Physics of Electronics:

1. Introduction to Quantum Mechanics (cont.)

July – December 2008

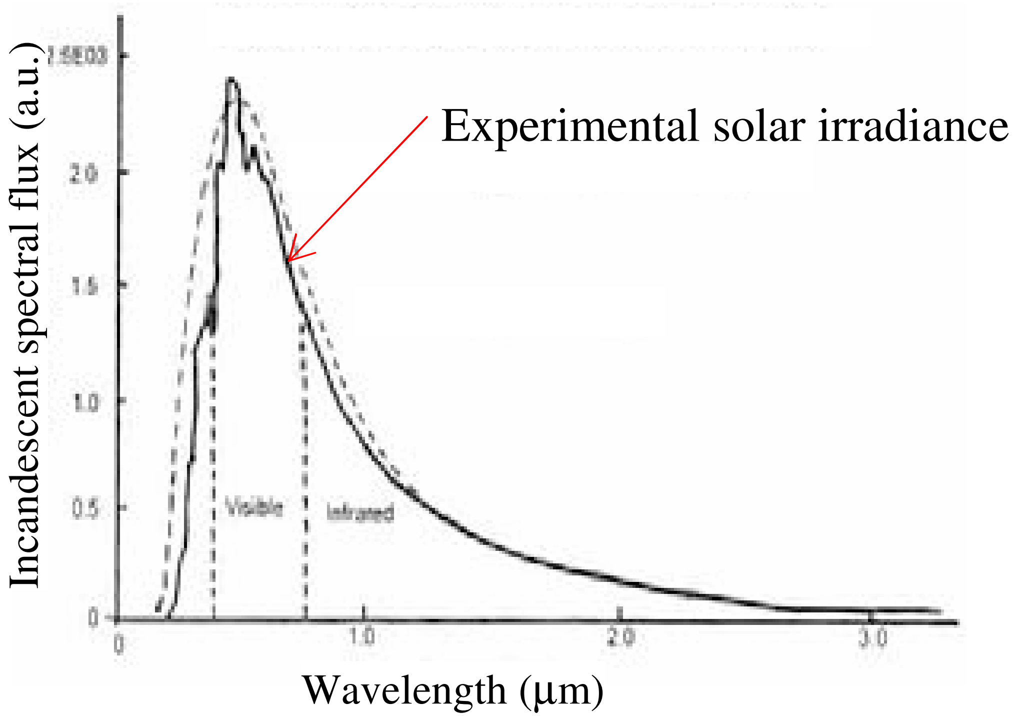
Contents overview

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

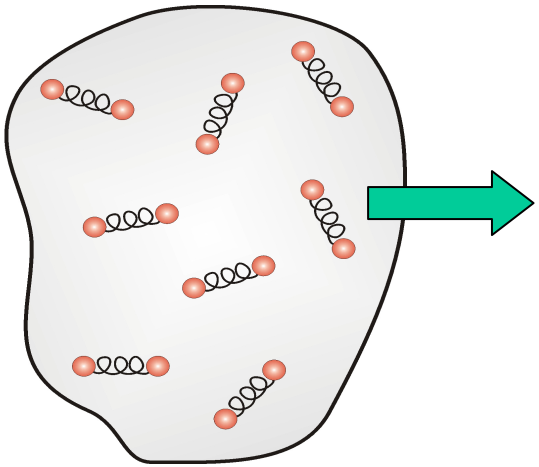
The English translation of some of the original articles can be seen at:
http://strangepaths.com/resources/fundamental-papers/en/

Blackbody Radiation

- Experiment



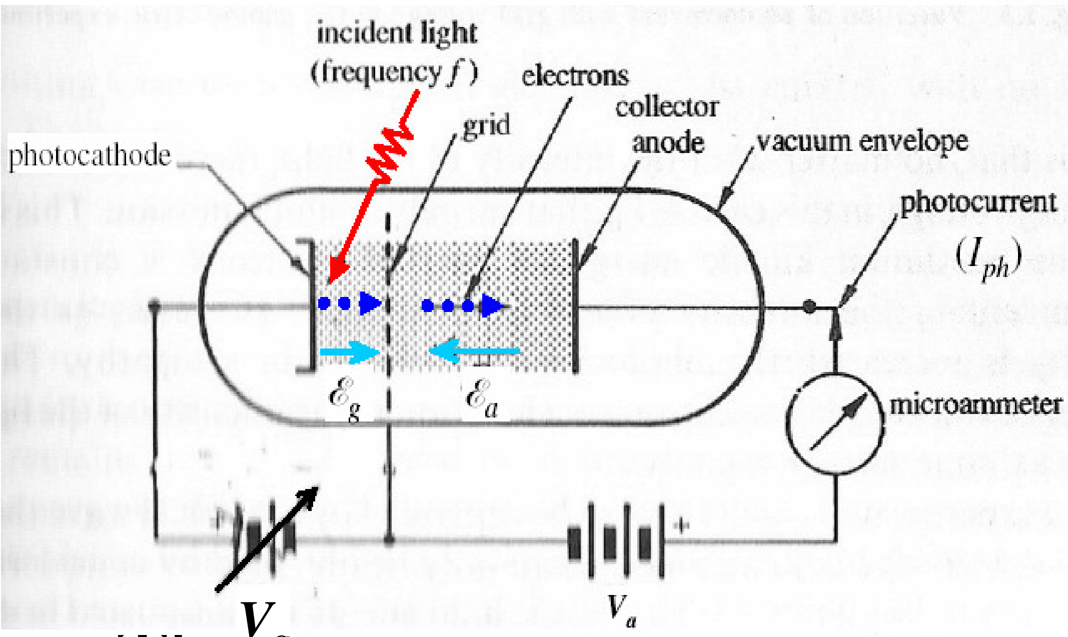
- Theory

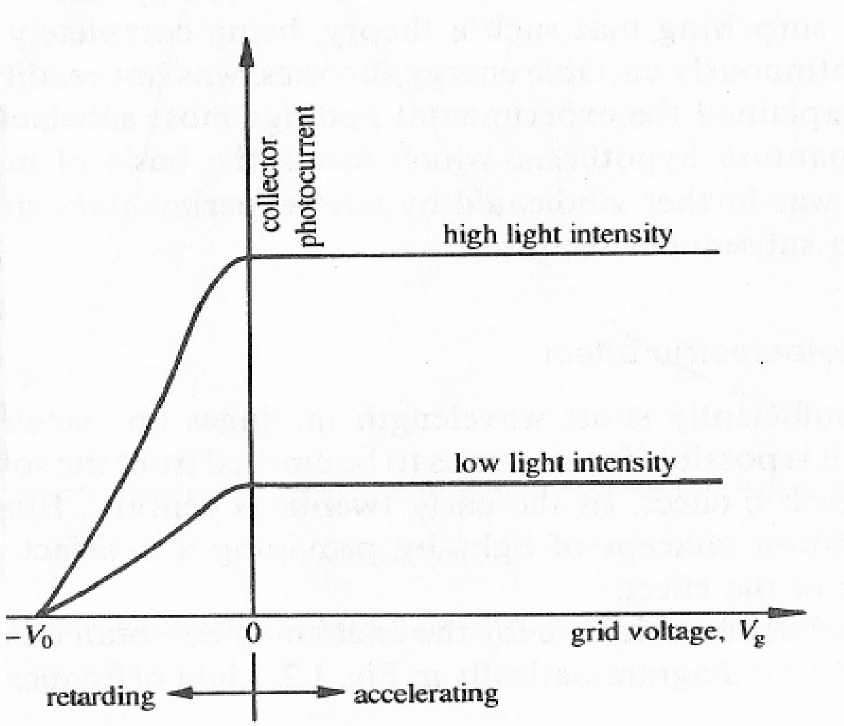


$$E = 0,\ \hbar\omega,\ 2\hbar\omega,\ 3\hbar\omega,\ \ldots,\ n\hbar\omega$$

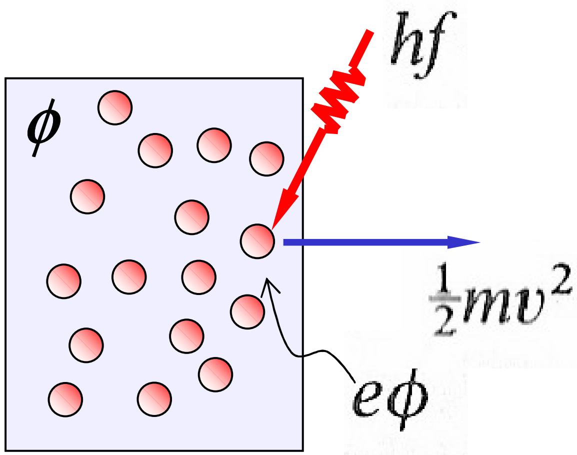
Photoelectric Effect

- Experiment





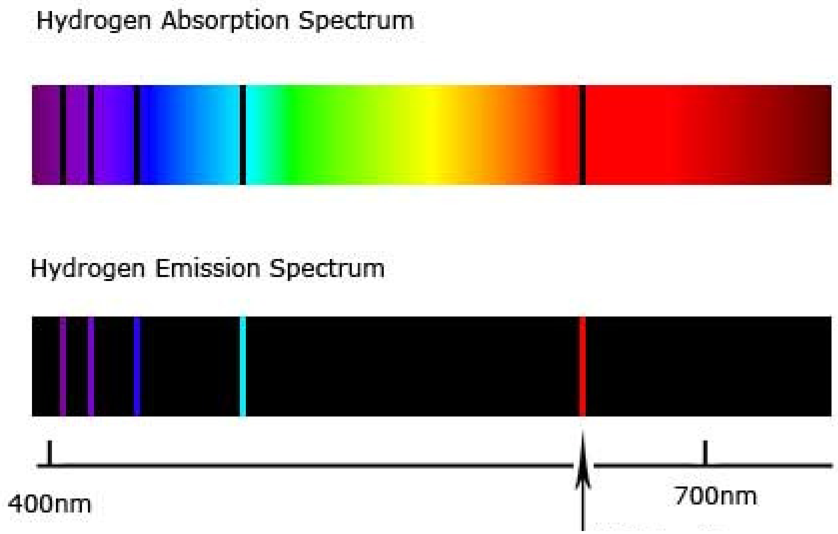
- Theory



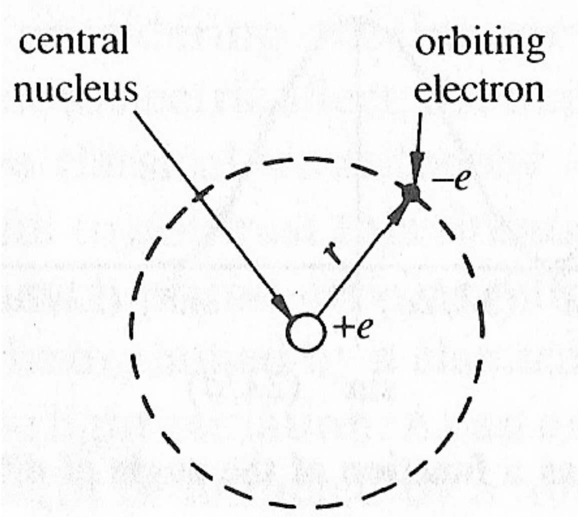
$$\tfrac{1}{2}mv^2 = hf - e\phi$$

Bohr Atom

- Experiment



- Theory

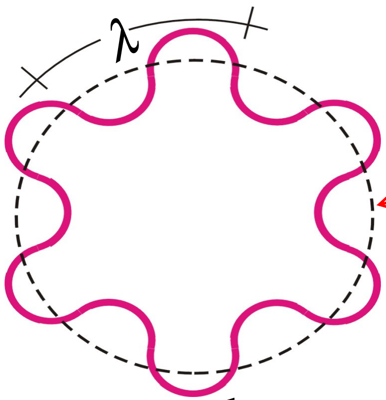


$$L = mvr = n\hbar \qquad \text{where } n = 1, 2, 3, \ldots$$

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

Particle-Wave Duality & Wavepackets

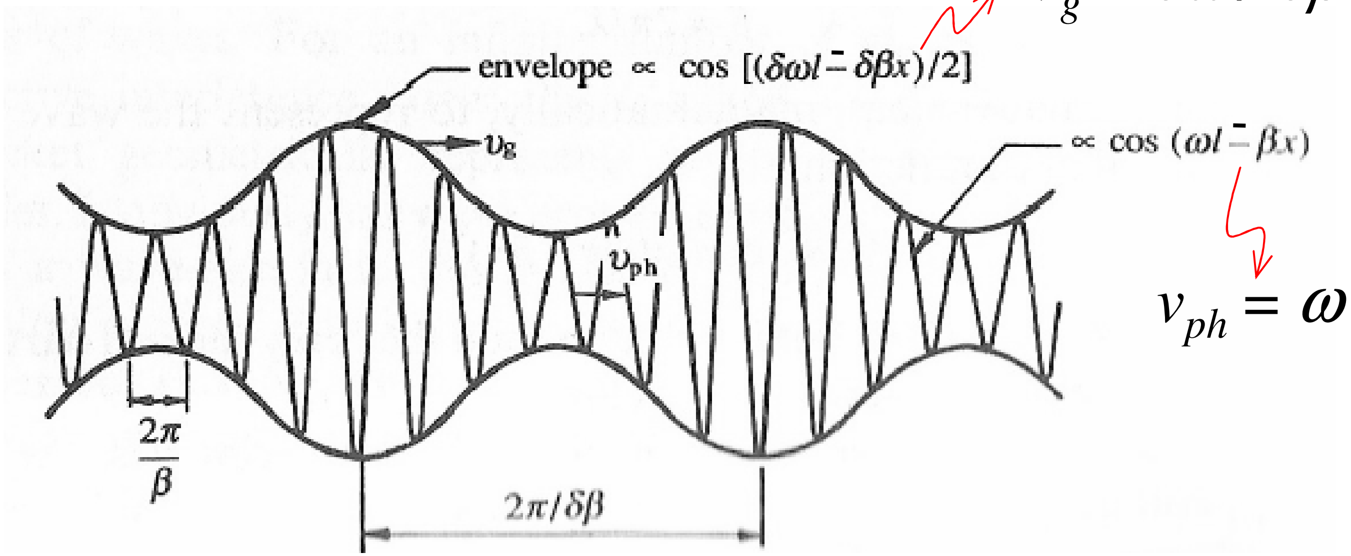
- De Broglie hypothesis:



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

- Phase and group velocity:

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



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

Wave function

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

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

$$\omega = \frac{2\pi T}{h} = \frac{T}{\hbar}$$

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

  - Phase and group velocity are:

$$v_{\mathrm{ph}} = \frac{\omega}{\beta} = \frac{T}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{v}{2} \qquad v_g = \partial\omega/\partial\beta = v$$

  - The wavepacket ψ is called **wave function**

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

Schrödinger Equation

- Time-dependent SE:

$$\boxed{\frac{\partial^2\psi}{\partial x^2}-\frac{2m}{\hbar^2}V\psi+\mathrm{j}\frac{2m}{\hbar}\frac{\partial\psi}{\partial t}=0}$$

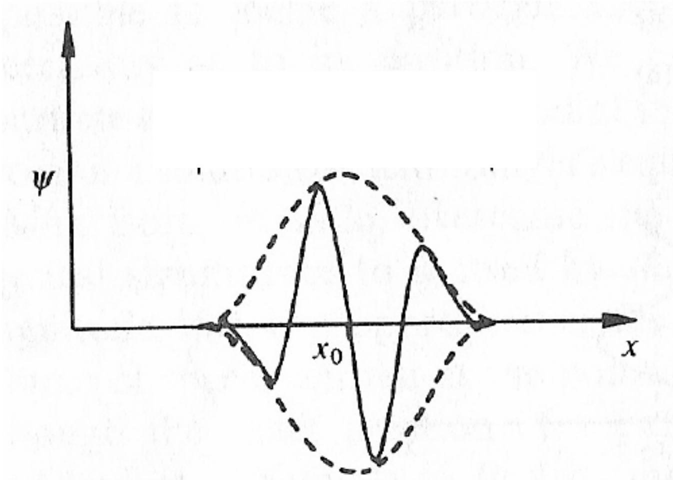
- Time-independent SE:

$$\boxed{\frac{\mathrm{d}^2\Psi}{\mathrm{d}x^2}+\frac{2m}{\hbar^2}(E-V)\Psi=0}$$

where the complete solution is: $\psi=\Psi(x)\exp(-\mathrm{j}Et/\hbar)$

Interpretation of the Wave Function

- Where is the particle?



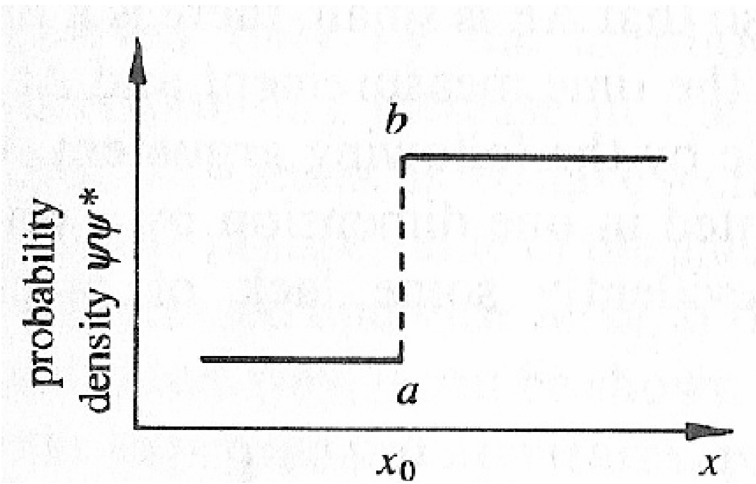
- Born interpretation:
  - The probability of finding the particle in the length interval $[x, x+\mathrm{d}x]$, at the time t, is given by:

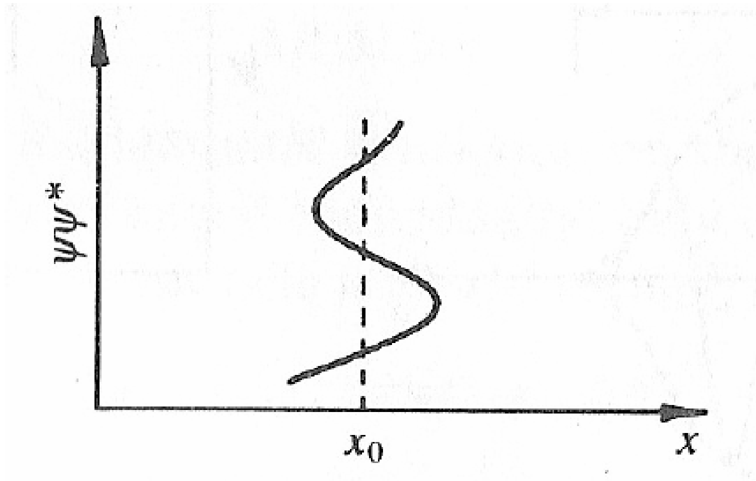
$$|\psi(x, t)|^2 \mathrm{d}x$$

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

Interpretation of the Wave Function

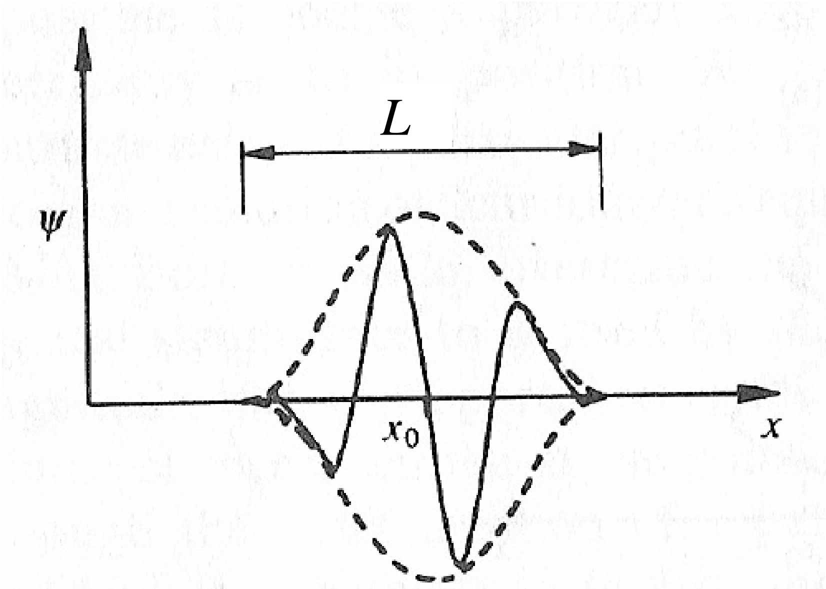
- Since $|\psi(x, t)|^2$ physical meaning, the w.f. has to comply various requirements:
  - Continuous on x.
  - Single valued on x.
  - Idem with its spatial first derivatives.
- Examples of improper w.f.





Heisenberg Principle

- Where is the particle?



$$L = N\lambda .$$

but λ is not well defined, therefore:

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

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

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

Heisenberg Principle

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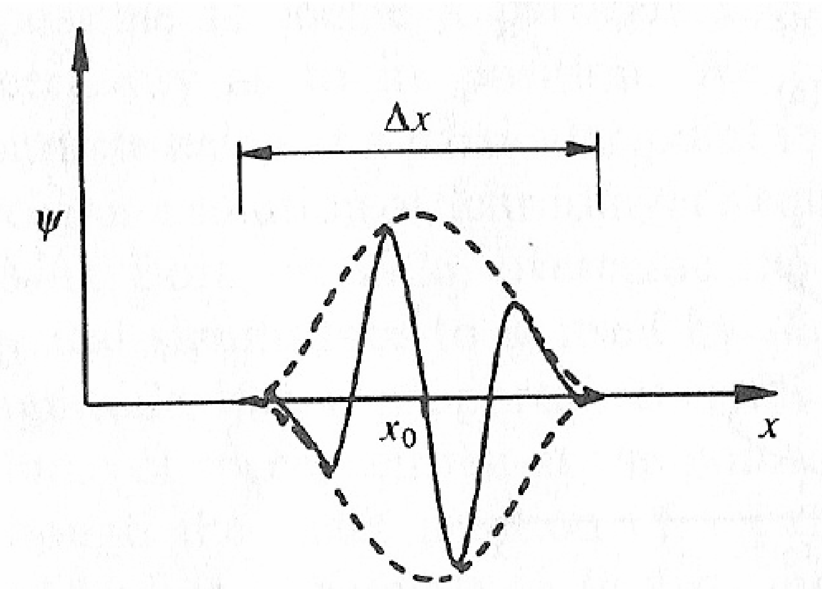

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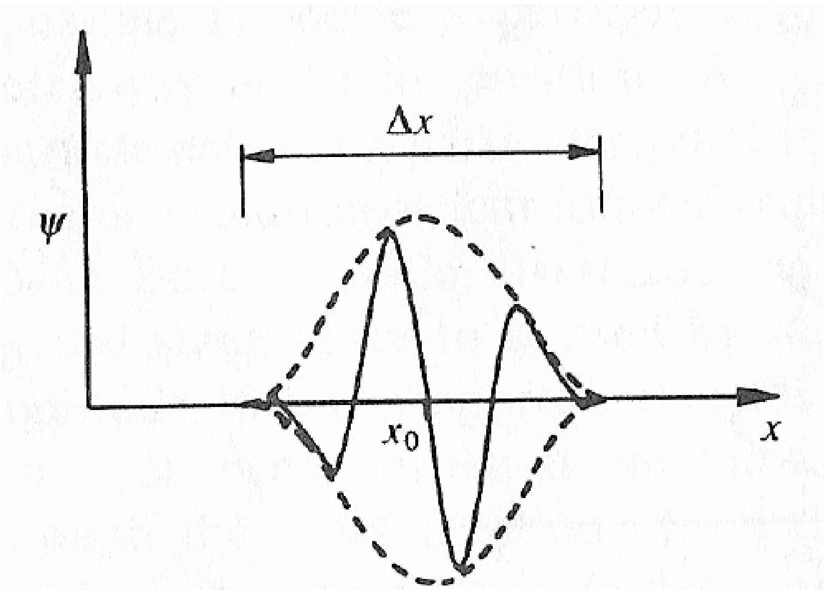
- A rigorous demonstration (no approximations) using matrix mechanics gives:

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

Heisenberg Principle

- Where is the particle?



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

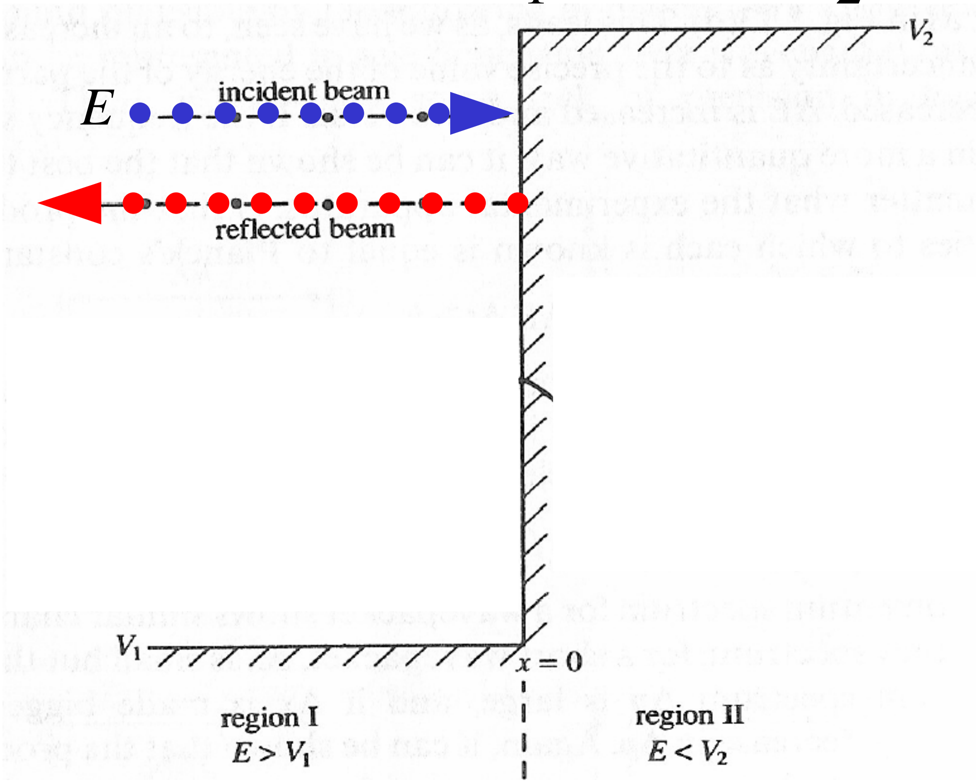
- In QM there are pair of physical quantities (called conjugates) for which this relation holds, e.g.:

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

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

Potential Barriers

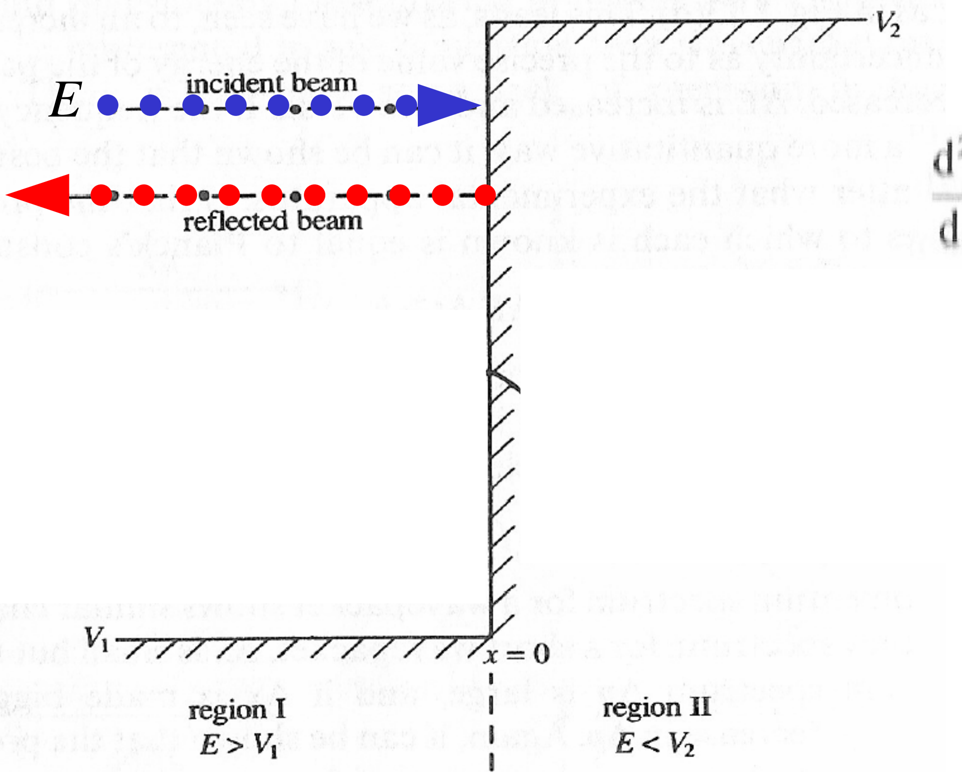
- Finite potential barrier ($V_1 < E < V_2$):



Potential Barriers

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

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



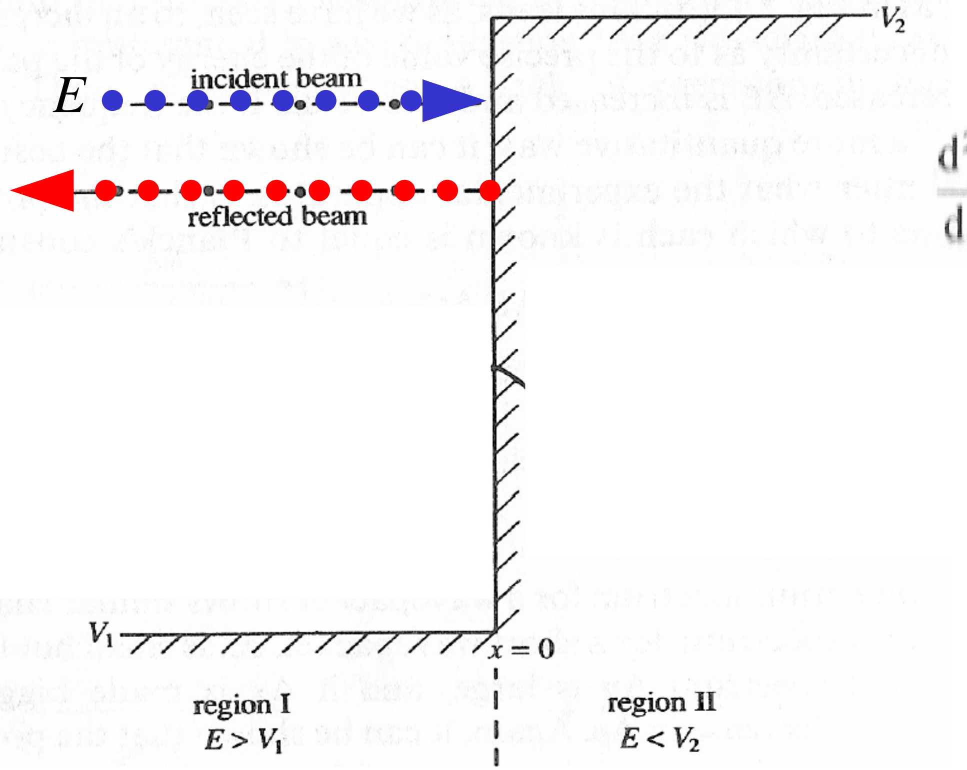
$$\frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2}(E - V_2)\Psi = 0$$

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

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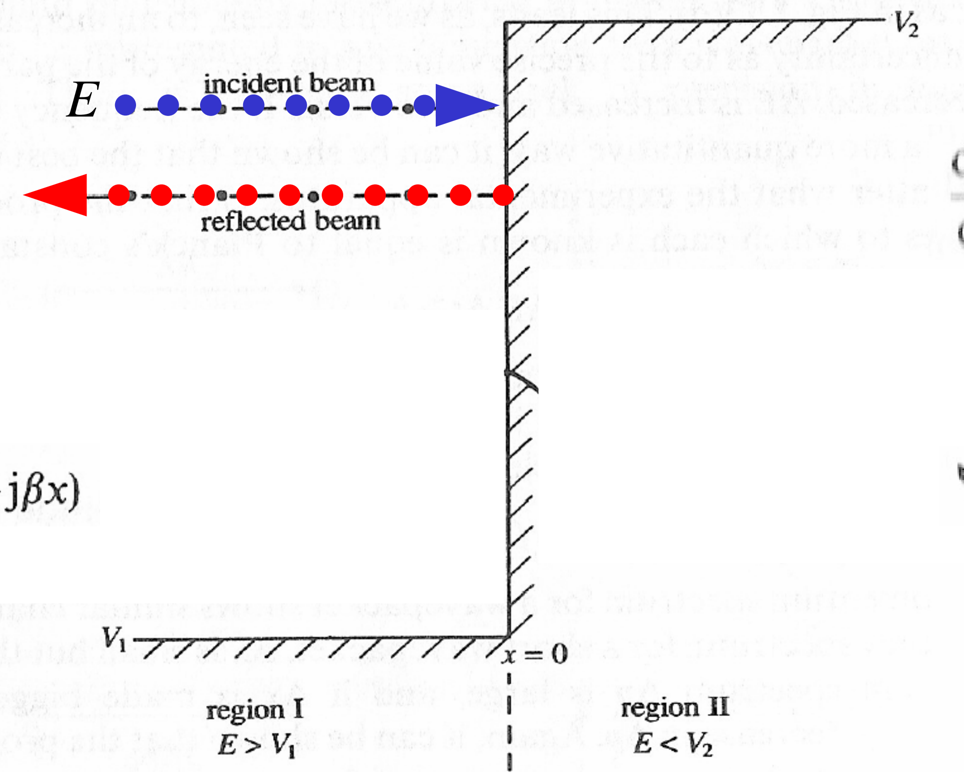

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$$\frac{d^2\Psi}{dx^2} + \beta^2\Psi = 0$$

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

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

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

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

Potential Barriers

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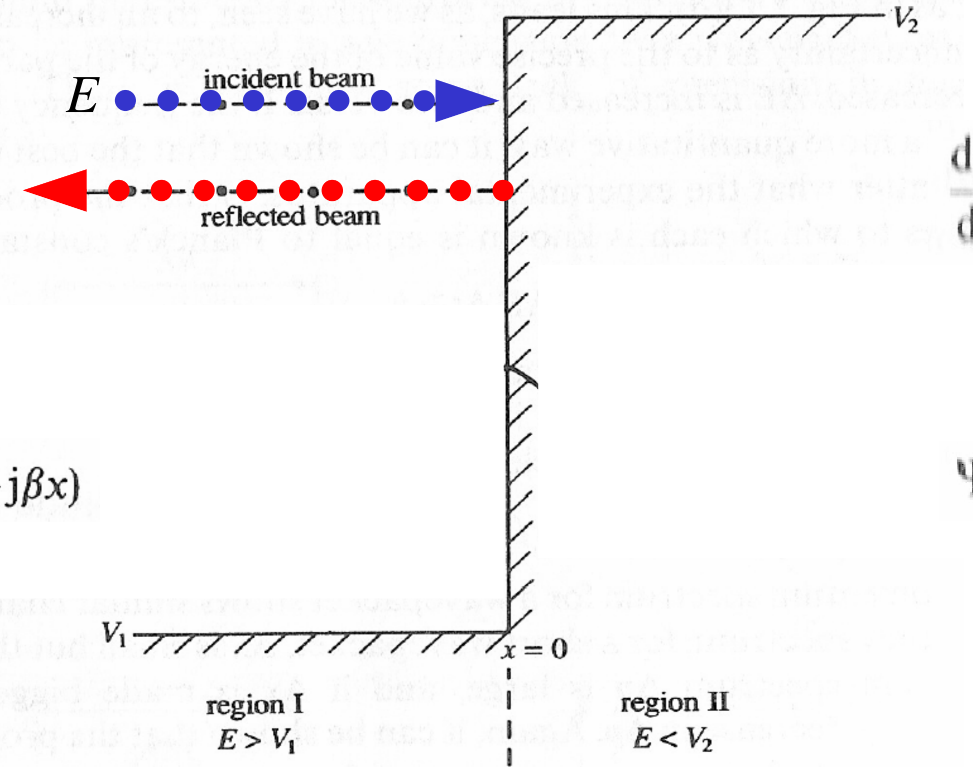

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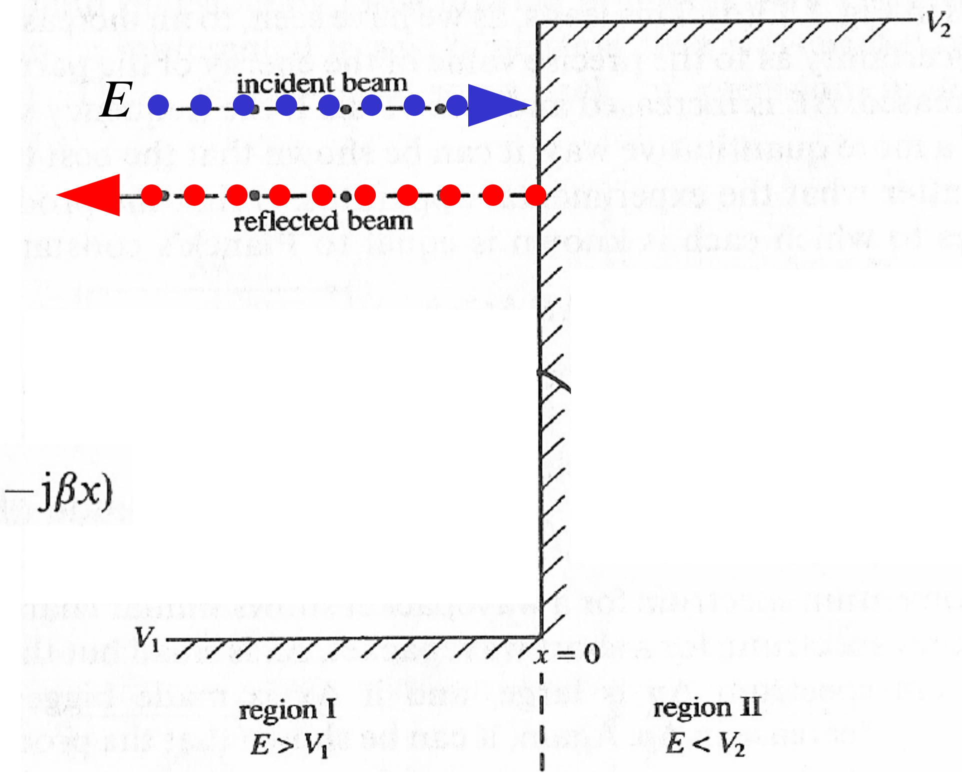

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$$\Psi_{II} = Ce^{-\alpha x} + \cancelto{0}{D}e^{\alpha x}$$

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

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

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

Notice that $|A| = |B|$

Potential Barriers

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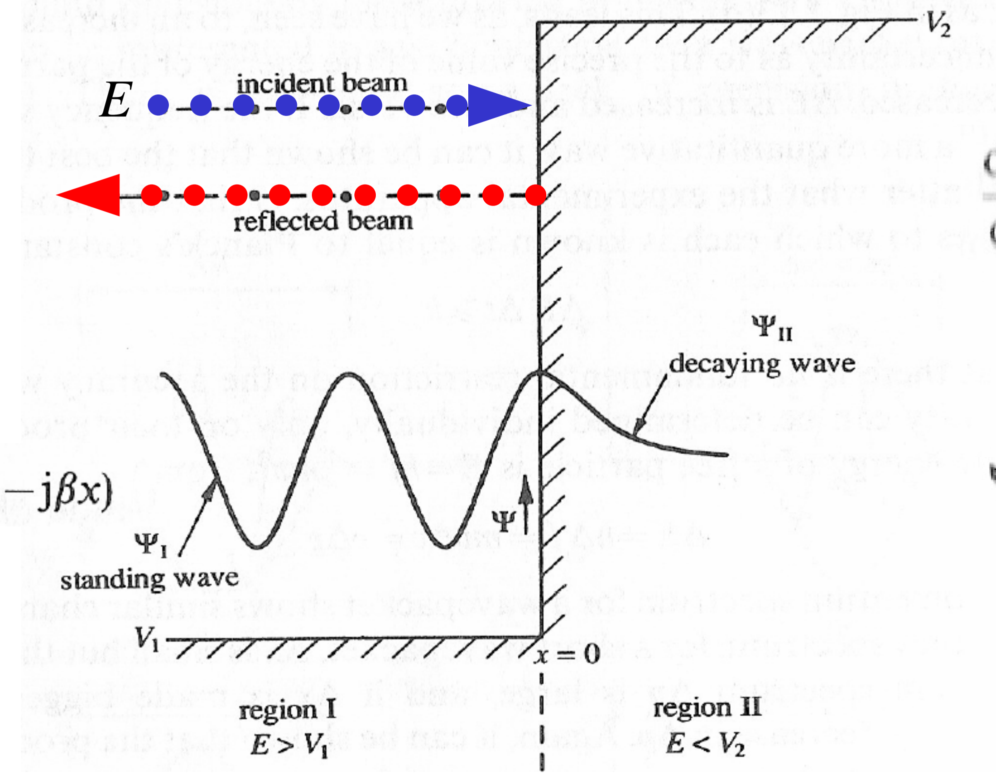

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$$\Psi_I|_{x=0} = \Psi_{II}|_{x=0} \qquad (\partial\Psi_I/\partial x)|_{x=0} = (\partial\Psi_{II}/\partial x)|_{x=0}$$

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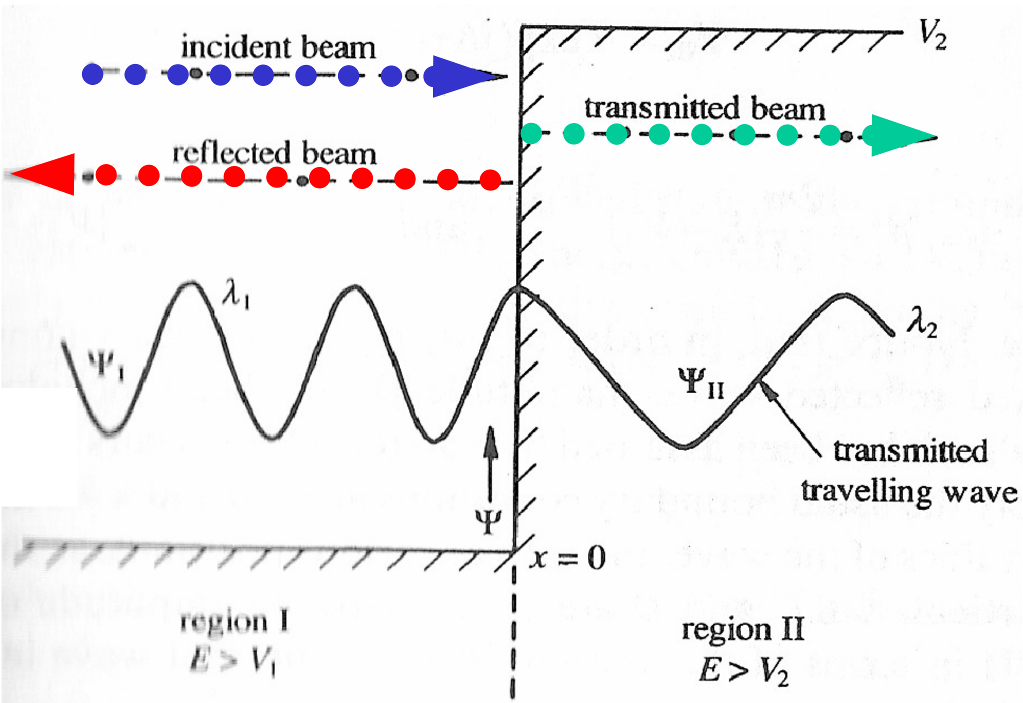
Notice that $|A| = |B|$

Potential Barriers

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



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

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

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

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

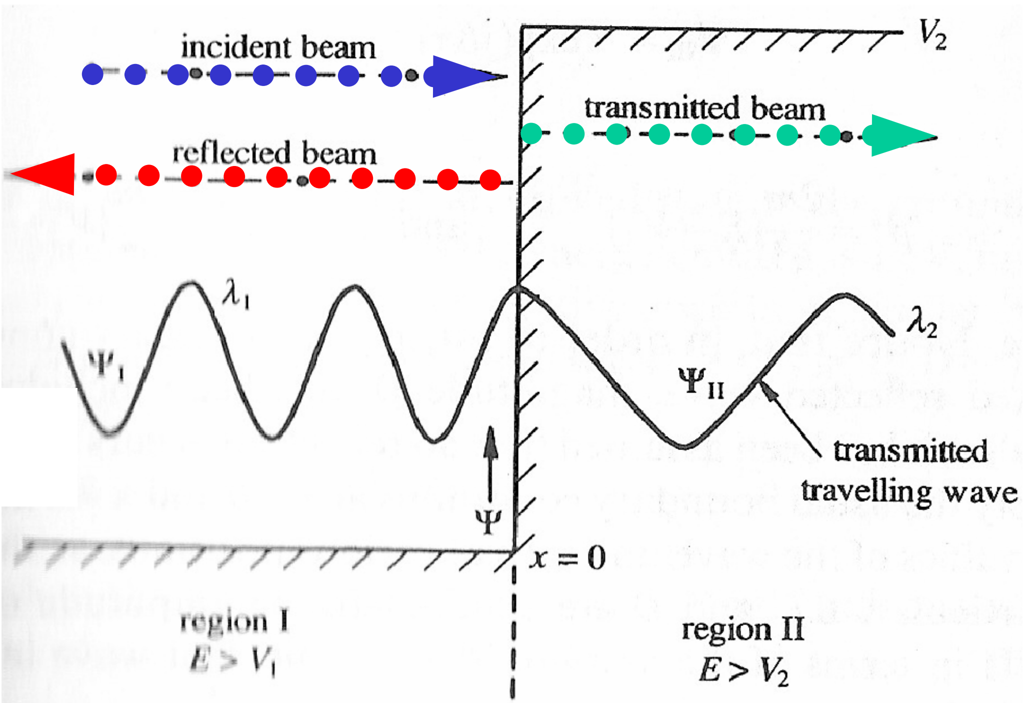
From continuity arguments:

$$A + B = C$$

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

Potential Barriers

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



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

From continuity arguments:

$$A + B = C$$

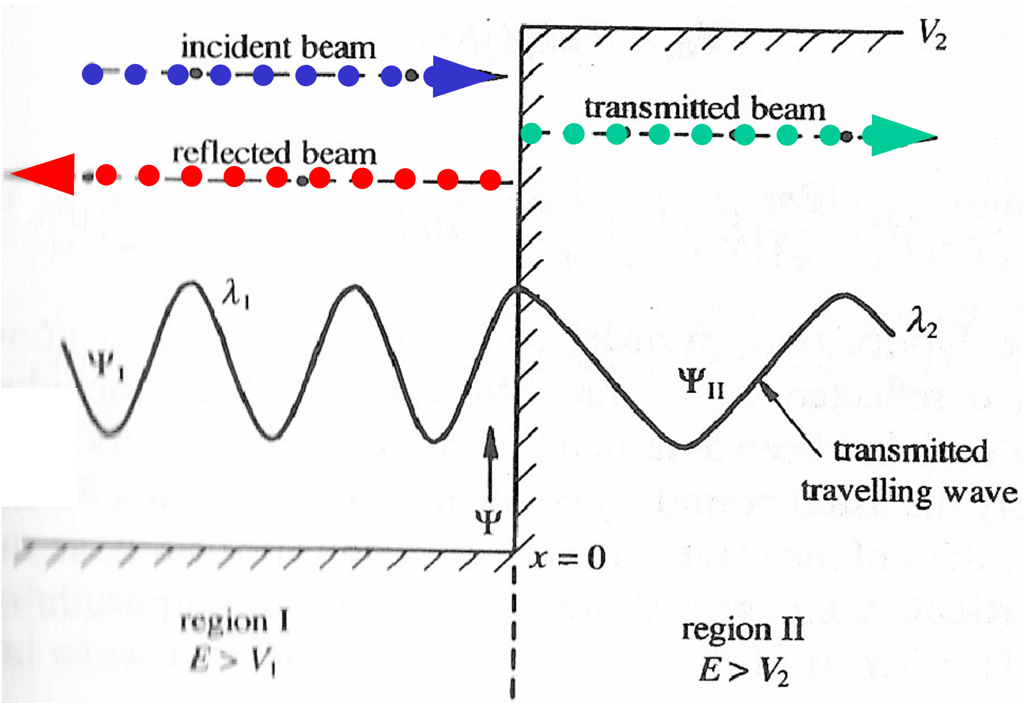
$$\beta_1(A - B) = \beta_2 C$$

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 ($V_1 < V_2 < E$):



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

From continuity arguments:

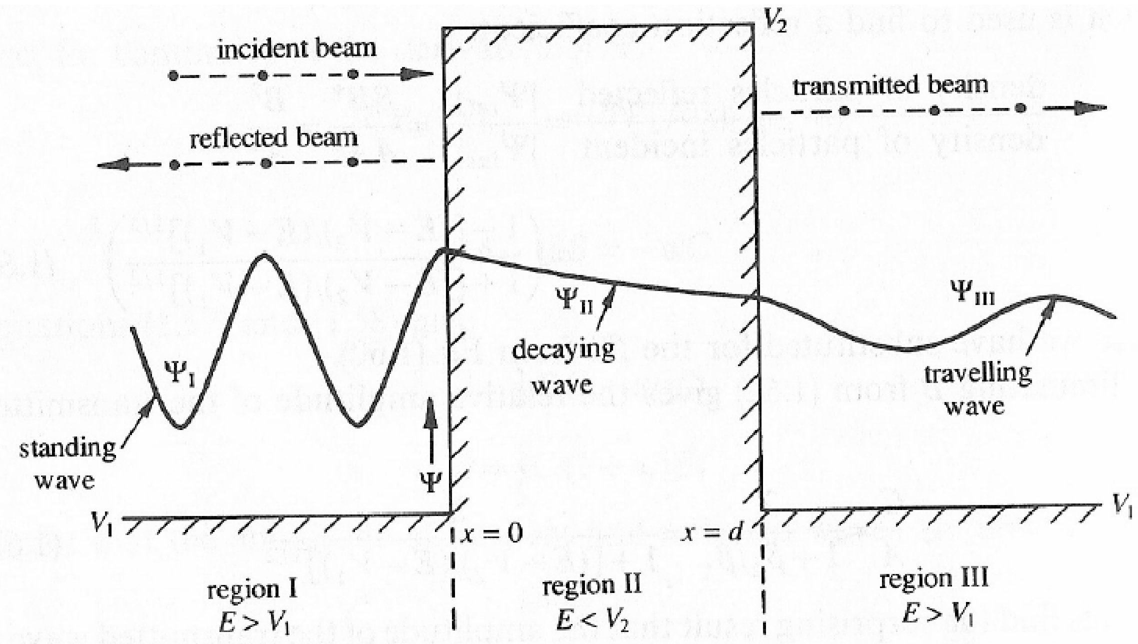
$$A + B = C$$
$$\beta_1(A - B) = \beta_2 C$$

Transmission coefficient:

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

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:

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

Potential Barriers

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

```
In[62]:= v2 = 2; (*volt*)
         ve = 1; (*volt*)
         Plot[ p13[α[v2 × qe, ve × qe], β[ve × qe], d], {d, 0, 10^-9},
          AxesLabel → {StyleForm["d(m)", FontSize → 16], StyleForm["P1-3", FontSize → 16]},
          PlotStyle → {Hue[0.9], Thickness[.01]} ];
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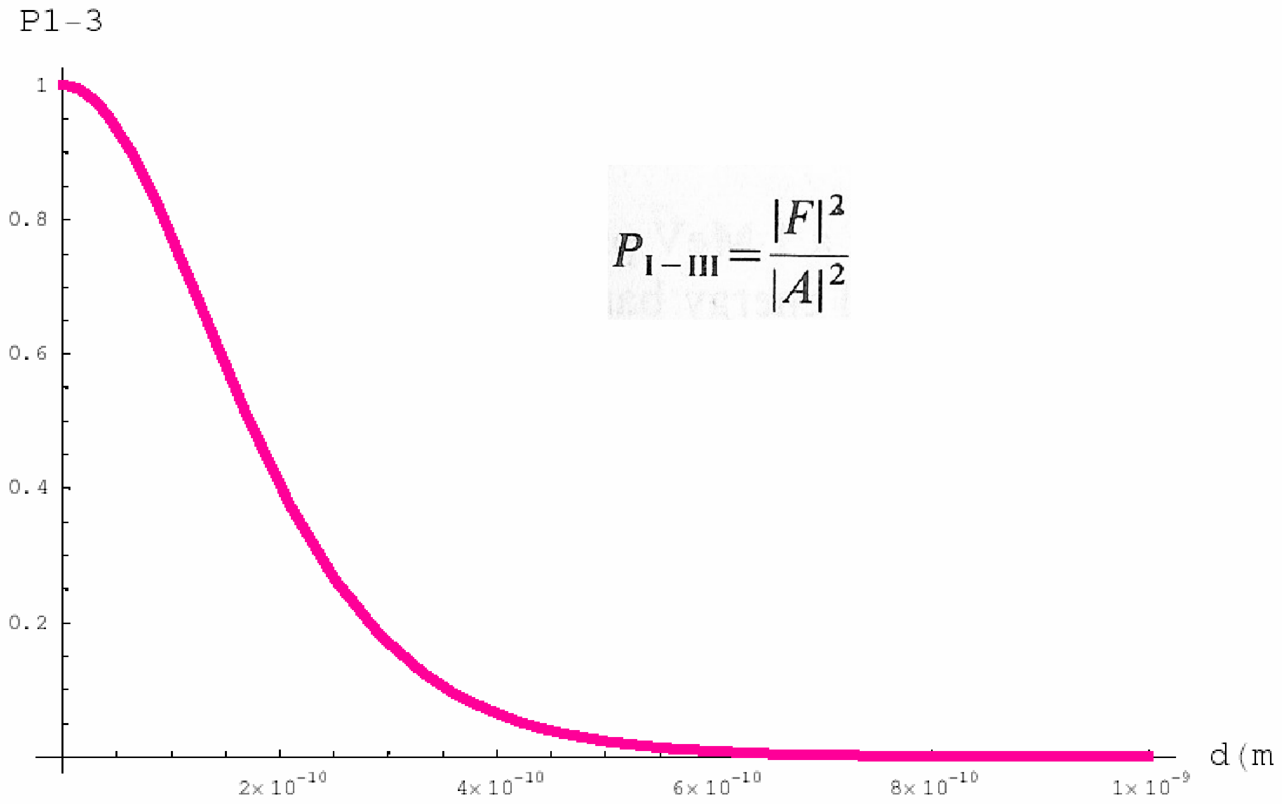


$$P_{\mathrm{I-III}} = \frac{|F|^2}{|A|^2}$$

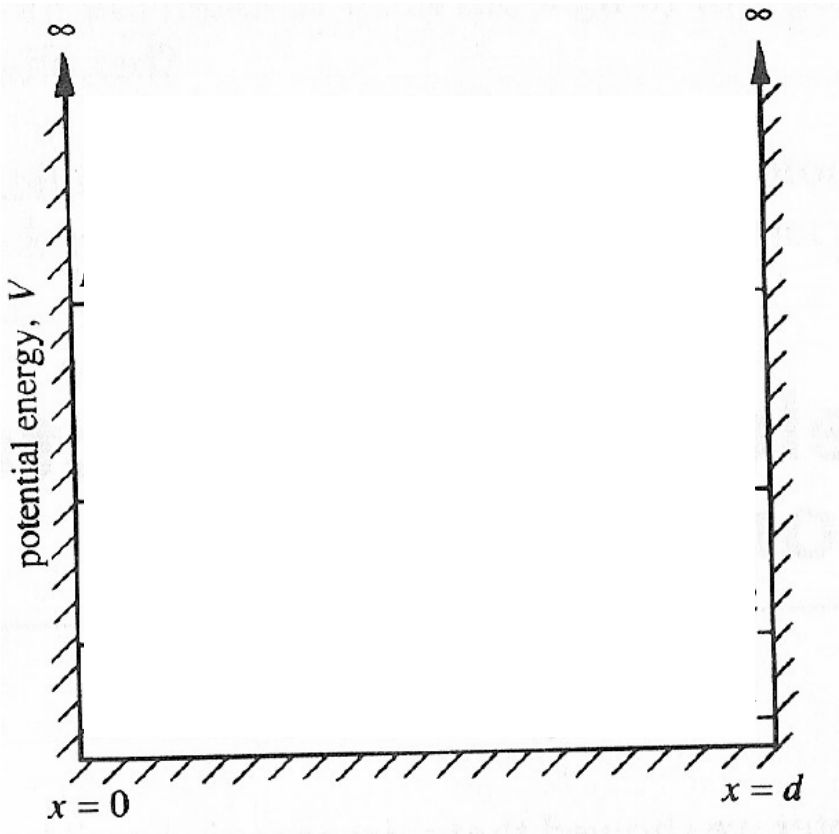
2. The Electronic Structure of Atoms

Contents overview

- A particle in a 1D potential well
- The hydrogen atom
- The exclusion principle

A Particle in a 1D Potential Well

- Infinite well:



$$V = \begin{cases} 0 \text{ for } 0 < x < d \\ \infty \text{ elsewhere} \end{cases}$$

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

$$\Rightarrow \frac{d^2\Psi}{dx^2} + \frac{2m}{\hbar^2} E\Psi = 0$$

$$\Rightarrow \Psi = Ae^{j\beta x} + Be^{-j\beta x} \qquad \beta^2 = (2m/\hbar^2)E$$

A Particle in a 1D Potential Well

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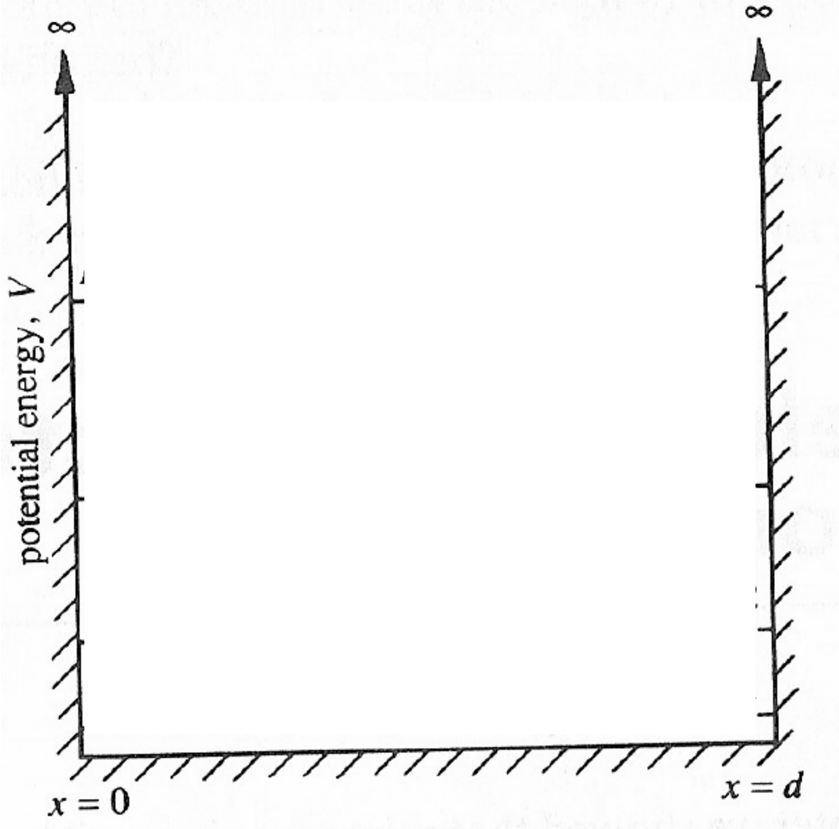

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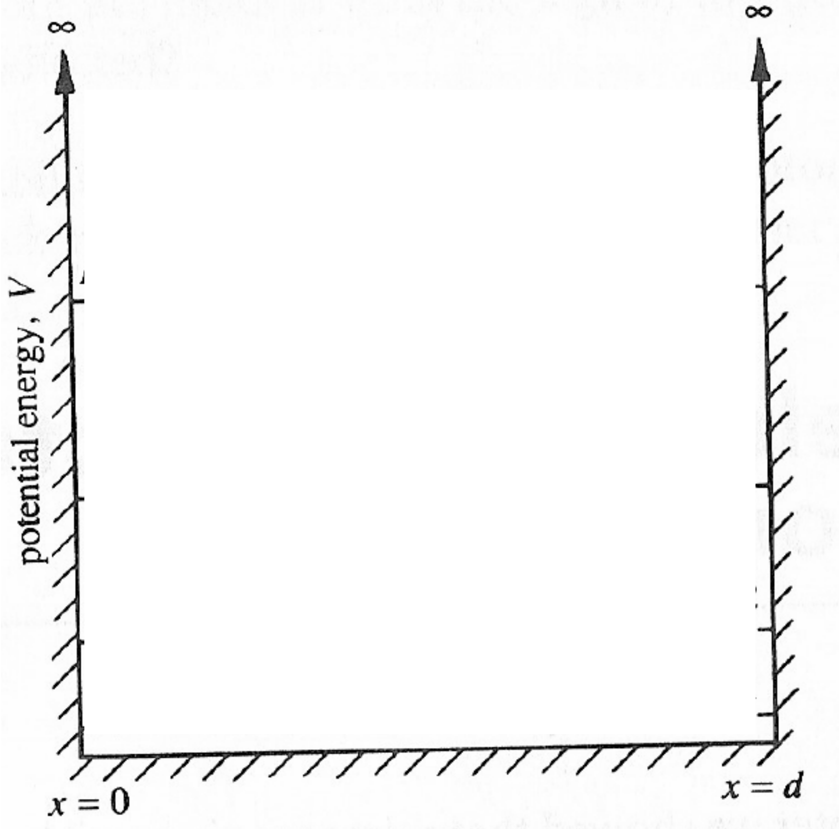
From continuity, i.e. $\Psi(0) = 0 = \Psi(d)$:

$$B = -A$$

$$0 = A(e^{j\beta d} - e^{-j\beta d})$$

A Particle in a 1D Potential Well

- Infinite well:



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From continuity, i.e. $\Psi(0) = 0 = \Psi(d)$:

$B = -A \Rightarrow \Psi = C\sin(\beta x)$ where $C = 2iA$

$0 = A(e^{j\beta d} - e^{-j\beta d}) \Rightarrow \sin(\beta d) = 0 \Rightarrow \beta d = [(2mE)^{1/2}/\hbar]\, d = n\pi$ where $n = 1,2,3,\ldots$

A Particle in a 1D Potential Well

- Infinite well:
  - C is obtained via normalization:

$$\int_0^d C^2 \sin^2(n\pi x/d)\,\mathrm{d}x = 1$$

$$\Psi = (2/d)^{1/2} \sin(n\pi x/d)$$

Each of these w.f. has an associated energy

$$E = \frac{\hbar^2 n^2 \pi^2}{2md^2} = \frac{n^2 h^2}{8md^2} \qquad n = 1,2,3,\ldots$$

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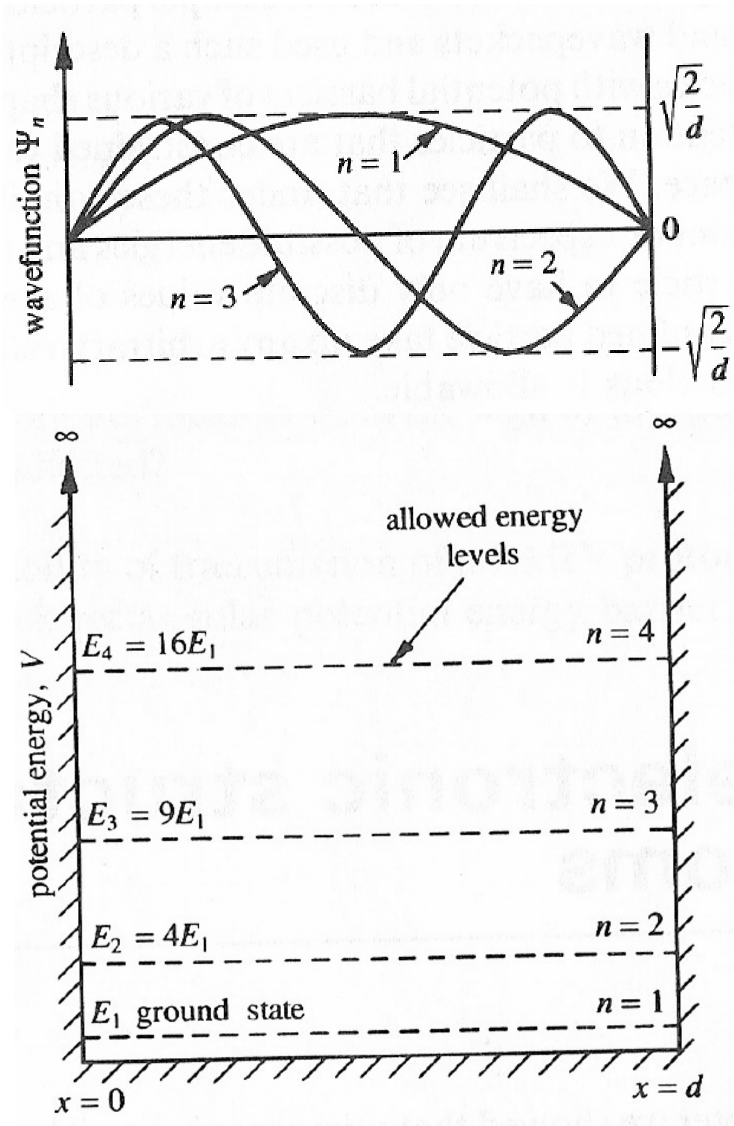
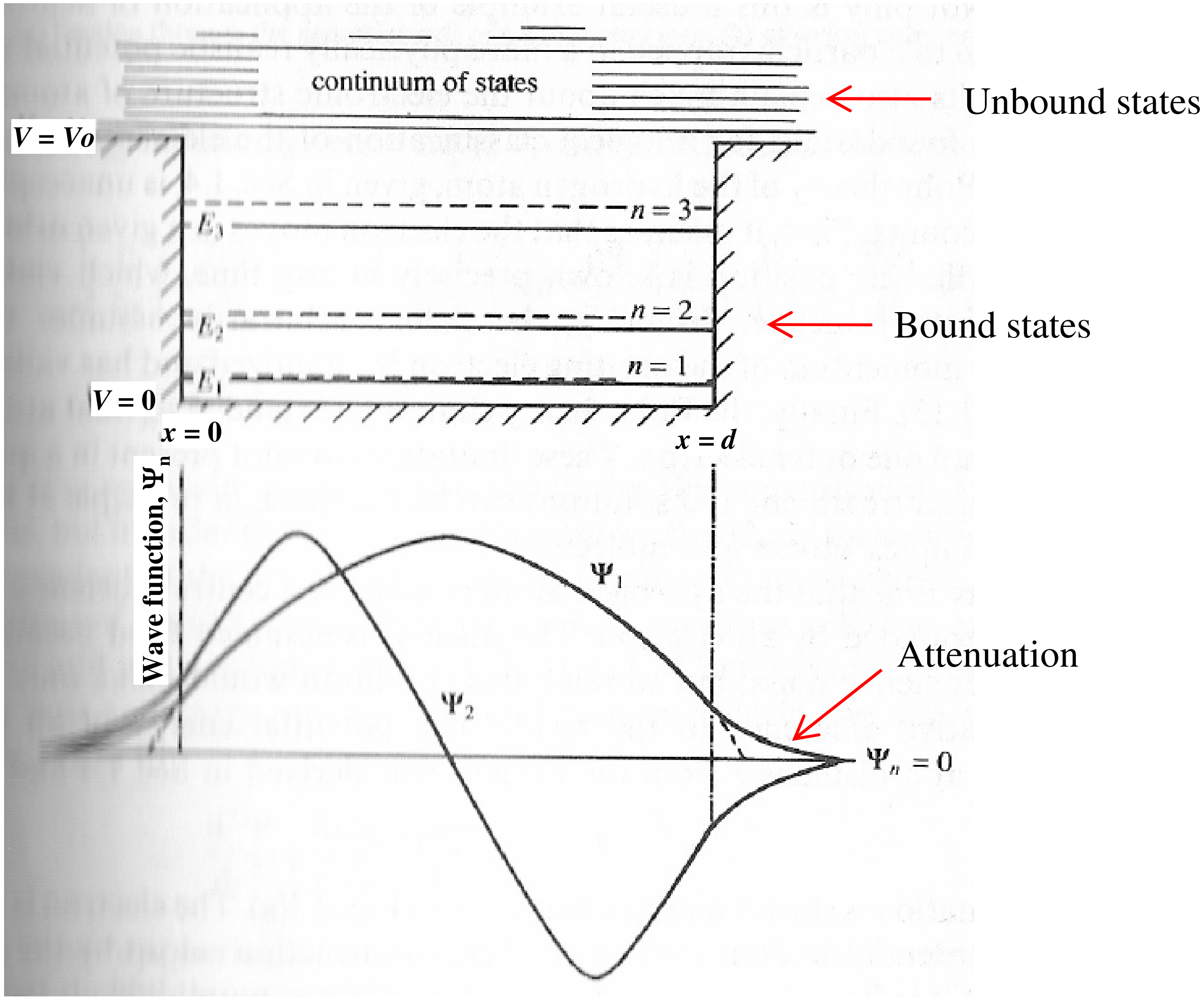


A Particle in a 1D Potential Well

- Finite well (left as an excercise):



http://www.youtube.com/watch?v=HKr9lSyL-Lo