Physics of Electronics:

1. Introduction to Quantum Mechanics

July – December 2008

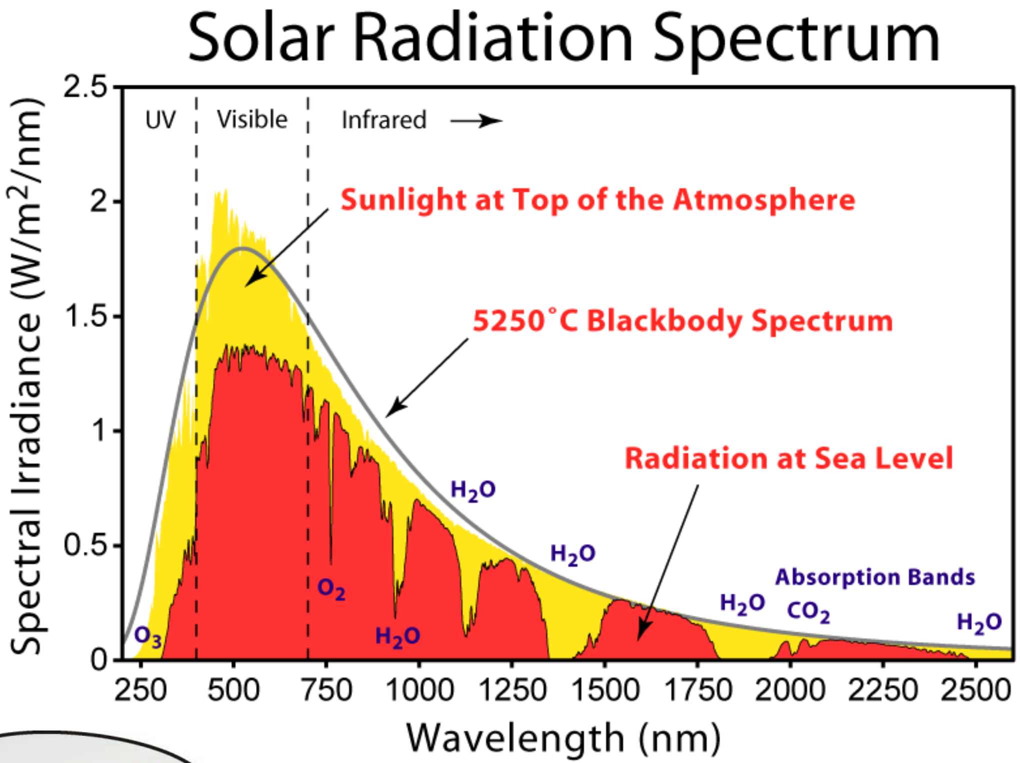
Contents overview

- Introduction
- Blackbody radiation
- Photoelectric effect
- Bohr atom
- Wavepackets
- Schrödinger equation
- Interpretation of wavefunction
- Uncertainty principle
- Beams of particles and potential barriers

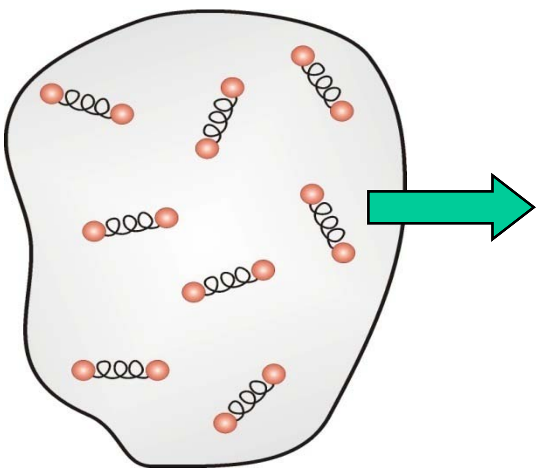
The English translation of some of the original articles can be seen at:
http://strangepaths.com/resources/fundamental-papers/en/

Blackbody Radiation

- Experiment



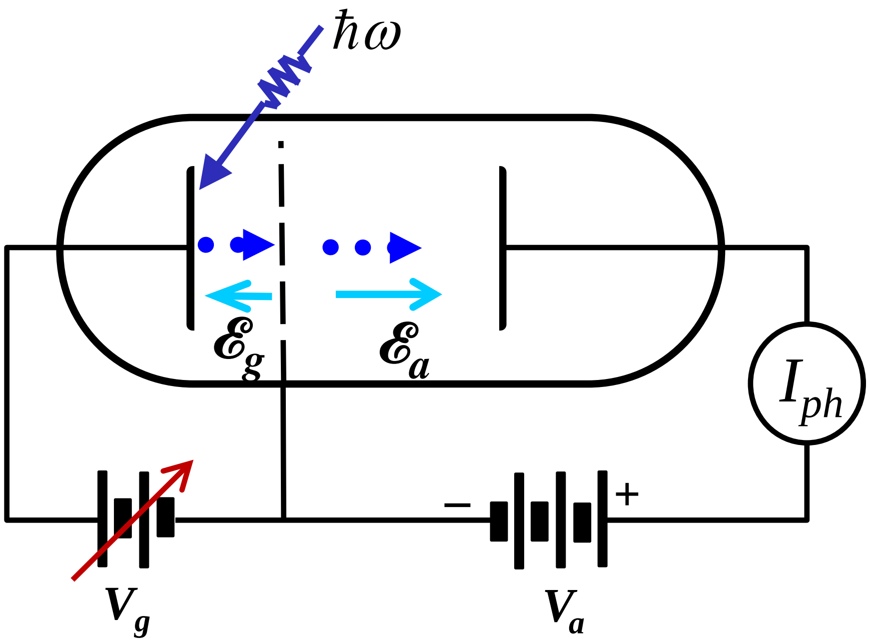
- Theory

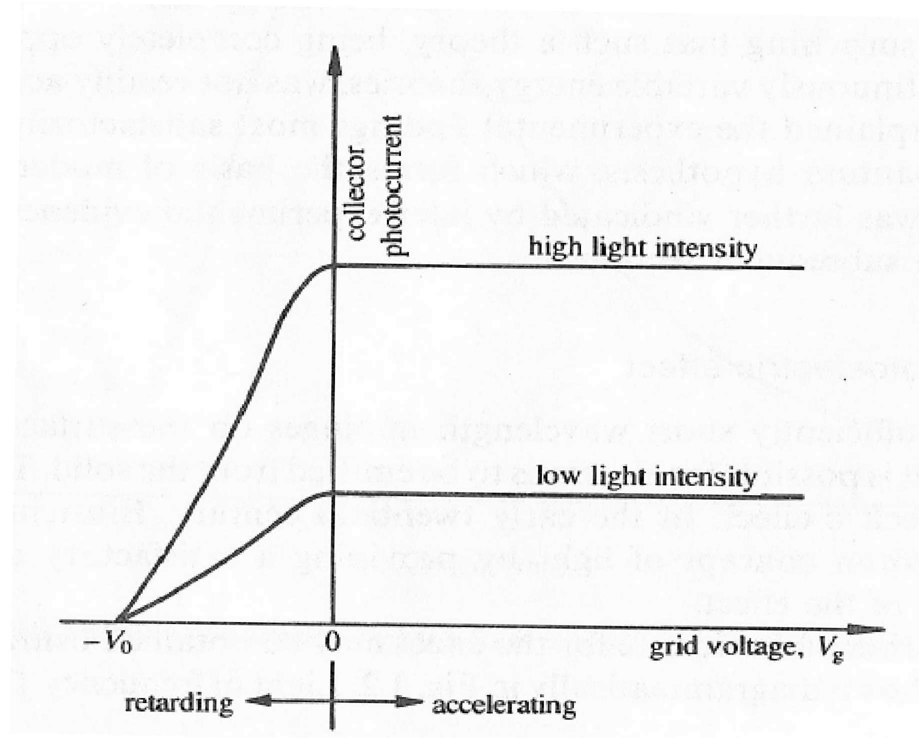


$$E = 0, \quad \hbar\omega, \quad 2\hbar\omega, \quad 3\hbar\omega, \quad \ldots, \quad n\hbar\omega$$

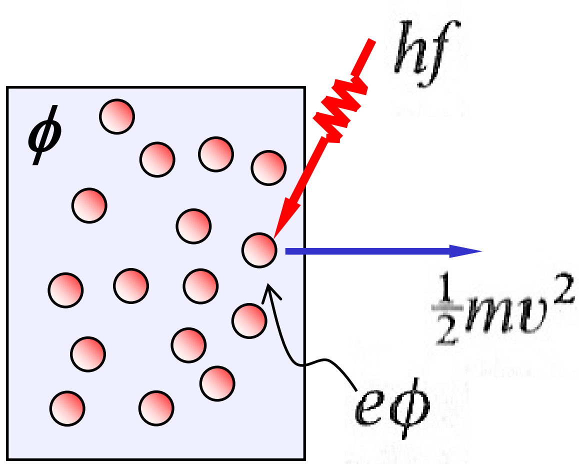
Photoelectric Effect

- Experiment





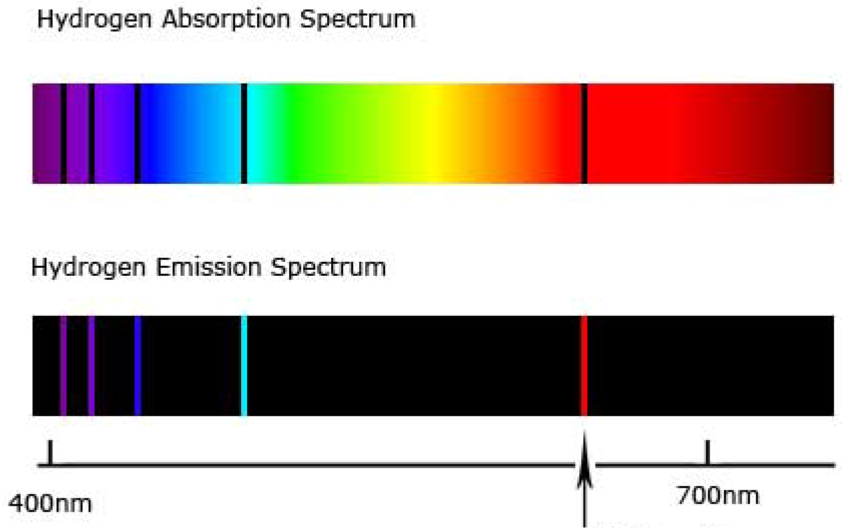
- Theory



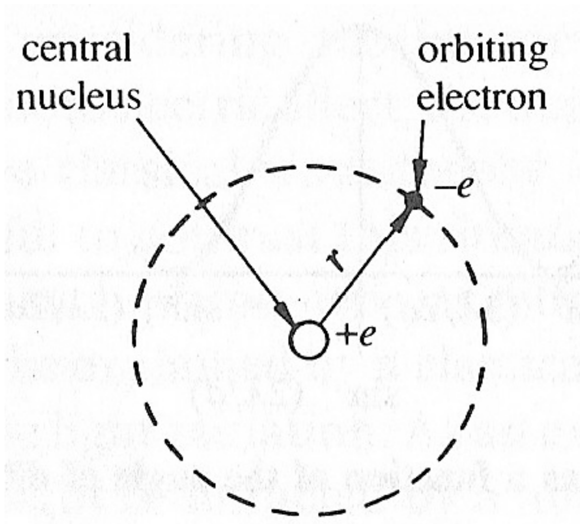
$$\tfrac{1}{2}mv^2 = hf - e\phi$$

Hydrogen and Bohr Atom

- Experiment



- Theory

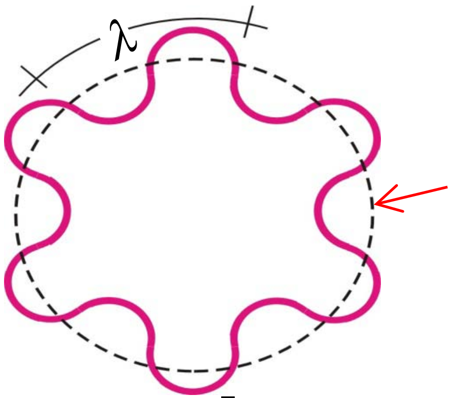


$$L = mvr = n\hbar \qquad \text{where } n = 1, 2, 3, \ldots$$

$$E_n = -\frac{e^2}{8\pi\epsilon_0}\frac{\pi e^2 m}{n^2 h^2 \epsilon_0} = -\frac{me^4}{8\epsilon_0^2 h^2 n^2} \simeq -\frac{13.6}{n^2}\,\text{eV}$$

Particle-Wave Duality & Wavepackets

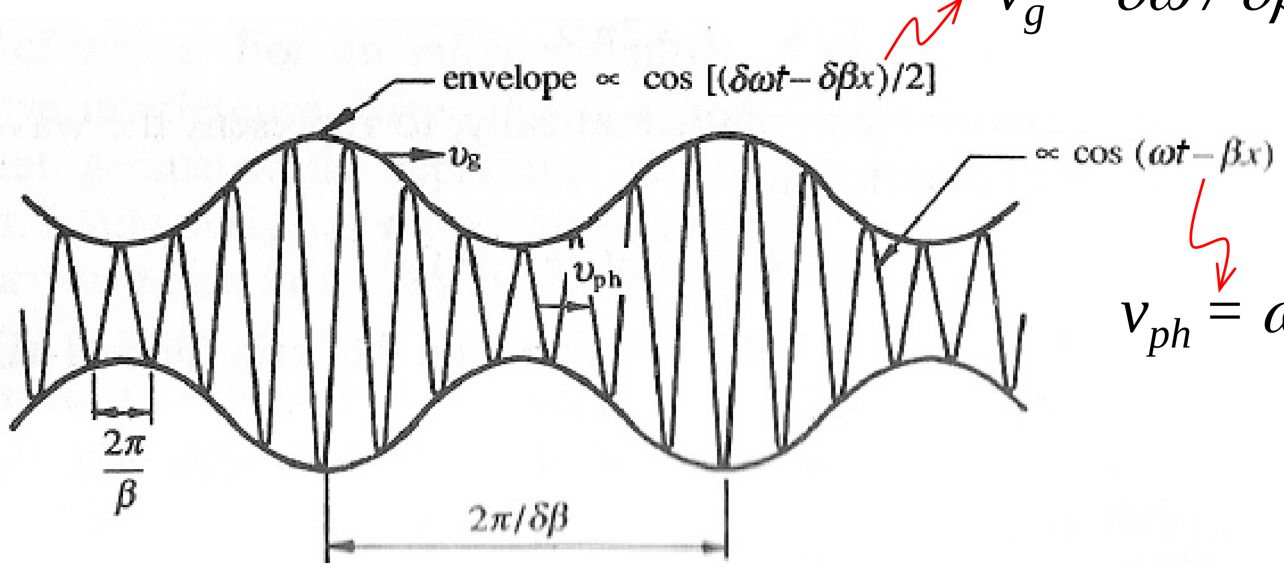
- De Broglie hypothesis:



$$2\pi r = n\lambda \;\Rightarrow\; p = h/\lambda$$

- Phase and group velocity:

$$v_g = \delta\omega / \delta\beta$$



$$v_{ph} = \omega / \beta$$

Wavepackets

- Associating a wavepacket to a particle:
  - From De Broglie and Bohr relations:

$$p = mv = h/\lambda \Rightarrow \beta = \frac{2\pi}{\lambda} = \frac{2\pi p}{h} = \frac{p}{\hbar}$$

$$T = \tfrac{1}{2}mv^2 = hf \Rightarrow \omega = \frac{2\pi T}{h} = \frac{T}{\hbar}$$

$$\Rightarrow \psi = A_0 \exp[-j(Tt - px)/\hbar]$$

  - In general a particle has also potential energy, therefore its wavefunction will be:

$$\psi = A_0 \exp[-j(Et - px)/\hbar]$$

where $E = T + V$

Schrödinger Equation

- It is similar to Newton’s equation. It describes the behavior of the wavefunction of a particle (and in general of any quantum system).

- Since we are describing a wave, SE should have the form of the well known wave equation that describe, for example, the EM field:

$$\frac{\partial^2 H}{\partial x^2} = \epsilon\mu \frac{\partial^2 H}{\partial t^2} \qquad \Longleftrightarrow \qquad H = H_0 \exp[-j(\omega t - \beta x)]$$

Schrödinger Equation

- “Derivation” of time-dependant SE:
  - Starting from $\psi = A_0 \exp[-j(Et - px)/\hbar]$
  - By deriving once respect to time

$$\frac{\partial \psi}{\partial t} = -j\frac{E}{\hbar}\psi \quad \Rightarrow \quad E\psi = \frac{\hbar}{j}\frac{\partial \psi}{\partial t}$$

  - Deriving twice respect to the position

$$\frac{\partial \psi}{\partial x} = j\frac{p}{\hbar}\psi \quad \Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \quad \Rightarrow \quad \frac{p^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

Schrödinger Equation

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  - Deriving twice respect to the position

$$\frac{\partial \psi}{\partial x} = j\frac{p}{\hbar}\psi \quad \Rightarrow \quad \frac{\partial^2 \psi}{\partial x^2} = -\frac{p^2}{\hbar^2}\psi \quad \Rightarrow \quad \frac{p^2}{2m}\psi = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

$$\left(\hat{p} \to \frac{\hbar}{j}\frac{\partial}{\partial x}\right)$$

Schrödinger Equation

- "Derivation" of time-dependant SE:
  - Starting from $\psi = A_0 \exp[-j(Et - px)/\hbar]$
  - Conservation of energy:

$$E = T + V = \frac{p^2}{2m} + V \quad \Rightarrow \quad \hat{E}\psi = \frac{\hat{p}^2}{2m}\psi + \hat{V}\psi$$

$$\Rightarrow \quad \boxed{\frac{\hbar}{j}\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \hat{V}\psi}$$

Schrödinger Equation

- "Derivation" of time-dependant SE:

$$\frac{\hbar}{j}\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} + \hat{V}\psi$$

  - Given a potential energy and the mass of the system, this equation can be solved.

  - Generalization to 3D:

$$\frac{\hbar}{j}\frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2 \psi + \hat{V}\psi$$

Schrödinger Equation

- Time-independent SE:
  - **If** V is time independent, we can assume the following form of the wavefunction (variable separation):

$$\psi = \Psi(x)\Gamma(t)$$

  - Then replacing it in the time-dependent SE:

$$\frac{\hbar}{j}\frac{1}{\Gamma(t)}\frac{\partial\Gamma(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2} + V(x)$$

Schrödinger Equation

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  - Then replacing it in the time-dependent SE:

$$\frac{\hbar}{j}\frac{1}{\Gamma(t)}\frac{\partial\Gamma(t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2} + V(x) = C$$

Schrödinger Equation

- Time-independent SE:
  - Solving the one in t:

$$\frac{\hbar}{j}\frac{1}{\Gamma(t)}\frac{\partial\Gamma(t)}{\partial t}=C \Rightarrow \Gamma(t)=\exp\left(-jCt/\hbar\right)$$

$$\Updownarrow$$

$$\psi=A_0\exp[-j(Et-px)/\hbar]$$

$$\Rightarrow \quad C=E \quad \Rightarrow \quad \boxed{\Gamma(t)=\exp(-jEt/\hbar)}$$

Schrödinger Equation

- Time-independent SE:
  - The one in x reduces to:

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2}+V(x)=E$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2}+V(x)\Psi(x)=E\Psi(x)}$$

Schrödinger Equation

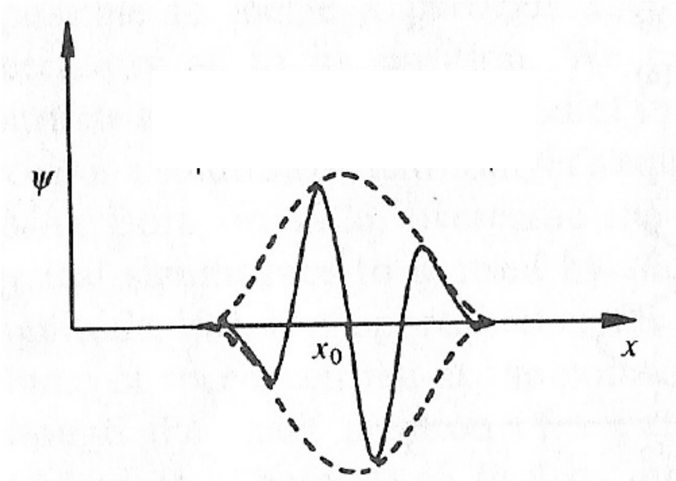
- Time-independent SE:
  - The one in *x* reduces to:

$$-\frac{\hbar^2}{2m}\frac{1}{\Psi(x)}\frac{\partial^2\Psi(x)}{\partial x^2}+V(x)=E$$

$$\Rightarrow \boxed{\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x)}{\partial x^2}}_{\frac{\hat{p}^2}{2m}}+\underbrace{V(x)\Psi(x)}_{\hat{V}}=E\Psi(x)}$$

Interpretation of the Wave Function

- Where is the particle?



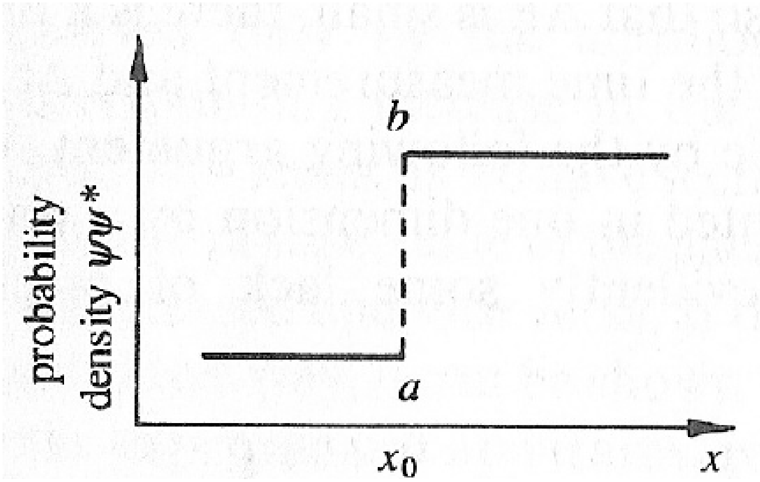
- Born interpretation:
  – The probability of finding the particle in the length interval [x, x+dx], at the time t, is given by:

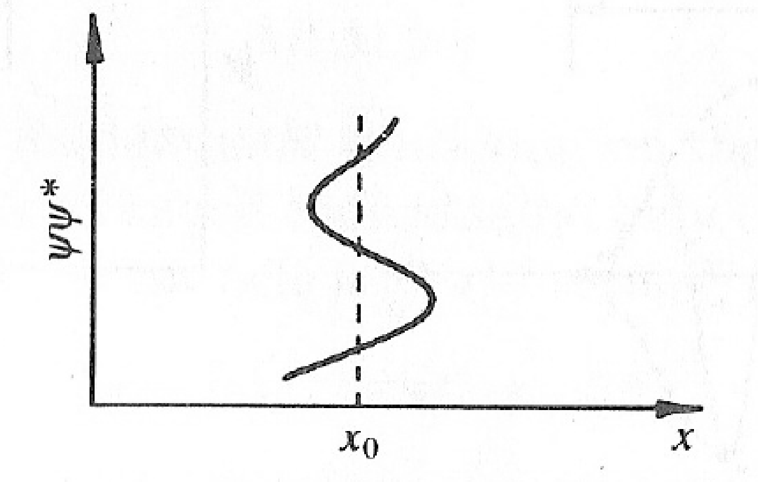
$$|\psi(x, t)|^2 \mathrm{d}x$$

  – Therefore: $\int_{\text{whole length}} \boldsymbol{|\psi(x, t)|^2 \mathrm{d}x = 1}$ (normalization)

Interpretation of the Wave Function

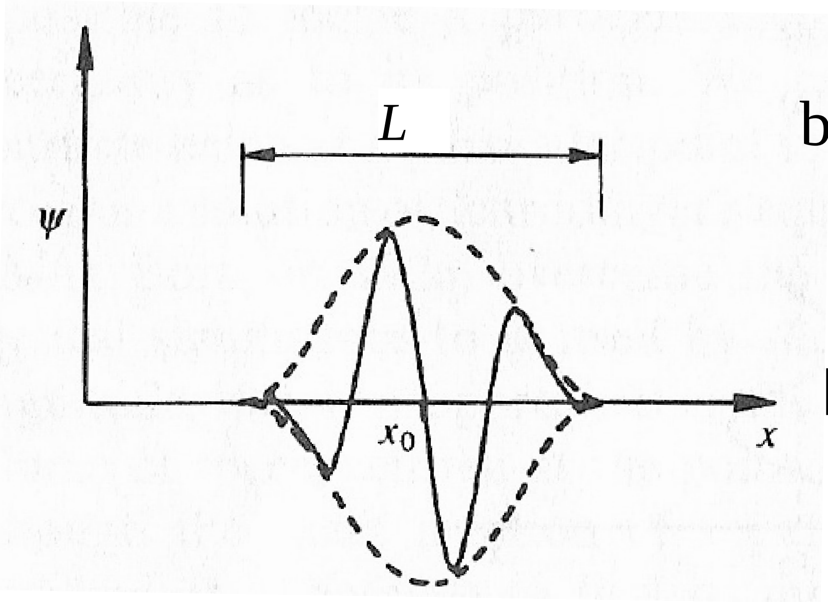
- Since $|\psi(x, t)|^2$ has physical meaning, the w.f. has to comply with various requirements:
  - Continuous on x.
  - Single valued on x.
  - Idem with its spatial first derivatives.
- Examples of improper w.f.





Heisenberg Principle

- Where is the particle?



$$L = N\lambda.$$

but L and λ are not well defined, therefore:

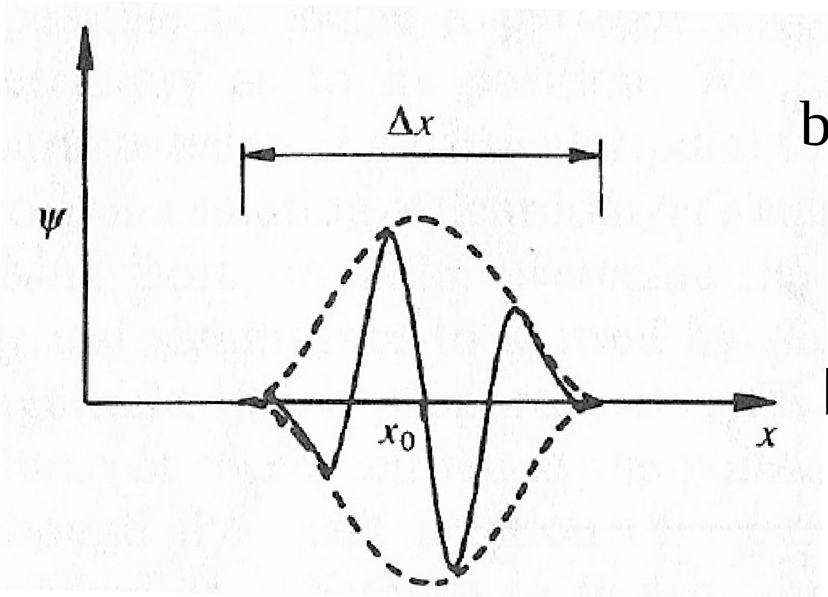
$$L + \Delta L \sim (N + \Delta N)(\lambda + \Delta\lambda),$$

$$\Rightarrow \quad L \sim \frac{-\lambda^2}{\Delta\lambda}. \quad \xrightarrow[p = h/\lambda]{\text{DeBroglie}} \quad L \sim \frac{h}{\Delta p}.$$

$$\Rightarrow \quad \Delta x \Delta p \sim h,$$

Heisenberg Principle

- Where is the particle?



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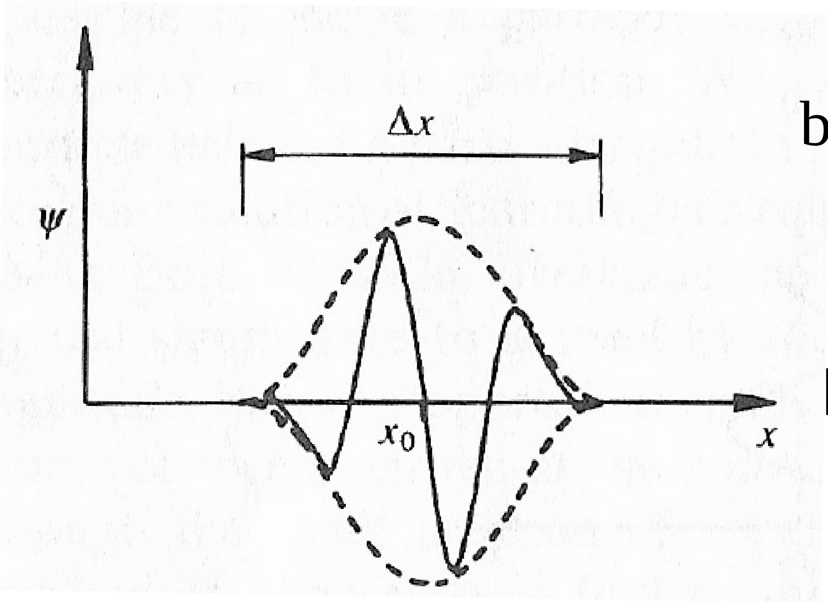
$$\Rightarrow \quad \Delta x \Delta p \sim h\,,$$

- A rigorous demonstration (no approximations) using matrix mechanics gives:

$$\boxed{\Delta p\,\Delta x \geq \hbar/2}$$

Heisenberg Principle

- Where is the particle?



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$$\Rightarrow \quad \Delta x \Delta p \sim h ,$$

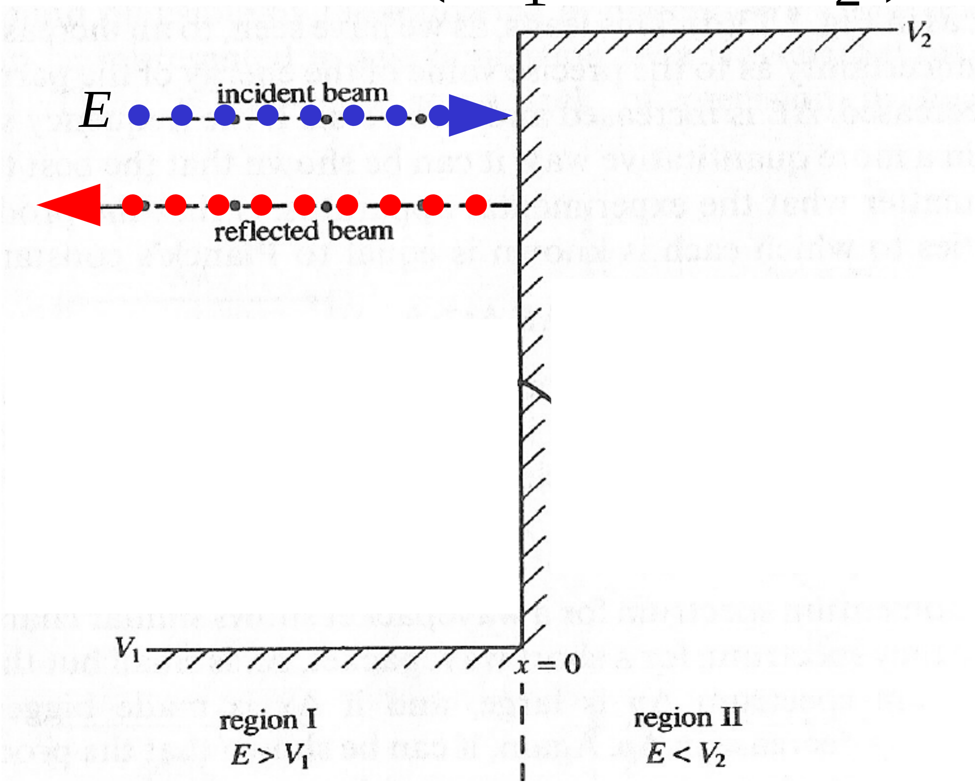
- In QM there are pair of physical quantities (called conjugates) for which this relation holds, e.g.:

$$\boxed{\Delta E\, \Delta t \geqslant h}$$

For an experimental demo: *Nature* **371**, 594 - 595 (13 October 2002)

Potential Barriers

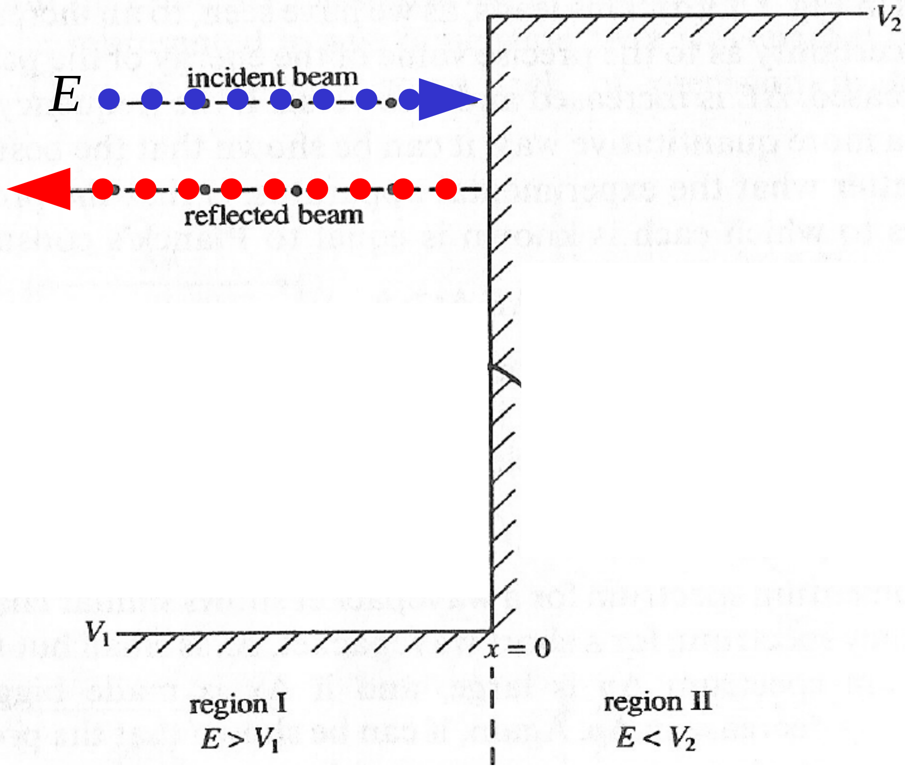
- Finite potential barrier ($V_1 < E < V_2$):



Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_1)\Psi = 0$$



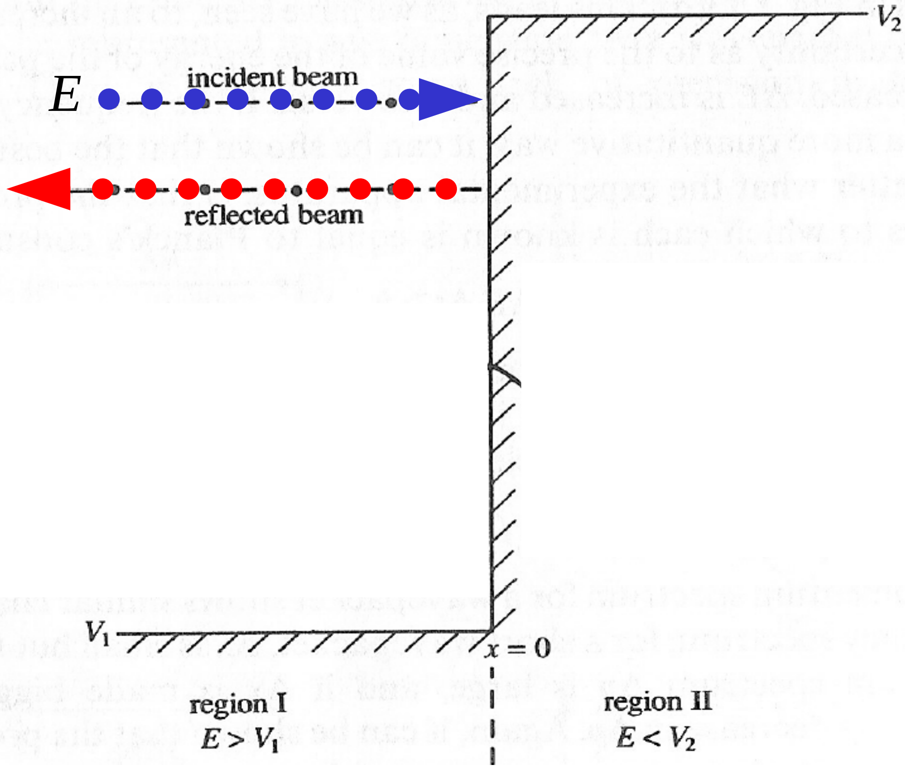
$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_2)\Psi = 0$$

Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_1)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + \beta^2\Psi = 0$$

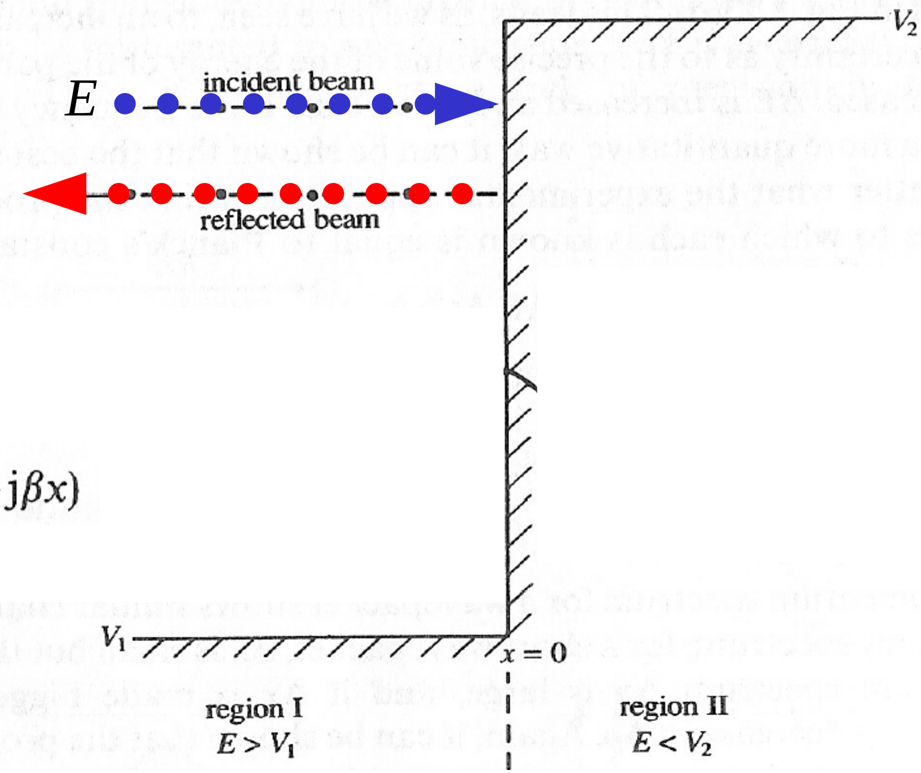


$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_2)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} - \alpha^2\Psi = 0$$

Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):



$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_1)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} + \beta^2\Psi = 0$$

$$\Psi_1 = A\exp(j\beta x) + B\exp(-j\beta x)$$

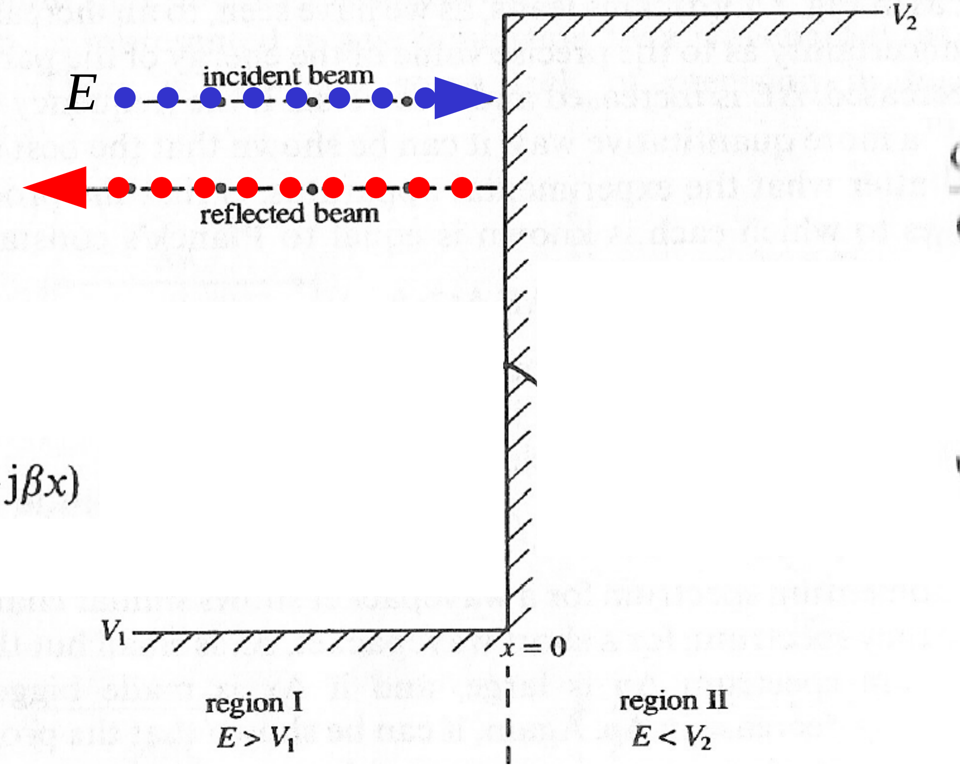
$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_2)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} - \alpha^2\Psi = 0$$

$$\Psi_{II} = Ce^{-\alpha x} + De^{\alpha x}$$

Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):



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$$\frac{d^2\Psi}{dx^2} - \alpha^2\Psi = 0$$

0

$$\Psi_{II} = Ce^{-\alpha x} + \cancel{D}e^{\alpha x}$$

Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):

$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_1)\Psi = 0$$

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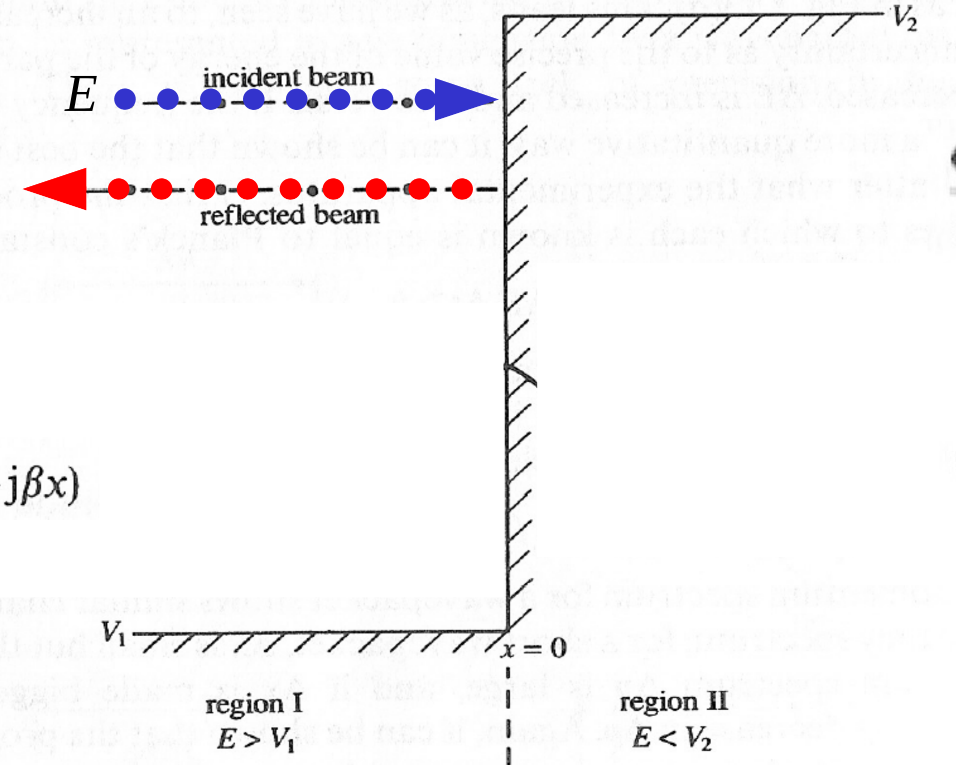


$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_2)\Psi = 0$$

$$\frac{d^2\Psi}{dx^2} - \alpha^2\Psi = 0$$

$$\Psi_{II} = Ce^{-\alpha x} + \cancelto{0}{D}e^{\alpha x}$$

  – A, B, C are found using continuity arguments and norm.

$$\Psi_I|_{x=0} = \Psi_{II}|_{x=0} \qquad (\partial\Psi_I/\partial x)|_{x=0} = (\partial\Psi_{II}/\partial x)|_{x=0}$$

$$A = \tfrac{1}{2}C(1 - \alpha/j\beta) \qquad B = \tfrac{1}{2}C(1 + \alpha/j\beta)$$

Notice that $|A| = |B|$

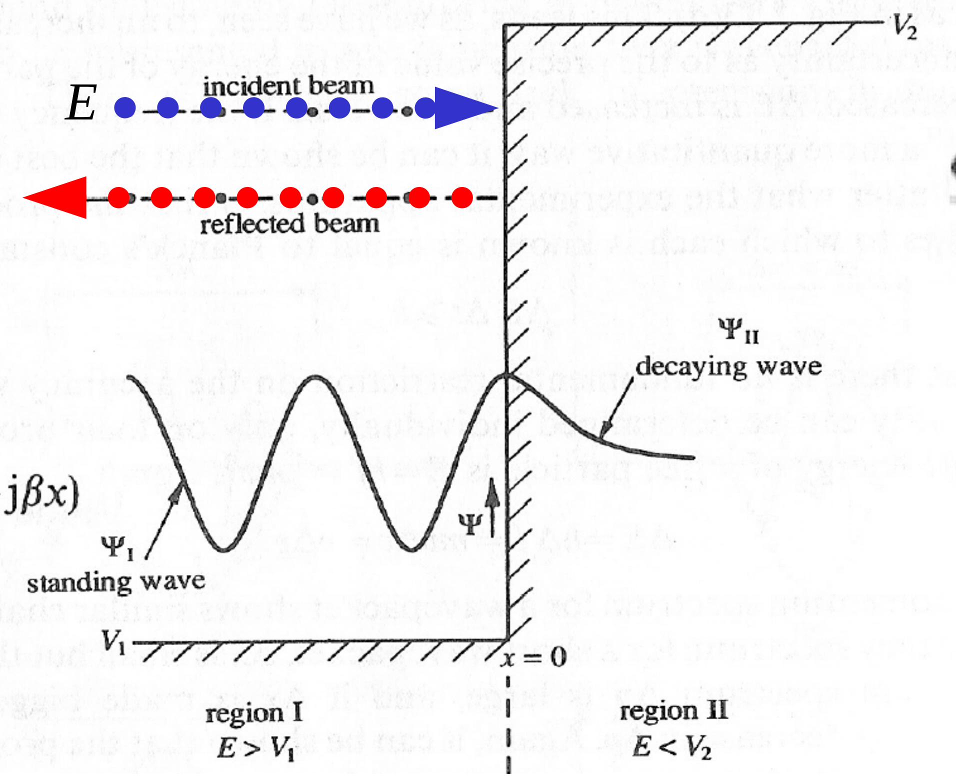
Potential Barriers

- Finite potential barrier ($V_1 < E < V_2$):

$$\frac{d^2\Psi}{dx^2}+\frac{2m}{\hbar^2}(E-V_1)\Psi=0$$

$$\frac{d^2\Psi}{dx^2}+\beta^2\Psi=0$$

$$\Psi_I = A\exp(j\beta x)+B\exp(-j\beta x)$$



$$\frac{d^2\Psi}{dx^2}+\frac{2m}{\hbar^2}(E-V_2)\Psi=0$$

$$\frac{d^2\Psi}{dx^2}-\alpha^2\Psi=0$$

$$\Psi_{II} = Ce^{-\alpha x}+\cancel{D}e^{\alpha x}$$

0

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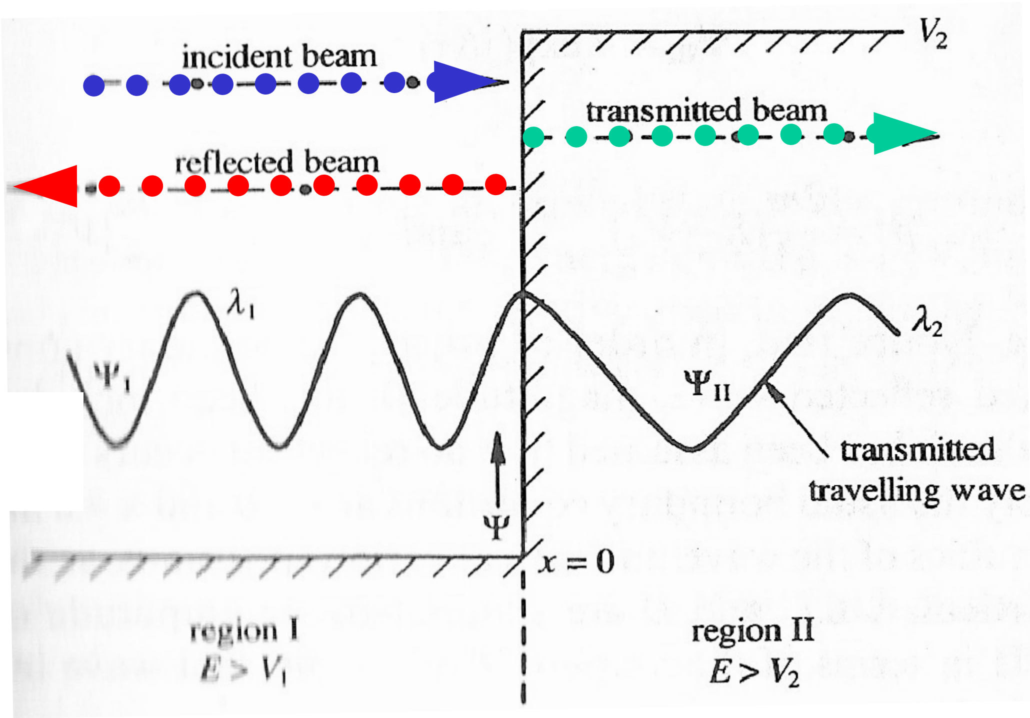
Notice that $|A| = |B|$

Potential Barriers

- Finite potential barrier ($V_1 < V_2 < E$):



$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_{1,2})\Psi = 0$$

$$\beta_{1,2}^2 = \frac{2m}{\hbar^2}(E - V_{1,2})$$

$$\Psi_1 = A\exp(j\beta_1 x) + B\exp(-j\beta_1 x)$$

$$\Psi_{II} = C\exp(j\beta_2 x)$$

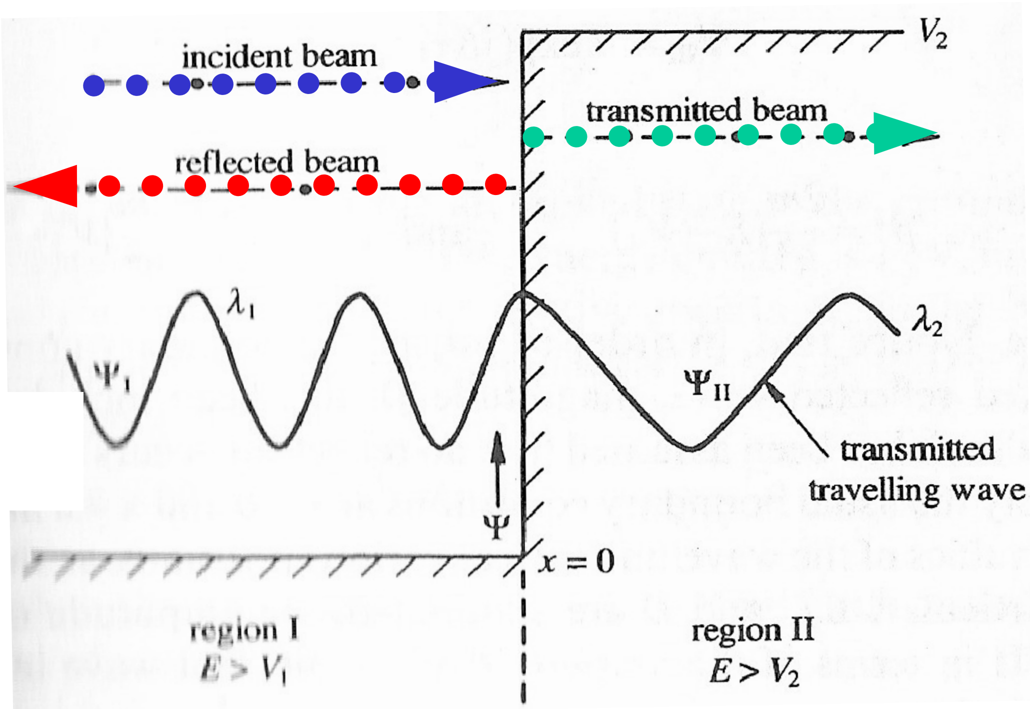
From continuity arguments:

$$A + B = C$$

$$\beta_1(A - B) = \beta_2 C$$

Potential Barriers

- Finite potential barrier ($V_1 < V_2 < E$):



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$$\beta_{1,2}^2 = \frac{2m}{\hbar^2}(E - V_{1,2})$$

$$\Psi_I = A\exp(j\beta_1 x) + B\exp(-j\beta_1 x)$$

$$\Psi_{II} = C\exp(j\beta_2 x)$$

From continuity arguments:

$$A + B = C$$

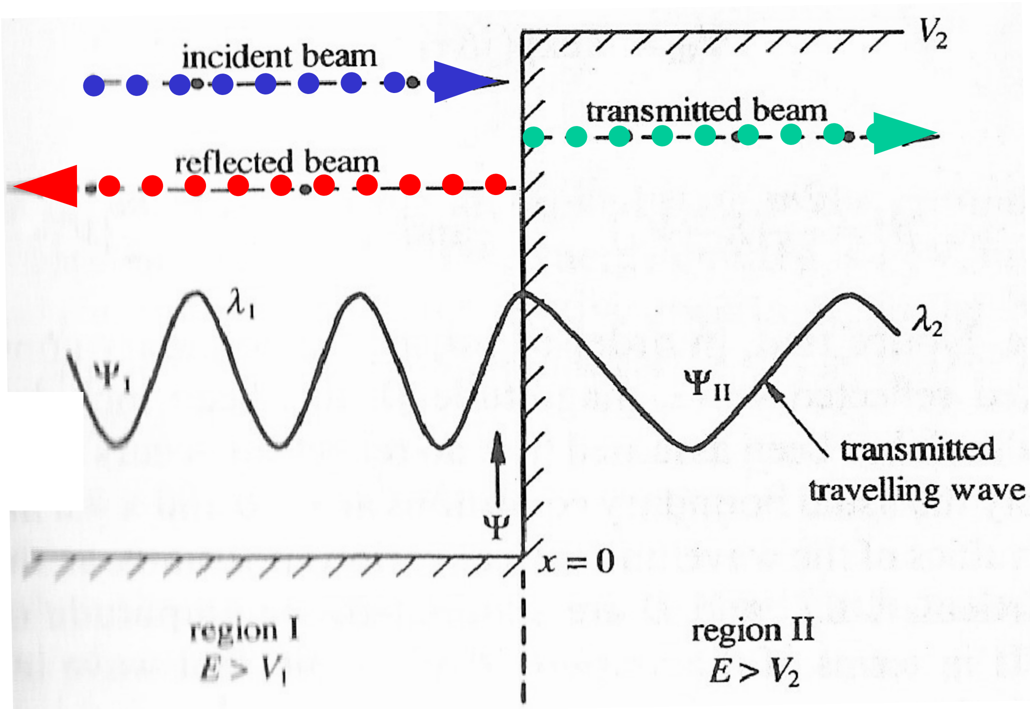
$$\beta_1(A - B) = \beta_2 C$$

Reflection coefficient:

$$\frac{\text{density of particles reflected}}{\text{density of particles incident}} = \frac{|\Psi_{ref}|^2}{|\Psi_{inc}|^2} = \frac{BB^*}{AA^*} = \frac{B^2}{A^2} = \left(\frac{1 - \beta_2/\beta_1}{1 + \beta_2/\beta_1}\right)^2$$

Potential Barriers

- Finite potential barrier ($V_1 < V_2 < E$):



$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_{1,2})\Psi = 0$$

$$\beta_{1,2}^2 = \frac{2m}{\hbar^2}(E - V_{1,2})$$

$$\Psi_1 = A\exp(j\beta_1 x) + B\exp(-j\beta_1 x)$$

$$\Psi_{II} = C\exp(j\beta_2 x)$$

From continuity arguments:

$$A + B = C$$

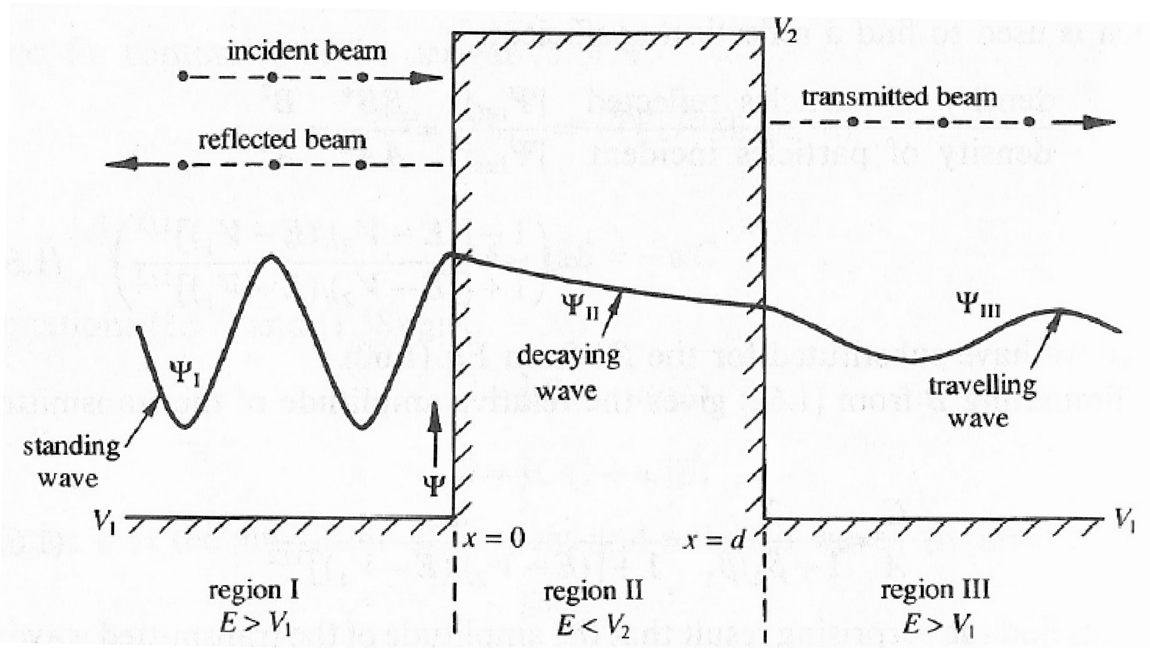
$$\beta_1(A - B) = \beta_2 C$$

Transmission coefficient:

$$\left|\frac{C}{A}\right|^2 = \left(\frac{2}{1 + \beta_2/\beta_1}\right)^2$$ but $\beta_1 > \beta_2$ $\Rightarrow$ $\left|\frac{C}{A}\right|^2 > 1$!

Potential Barriers

- Narrow potential barrier ($V_1 < E < V_2$):



$$\Psi_I = A\exp(j\beta x) + B\exp(-j\beta x)$$
$$\Psi_{II} = C\exp(-\alpha x) + D\exp(\alpha x)$$
$$\Psi_{III} = F\exp(j\beta x)$$

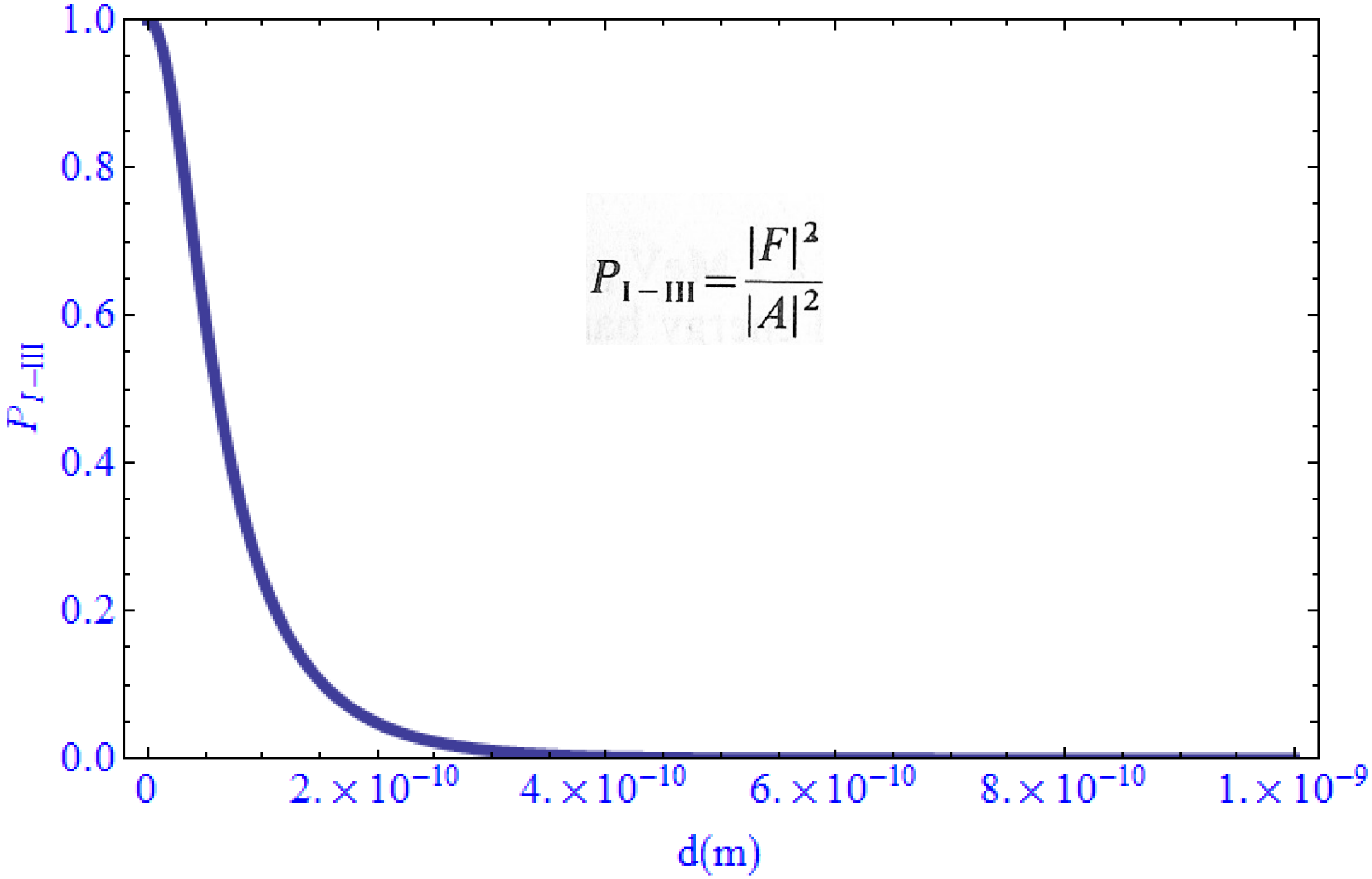
α and β as before

As before, A,B,C,D,F to be obtained from continuity and normalization. In particular:

$$F = A\exp(-j\beta d)\left[\cosh(\alpha d) + \frac{j}{2}\left(\frac{\alpha}{\beta} - \frac{\beta}{\alpha}\right)\sinh(\alpha d)\right]^{-1}$$

Potential Barriers

- Narrow potential barrier ($V_1 < E < V_2$):
  - Transmission from I to III



Conclusions

- The Schrodinger equation (SE) was studied.
- It was “deduced” from the particle wavefunction but it is applicable to any quantum system.
- The SE was applied to different potentials.