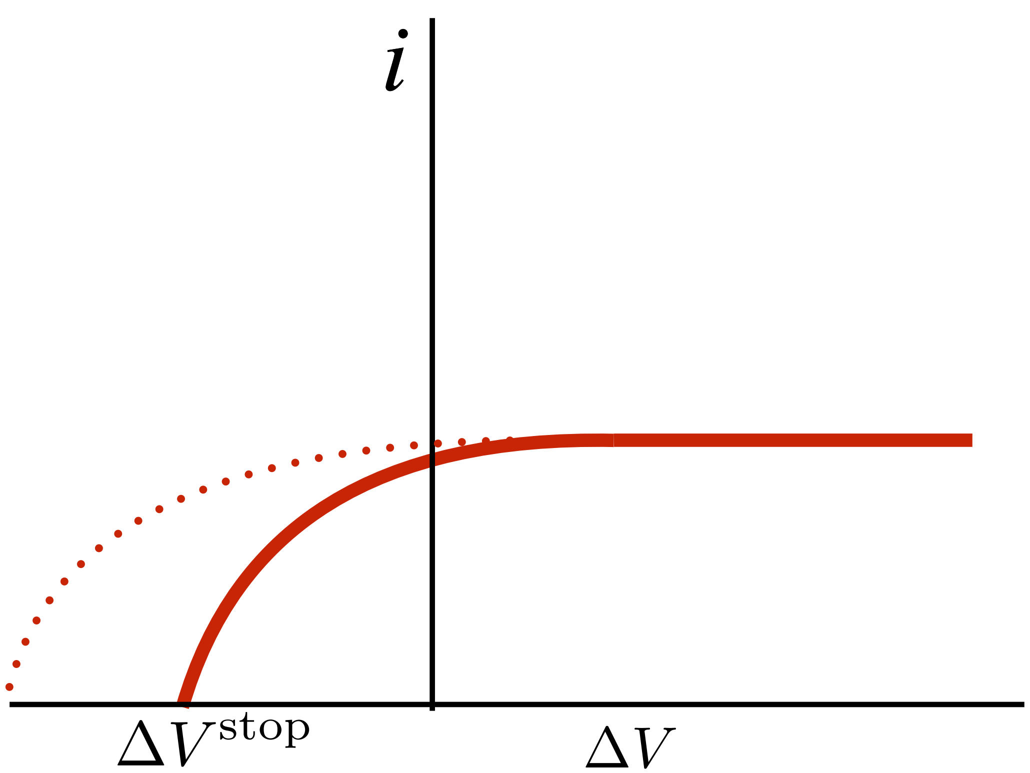
$$E_x = -\Delta V/d$$

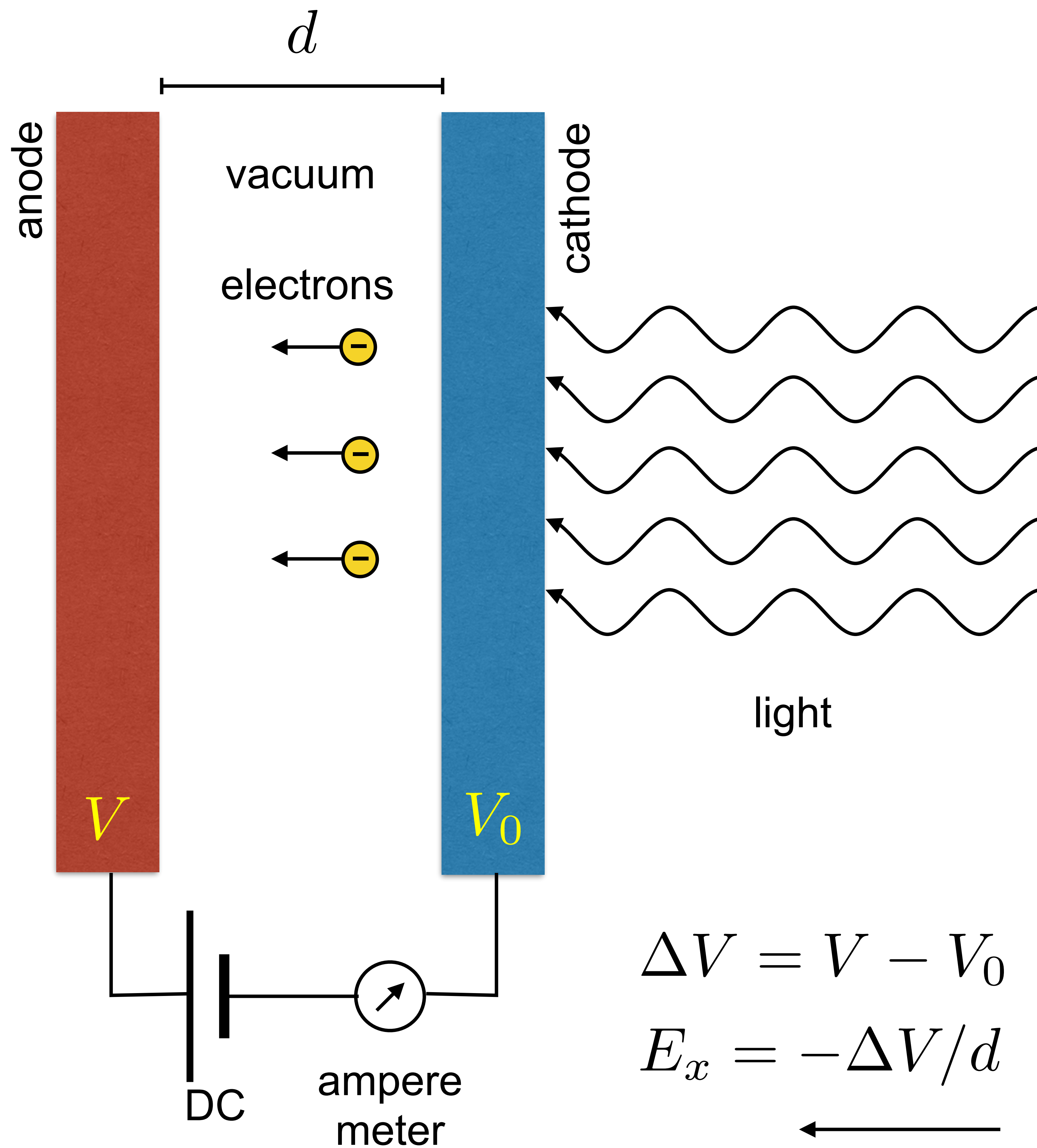
x

Photoelectric effect

experimental observations

- threshold frequency
  - independent of intensity
- maximum photocurrent
  - linear in intensity
- stopping potential
  - frequency dependent





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Photoelectric effect

experimental observations

threshold frequency

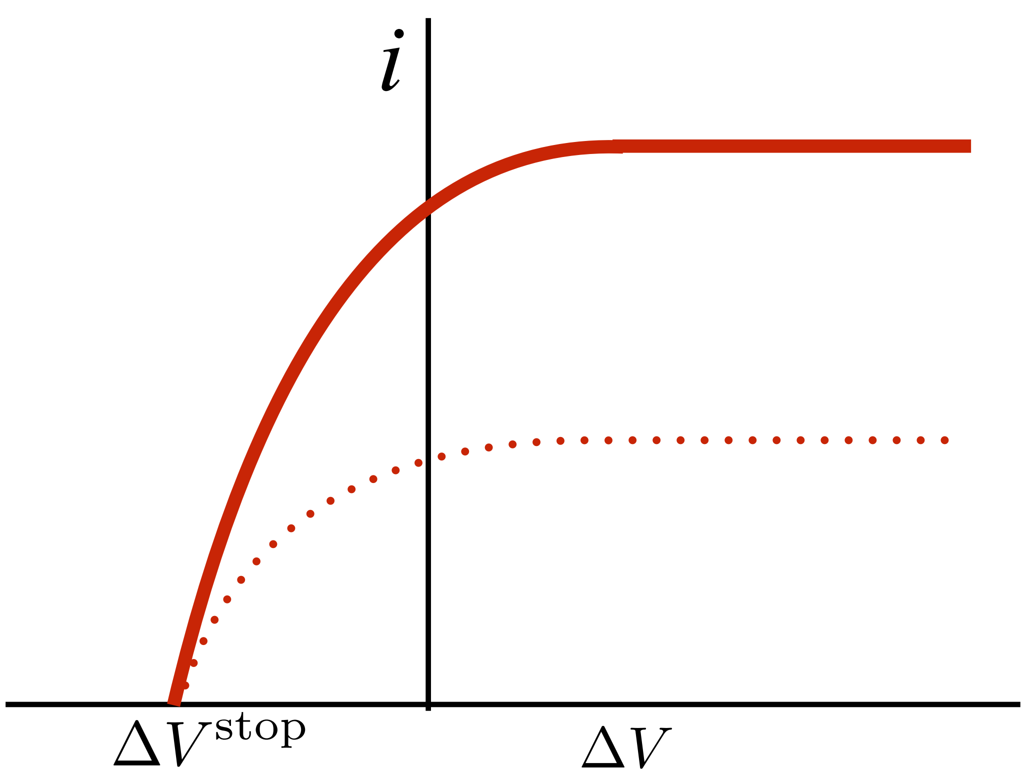
- independent of intensity

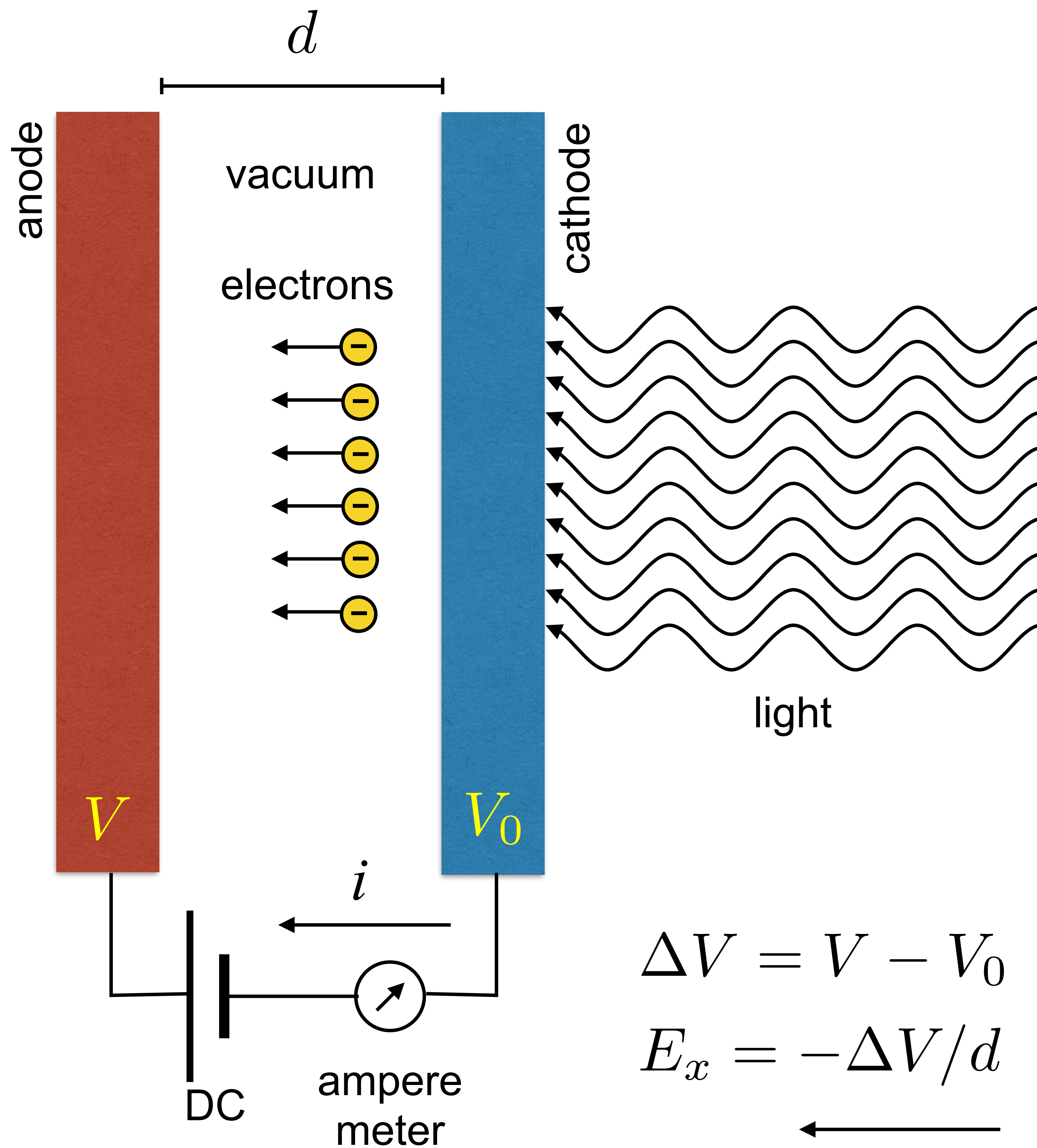
maximum photocurrent

- linear in intensity

stopping potential

- frequency dependent
- independent of intensity





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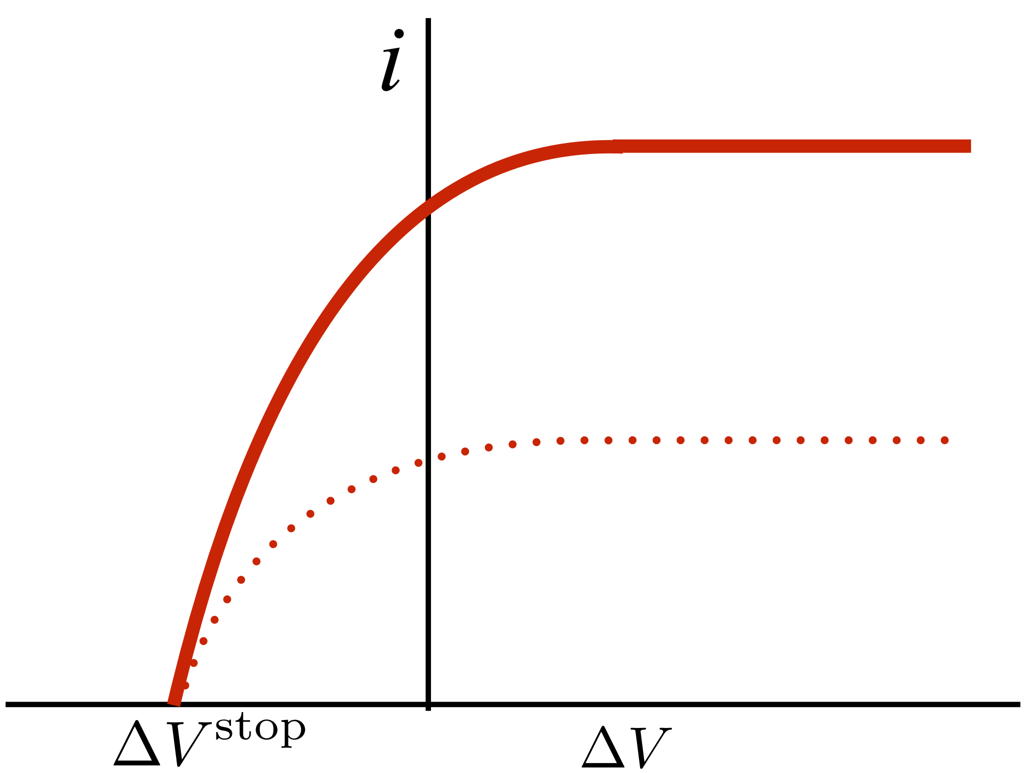
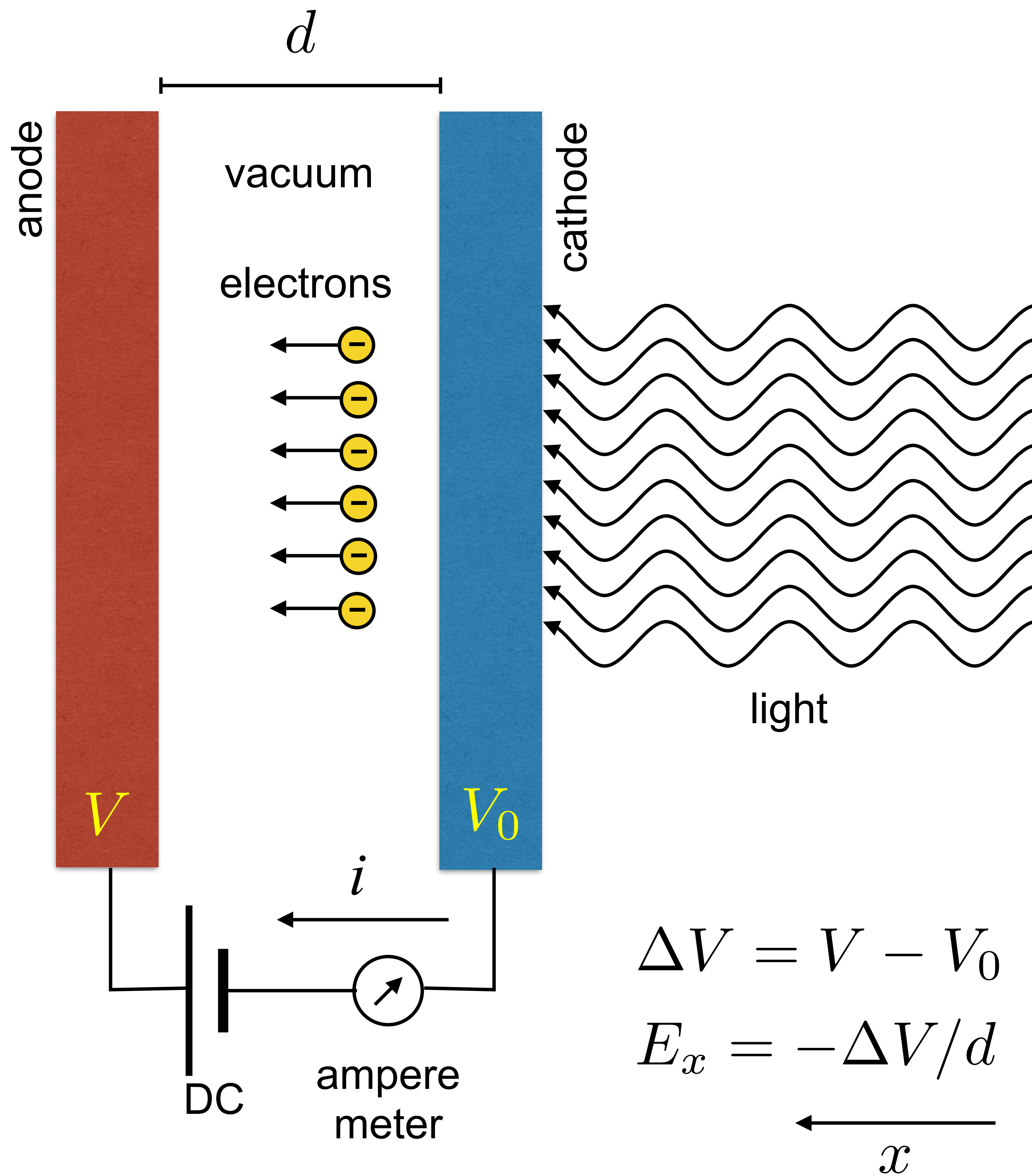
Photoelectric effect

experimental observations

- threshold frequency
  - independent of intensity
- maximum photocurrent
  - linear in intensity
- stopping potential
  - frequency dependent
  - independent of intensity
- instantaneous





$$\Delta V = V - V_0$$

$$E_x = -\Delta V / d$$

Photoelectric effect

conflict between experimental observations and predictions

1. no photoemission below minimum frequency
2. kinetic energy proportional to frequency of light, independent of intensity
3. maximum photocurrent proportional to intensity
4. instantaneous

Photoelectric effect

Einstein:

electromagnetic radiation is composed of quanta with discrete energies

'photon'

$$E = h\nu$$

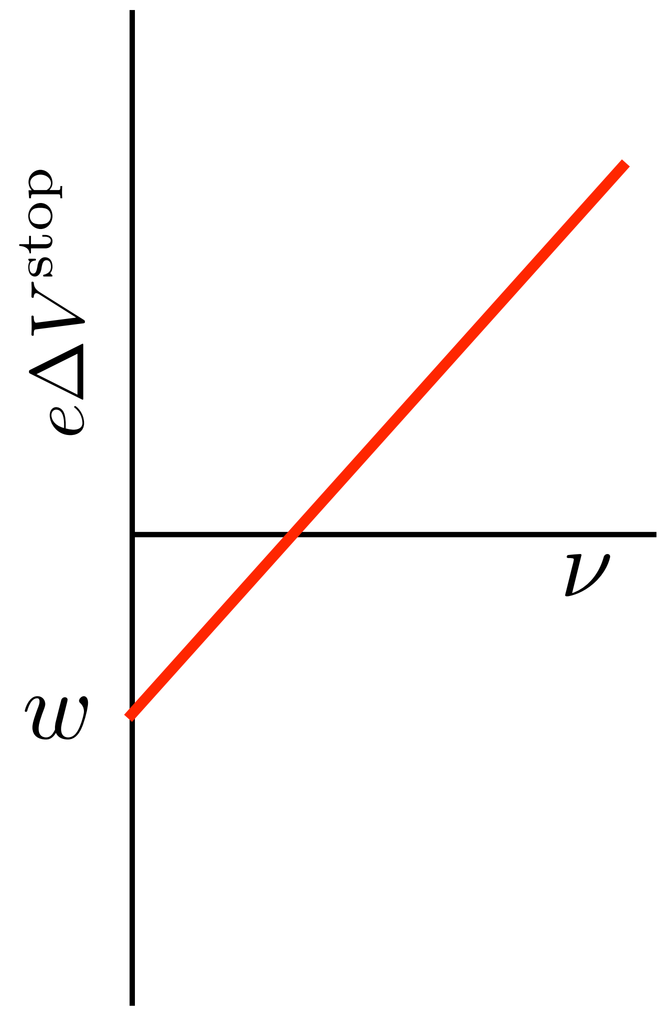
Photoelectric effect

Einsteins prediction for photoelectric effect

electrons interact with one photon at the time and take up all energy

photons converted into kinetic energy plus work required to escape

$$h\nu = \frac{1}{2}m_e v^2 + w$$



Schrödinger equation (1926)

Photoelectric effect

Einsteins prediction for photoelectric effect

electrons interact with one photon at the time and take up all energy

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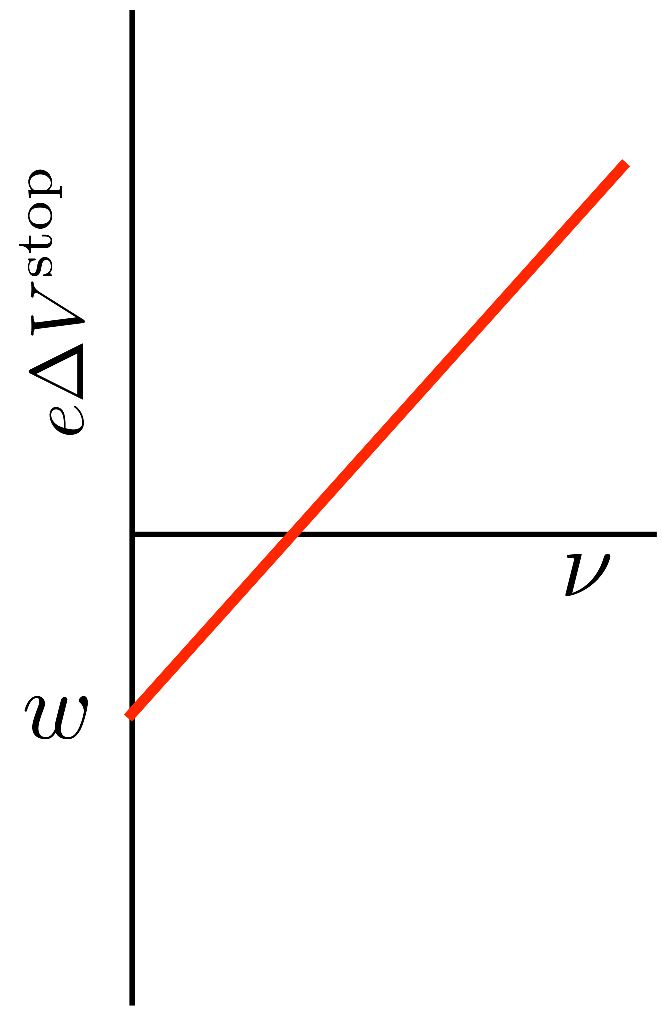
$$h\nu = \frac{1}{2} m_e v^2 + w$$

simple linear relation ship between frequency and stopping potential

$$e\Delta V^{\mathrm{stop}} = h\nu - w$$

experimental confirmation

Millikan, 1909



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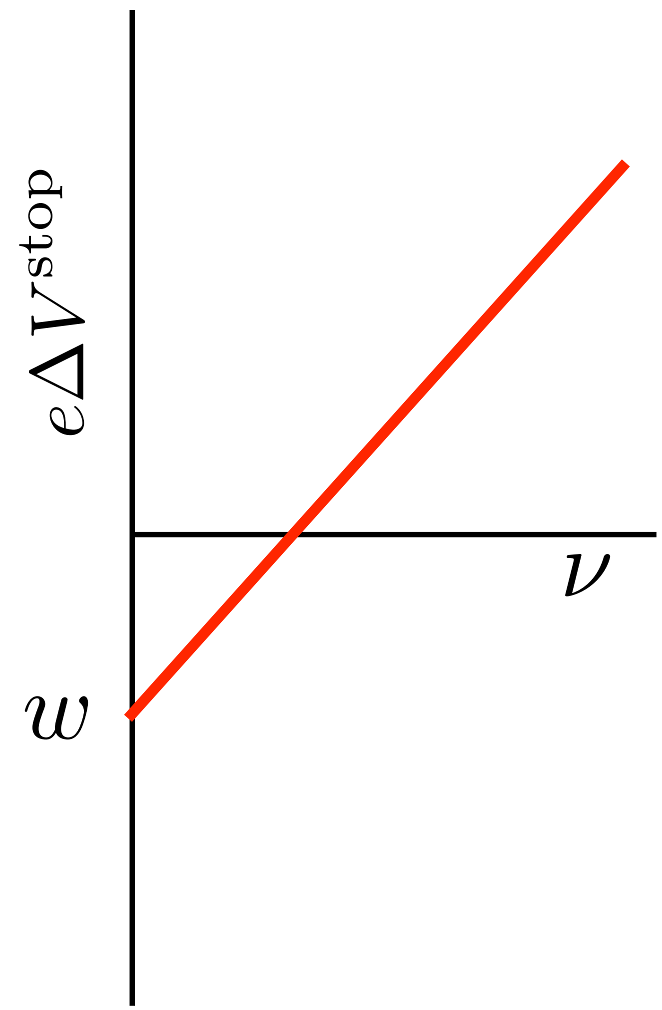


experimental confirmation

Millikan, 1909

implications

if waves can be particles, can particles be waves?

wave-particle duality

de-Broglie (1923)

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

Schrödinger equation (1926)

Photoelectric effect

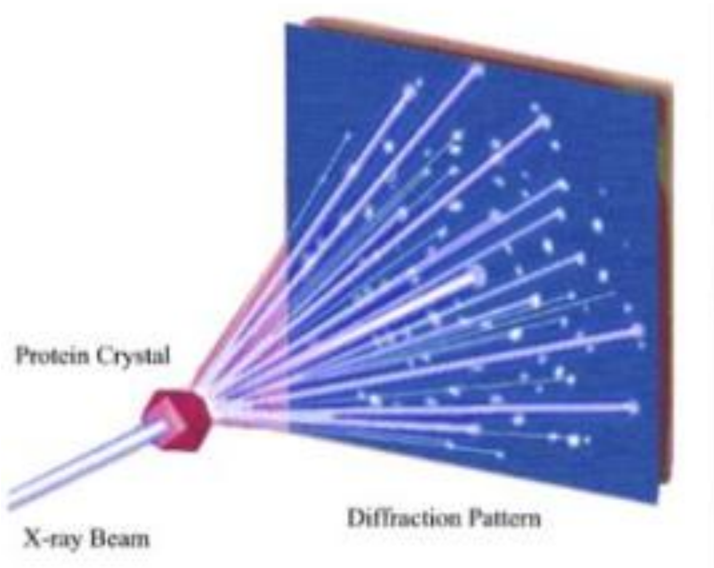
- photon multipliers
  - release of electron is amplified to get signal
  - night-vision
- material science: photo-emission spectroscopy
  - energy levels of bound electrons
    - electronic structure of atoms, molecules and materials
- biology
  - photo-ionization
    - UV exposure leads to free electrons and reactive radicals in DNA: damage and/or mutations
- crystallography
  - determine structure from x-ray diffractions

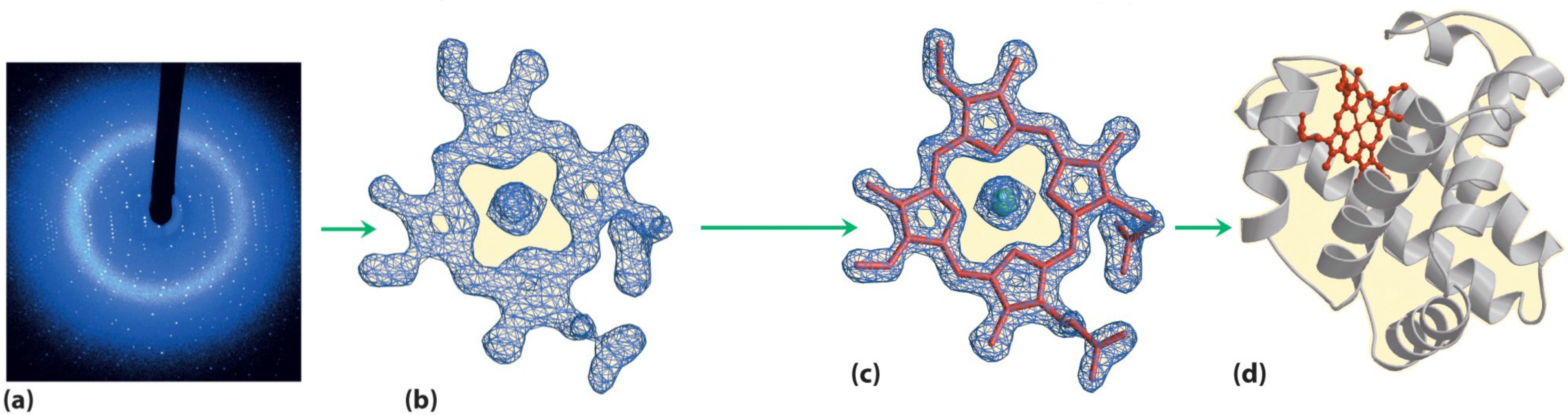
Photoelectric effect

off-topic: crystallography

determine structure from x-ray diffraction

x-ray energies: 10 keV





new: diffract and destroy!

outrun photoelectric effect

Photoelectric effect

the experiment

electrons released by light

from cathode to anode

kinetic energy

$$E_{\rm kin} = \frac{1}{2} m_e v^2$$

photocurrent

$$i \propto v$$

stopping potential

make cathode positief

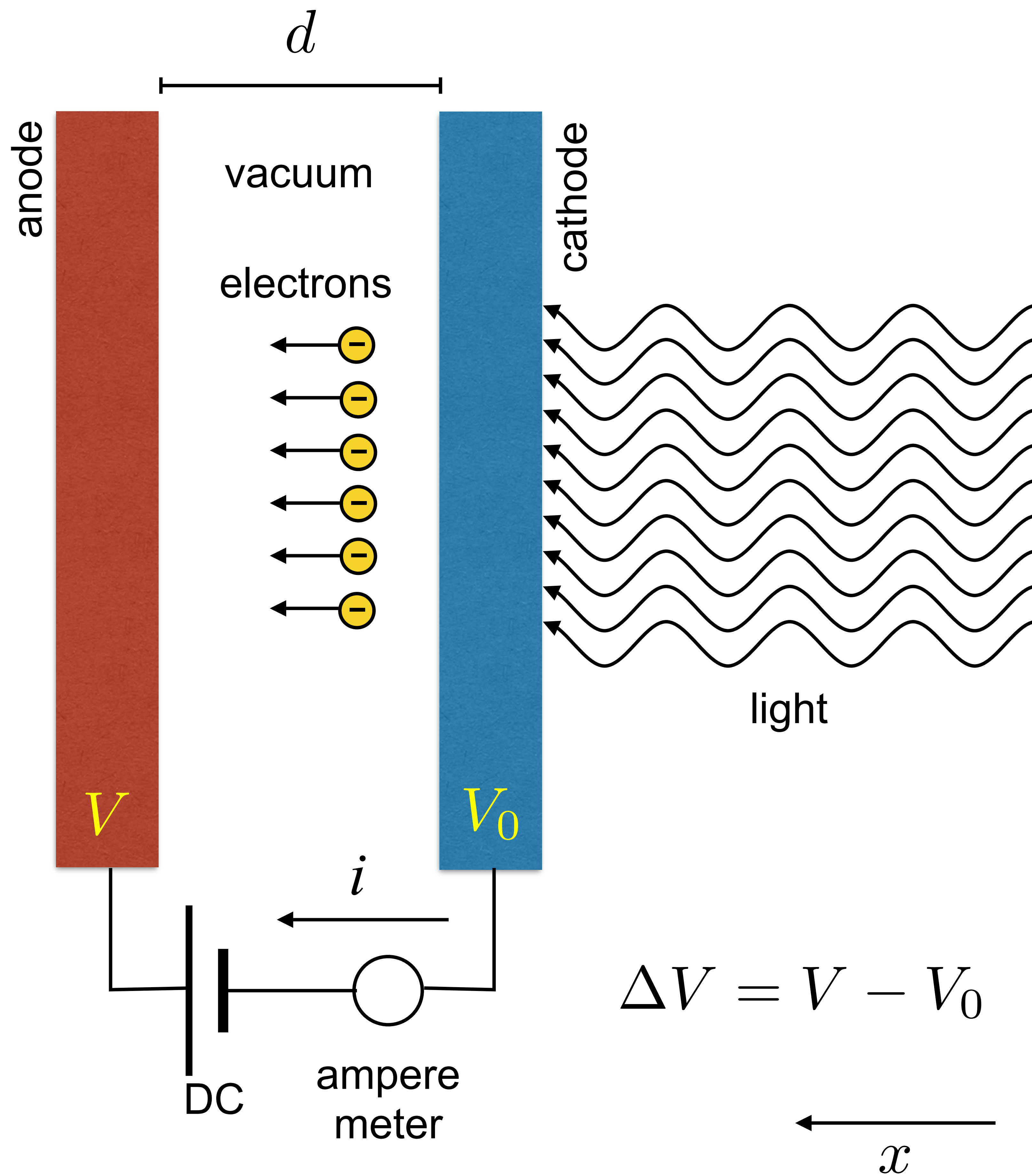
work on electron

$$E_{\rm pot}(x) = e\frac{\Delta V}{d}x$$

stop electron just before anode

$$E_{\rm pot}(d) = K_{\rm kin}$$

$$\Delta V^{\rm stop} = \frac{m_e v^2}{2e}$$



Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

linear operators

$$\hat{\Omega}(af) = a\hat{\Omega}f$$

eigenfunctions & eigenvalues

$$\hat{\Omega}f = \omega f$$

complete set

$$\hat{\Omega}f_n = \omega_n f_n$$

linear combination

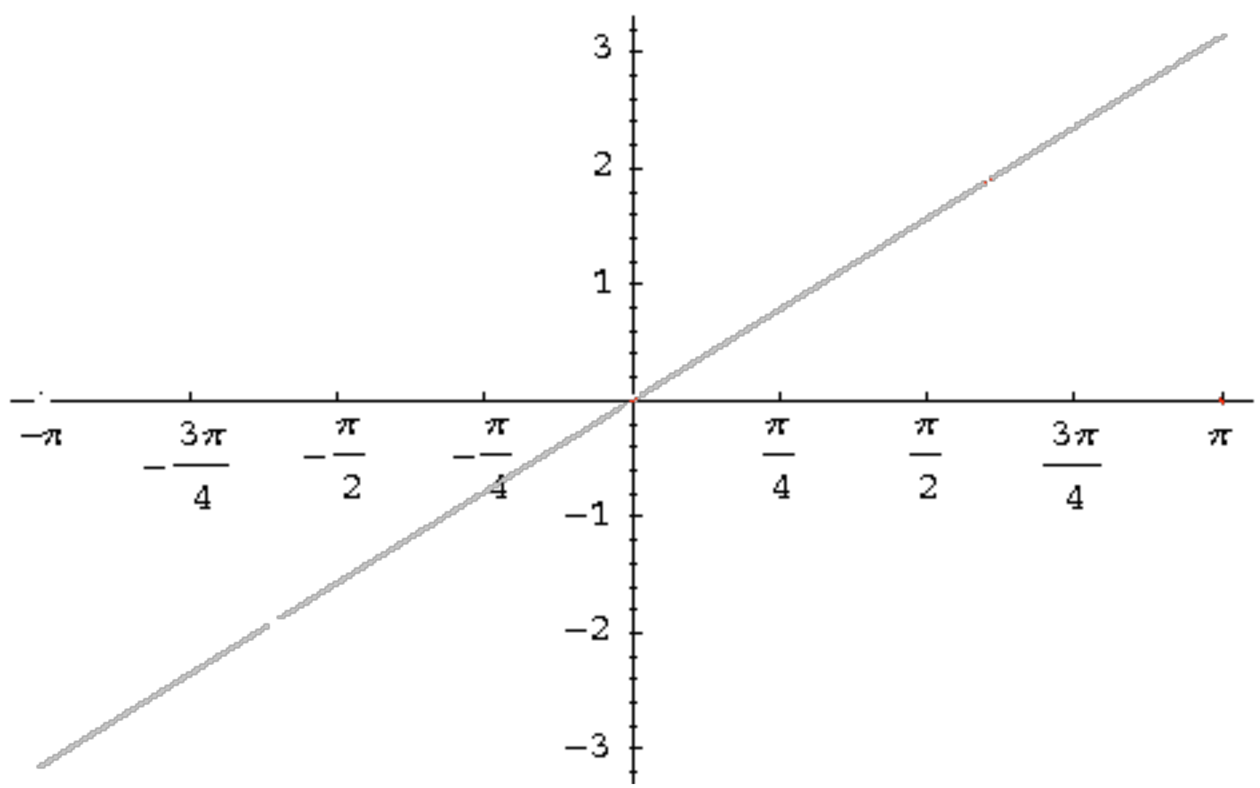
$$g = \sum_n c_n f_n$$

Recall from Mathematics: Fourier Series

Linear combination of Cosine and Sine functions

example

$$f(x) = x \qquad -\pi \leq x \leq \pi$$



Recall from Mathematics: Fourier Series

Linear combination of Cosine and Sine functions

example

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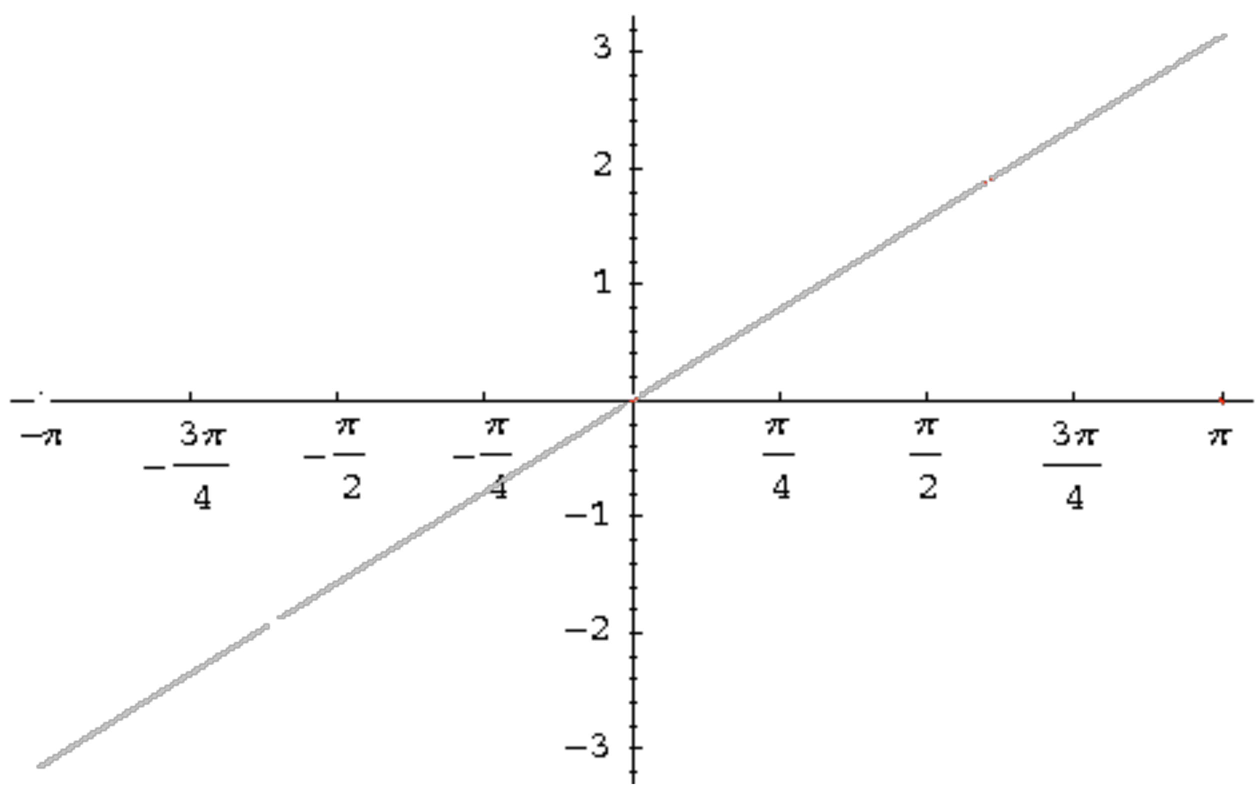
Fourier series

$$f(x) = \sum_{n=1} a_n \sin[nx] \qquad a_n = \frac{2}{n}(-1)^{n+1}$$

$$f(x) \approx 2\left(\sin[x] - \frac{1}{2}\sin[2x] + \frac{1}{3}\sin[3x] - \frac{1}{4}\sin[4x] + \ldots\right)$$



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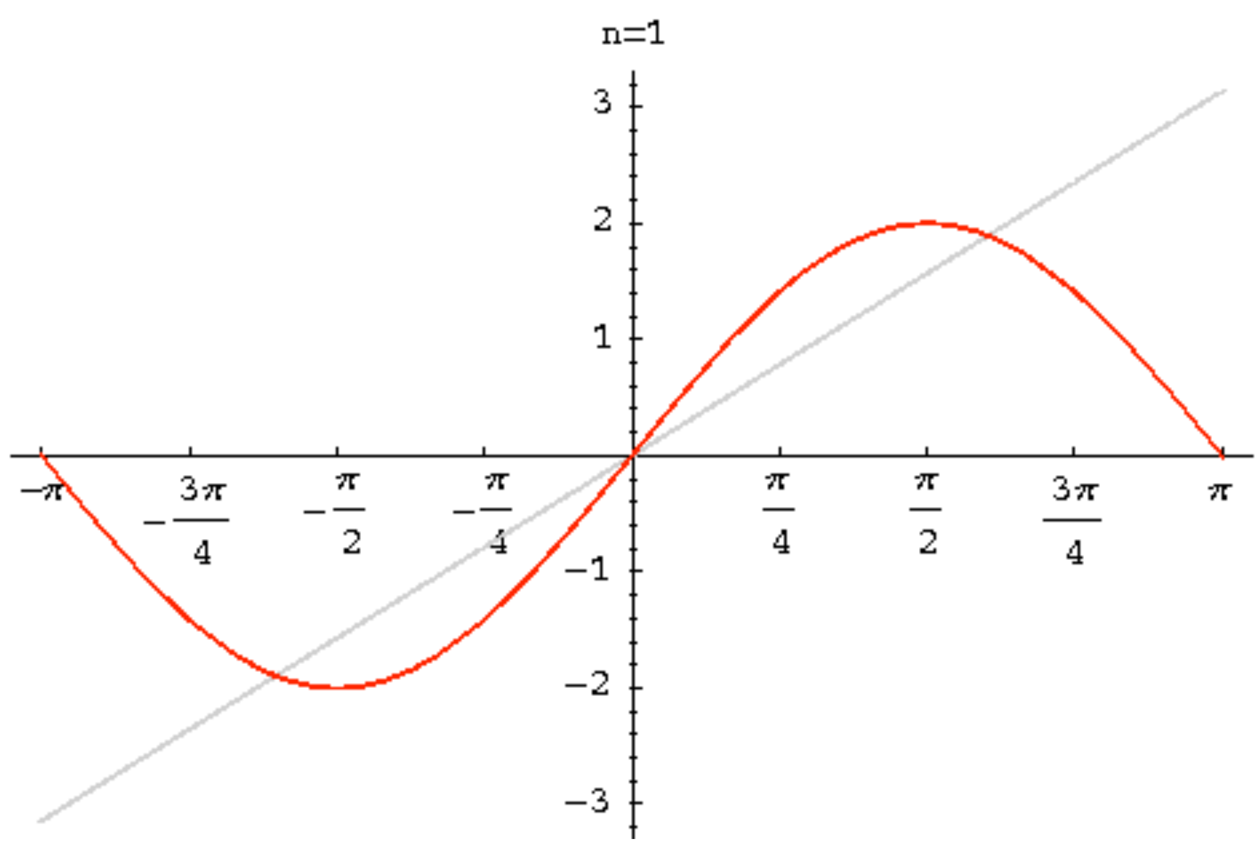
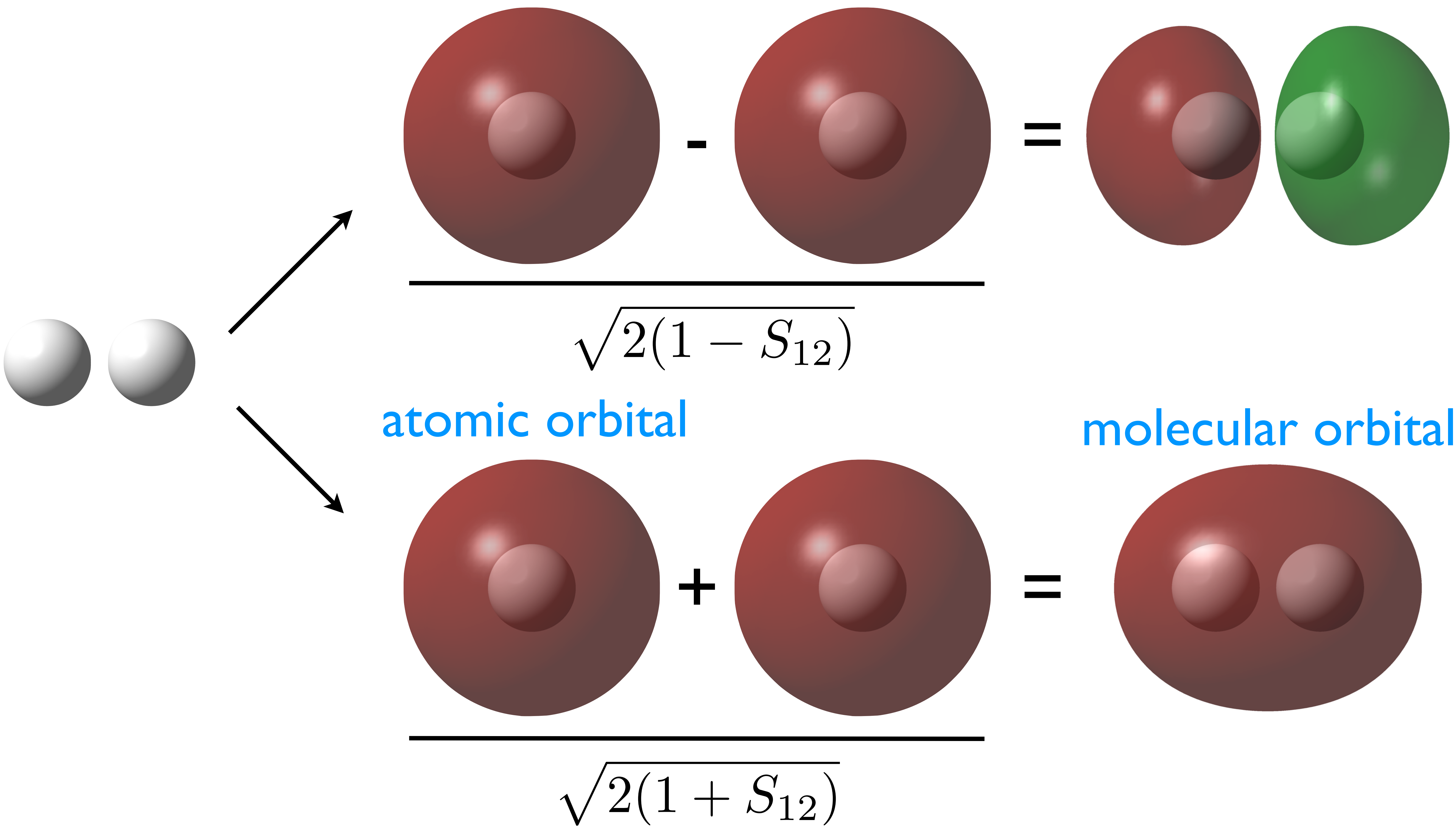


Hydrogen molecule

Linear Combination of single hydrogen orbitals



Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

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$$g = \sum_n c_n f_n$$

$$\hat{\Omega}g = f_n = \hat{\Omega}\sum_n c_n f_n = \sum_n c_n \hat{\Omega} f_n = \sum_n c_n \omega_n f_n$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

representation

$$\hat{x} f \to x \times f \qquad \hat{p}_x f \to -i\hbar \frac{\partial}{\partial x} f$$

commutation

$$[\hat{A}, \hat{B}] f = \hat{A}\hat{B} f - \hat{B}\hat{A} f$$

position and moment *do not* commute

$$[\hat{x}, \hat{p}_x] f = i\hbar f$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

representation

$$\hat{x} f \to x \times f \qquad \hat{p}_x f \to -i\hbar \frac{\partial}{\partial x} f$$

from classical to quantum

replace x and p by their operators

e.g., total energy (Hamiltonian)

$$H = T + V = \frac{p_x^2}{2m} + V(x)$$

$$\hat{H} = \hat{T} + \hat{V} = \frac{\hat{p}_x^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(\hat{x})$$

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chapter 1, abstract introductory stuff

integrals over operators

$$I = \int f_m^* \hat{\Omega} f_n d\tau = \langle m|\hat{\Omega}|n\rangle = \Omega_{mn}$$

bracket notation

$$f_n^* = \langle n| \qquad f_m = |m\rangle \qquad \langle m|n\rangle = \langle n|m\rangle^*$$

completeness of a basis

$$\sum_n |n\rangle\langle n| = 1$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

Hermitian operators

$$\int f_m^* \hat{\Omega} f_n d\tau = \int \underline{(\hat{\Omega} f_m)^*} f_n d\tau = \left(\int f_n^* \hat{\Omega} f_m d\tau \right)^*$$

bracket notation

$$\langle m|\hat{\Omega}|n\rangle = \langle n|\hat{\Omega}|m\rangle^*$$

eigenvalues are real

eigenfunctions are orthogonal

$$\langle n|m\rangle = \delta_{nm}$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

Hermitian operators

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eigenvalues are real

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$$\langle n|m\rangle = \delta_{nm}$$

observables have Hermitian operators

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

wave function

probability function

$$P(x) = \psi^*(x)\psi(x)dx$$

brackets

$$|s\rangle = \psi_s(x) \qquad \langle s| = \psi_s^*(x) \qquad \langle s|q\rangle = a \qquad \langle q|s\rangle = a^* \qquad |s\rangle\langle q| = \hat{O}$$

superposition principle

$$\Psi(x) = \sum c_i |s_i\rangle$$

operators

$$\hat{A}|s\rangle = a|q\rangle \qquad \langle s|\hat{A}^\dagger = a^*\langle q|$$

hermitian operators

$$\langle r|\hat{A}|s\rangle = a\langle r|q\rangle = \left(a * \langle q|r\rangle\right)^* = \left(\langle s|\hat{A}^\dagger|r\rangle\right)^* = \left(\langle s|\hat{A}|r\rangle\right)^*$$

eigenfunction/values

$$\hat{A}|a\rangle = \alpha|a\rangle$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

Dirac quantum conditions

classical Poisson bracket

$$\{f, g\} = \frac{\partial f}{\partial x}\frac{\partial g}{\partial p} - \frac{\partial g}{\partial x}\frac{\partial f}{\partial p}$$

quantum mechanics operators corresponding to observables

$$[\hat{f}, \hat{g}] = i\hbar\{f, g\}$$

commuting operators & simultaneous eigenfunctions

expectation values & averages

$$\langle A \rangle = \langle S | \hat{A} | S \rangle$$

uncertainty relations

$$(\Delta f)(\Delta g) \geq \frac{1}{2} | \langle -i[\hat{f}, \hat{g}] \rangle |$$

Quantum Mechanics (KEMS401)

chapter 1:

the postulates

state of a system is fully described by its wave function

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3, .., t)$$

observables are represented by *Hermitian* operators

commutation relation

$$[x, p_x] = i\hbar$$

value of observable is expectation value of wave function

$$\langle O \rangle = \frac{\int_{-\infty}^{\infty} \psi^* \hat{O} \psi d\tau}{\int_{-\infty}^{\infty} \psi^* \psi d\tau} = \frac{\langle \psi | \hat{O} | \psi \rangle}{\langle \psi | \psi \rangle}$$

probability density

$$P(x)dx = \psi^*(x)\psi(x)dx$$

time evolution

Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi(x, t) = \hat{H}(x, t)\psi(x, t)$$

Quantum Mechanics (KEMS401)

chapter 1:

Bohr conditions

$$P(x)dx = \psi^*(x)\psi(x)dx$$

wave function is probability function with following properties

- wave function must be finite everywhere
- wave function must be single-valued everywhere
- wave function must be continuous
- wave function must be differentiable everywhere

boundary conditions

- only certain solutions are possible, e.g. wave function goes to zero at infinity
- quantisation: discrete energy levels

$$E_n = \frac{n^2h^2}{8L^2m}$$

Quantum Mechanics (KEMS401)

chapter 1:

Schrödinger equation

time dependent

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \hat{H}(x,t)\psi(x,t)$$

time independent

$$\hat{H}(x)\psi(x,t) = E\psi(x,t)$$

Hamiltonian

$$\hat{H}(x,t) = \frac{1}{2m}\hat{p}^2 + V(x,t) = -\frac{1}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$$

free particle & wave packet (lecture 2)

time-dependence of expectation values

particle in box

tunneling

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

simultaneous observables

corresponding operators commute

$$[\hat{A}, \hat{B}] = 0$$

observables A and B can be observed

$$\hat{A}\hat{B}\psi = b\hat{A}\psi = ab\psi$$

$$\hat{B}\hat{A}\psi = a\hat{B}\psi = ab\psi$$

if they do not commute:

$$\hat{A}\hat{B}\psi = \hat{A}\phi \qquad \hat{A}\phi \neq a\phi$$

$$\hat{B}\hat{A}\psi = a\hat{B}\psi = a\phi$$

Quantum Mechanics (KEMS401)

chapter 1, abstract introductory stuff

expectation value

eigenfunctions of operator

$$\langle A \rangle = \langle \psi | \hat{A} | \psi \rangle = \langle \psi | a | \psi \rangle = a$$

observables A and B can be observed

$$\hat{B} | \psi \rangle = | \phi \rangle$$

$$\hat{B} | \varphi_n \rangle = b_n | \varphi_n \rangle$$

complete set

$$\phi = \sum_n c_n | \varphi_n \rangle$$

$$\langle B \rangle = \langle \phi | \hat{B} | \phi \rangle = \sum_m \sum_n c_m^* c_n \langle \varphi_m | \hat{B} | \varphi_n \rangle = \sum_n b_n |c_n|^2$$