PC2232 Physics for Electrical Engineers
Lecture 8: Quantum Harmonic Oscillator, Tunneling

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February 13, 2015

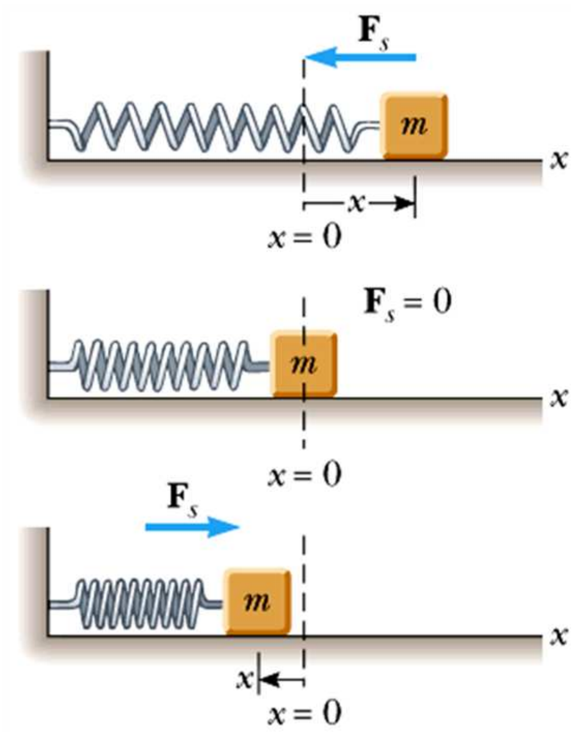
Classical Harmonic Oscillator

- A one-dimensional, nonrelativistic classical harmonic oscillator obeys Newton's second law

$$m\frac{d^2x}{dt^2} = F, \tag{1}$$

with a restoring force

$$F = -\kappa x. \tag{2}$$



- Solution:

$$x(t) = A\cos(\omega_0 t + \theta), \tag{3}$$

A and θ determined by initial conditions of x and dx/dt.

$$m\frac{d^2x}{dt^2} = -m\omega_0^2 x = -\kappa x, \tag{4}$$

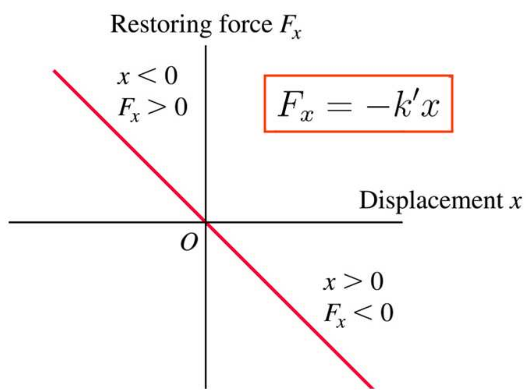
There is a resonance frequency:

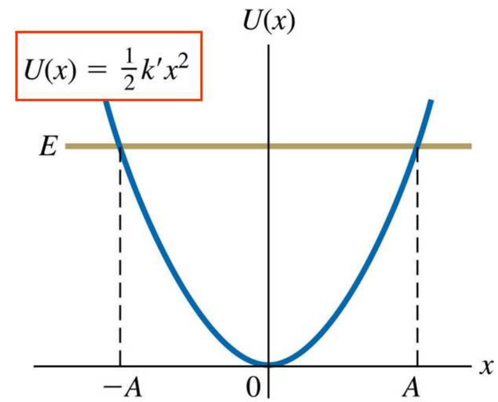
$$\omega_0 = \sqrt{\frac{\kappa}{m}}. \tag{5}$$

Energy of Harmonic Oscillator

- In quantum mechanics, energy is more important than force.
- The total energy of a classical harmonic oscillator is

$$E = \frac{p^2}{2m} + \frac{1}{2}\kappa x^2, \qquad p = m\frac{dx}{dt}, \qquad F = -\frac{dU}{dx} = -\frac{d}{dx}\left(\frac{1}{2}\kappa x^2\right). \tag{6}$$





- The first term is the kinetic energy, the second term is the potential energy. For $x = A\cos(\omega_0 t + \theta)$ for example,

$$\frac{p^2}{2m} = \frac{\kappa A^2}{2}\sin^2(\omega_0 t + \theta), \qquad \frac{\kappa x^2}{2} = \frac{\kappa A^2}{2}\cos^2(\omega_0 t + \theta), \qquad E = \frac{\kappa A^2}{2}. \tag{7}$$

  Energy $\propto A^2$. Any initial condition is allowed, meaning that A can be any value and E can be any nonnegative number.
- Averaged over time, one-half of energy is kinetic and one-half is potential.

Quantum Harmonic Oscillator

- In the quantum case, the time-independent Schrödinger equation becomes (replace p by operator $-i\hbar\frac{\partial}{\partial x}$)

$$\boxed{E\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\kappa x^2\right)\psi.} \tag{8}$$

- The quantum harmonic oscillator is extremely important for multiple reasons:
  - It is analytically solvable and can serve as an approximation for more complicated potentials near a local minimum; e.g., vibrations of atoms in a molecule.

$$U(x) \approx U(x_0) + \frac{1}{2}U^{(2)}(x_0)(x - x_0)^2. \tag{9}$$

  - Classically, it turns out that electromagnetic fields can be considered as an infinite number of harmonic oscillators. Quantum electromagnetism is essentially a general theory of quantum harmonic oscillators.
- We won't show the details of how to solve it, we will just tell you the solutions and the general properties.

Hermite-Gaussian functions

- Given

$$E\psi = \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + \frac{1}{2}\kappa x^2\right)\psi, \qquad (10)$$

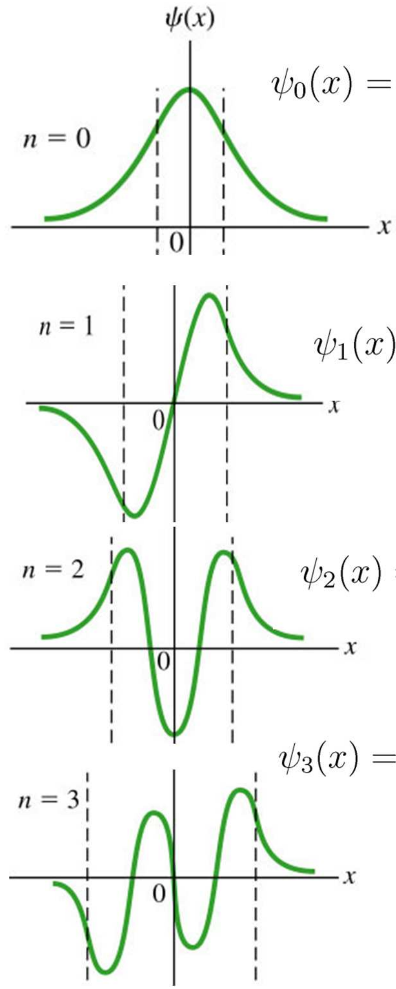
the general solution is

$$\psi_n(x) = A_n H_n(\beta x)\exp\left(-\frac{1}{2}\beta^2 x^2\right), \quad (11)$$

$$\beta \equiv \left(\frac{m\kappa}{\hbar^2}\right)^{1/4}, \qquad (12)$$

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0, \quad n = 0, 1, 2, \ldots \qquad (13)$$

$H_n(\beta x)$ is Hermite polynomial, A_n is a normalization constant.



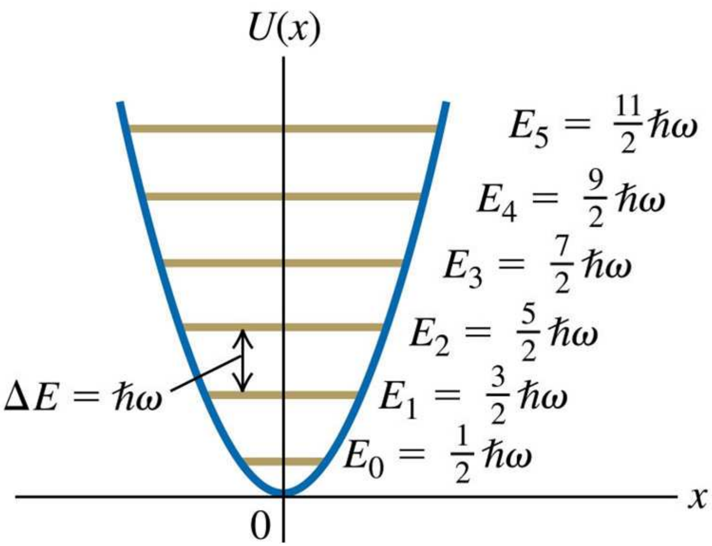
$$\psi_0(x) = \left(\frac{\beta}{\sqrt{\pi}}\right)^{1/2} e^{-\frac{1}{2}\beta^2 x^2}$$

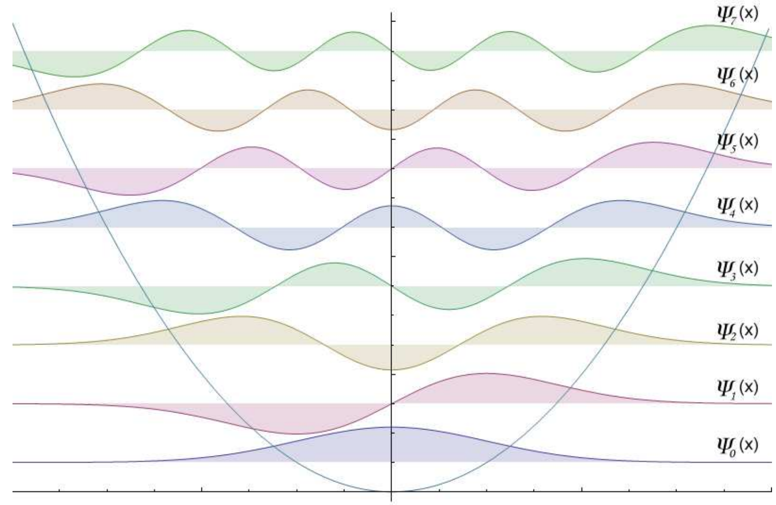
$$\psi_1(x) = \left(\frac{\beta}{2\sqrt{\pi}}\right)^{1/2} (2\beta x)e^{-\frac{1}{2}\beta^2 x^2}$$

$$\psi_2(x) = \left(\frac{\beta}{8\sqrt{\pi}}\right)^{1/2} (4\beta^2 x^2 - 2)e^{-\frac{1}{2}\beta^2 x^2}$$

$$\psi_3(x) = \left(\frac{\beta}{48\sqrt{\pi}}\right)^{1/2} (8\beta x^3 - 12\beta x)e^{-\frac{1}{2}\beta^2 x^2}$$

Discrete Energy of Quantum Harmonic Oscillator





http://en.wikipedia.org/wiki/File:HarmOsziFunktionen.png

- The most important property of the solutions is the discrete energies:

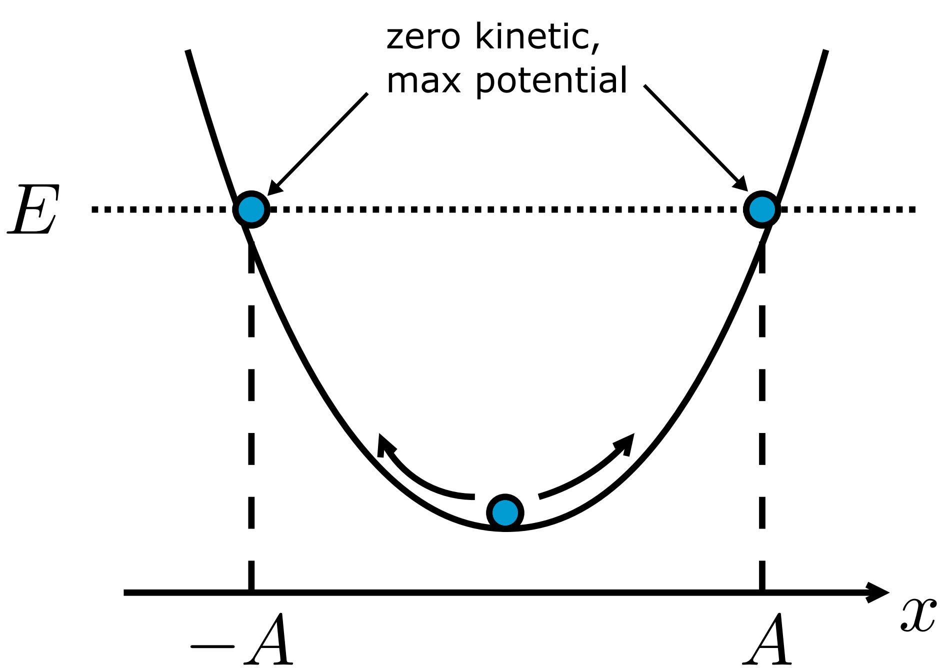
$$\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega_0, \quad n = 0, 1, 2, \ldots} \tag{14}$$

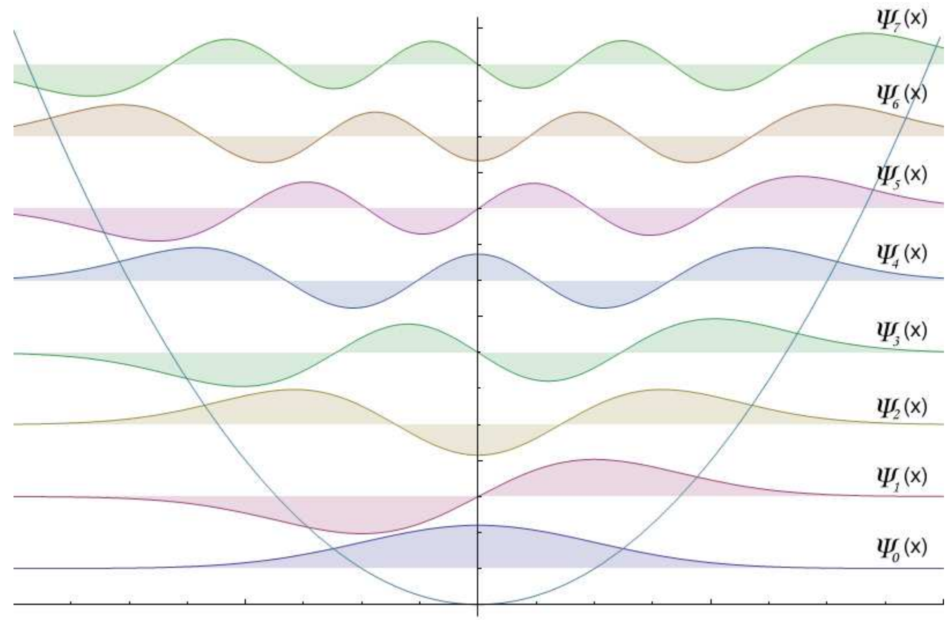
  It depends on the resonance frequency of the harmonic oscillator. n is the number of energy quanta above the ground-state energy $E_0 = \hbar\omega_0/2$, which is nonzero.
- The energies have equal spacing:

$$E_{n+1} - E_n = \hbar\omega_0. \tag{15}$$

- $\hbar\omega_0$ is an extremely small energy for everyday-life frequencies. It becomes observable only when ω_0 becomes very high or E becomes very low.

Classical versus Quantum





- Energy can be arbitrary (≥ 0).
- At $E = U(x)$, the particle has maximum potential energy and zero kinetic energy.
- Position cannot exist in regions where $E < U(x)$
- At potential minimum, speed is highest. Maximum speed $= \sqrt{2E/m}$.

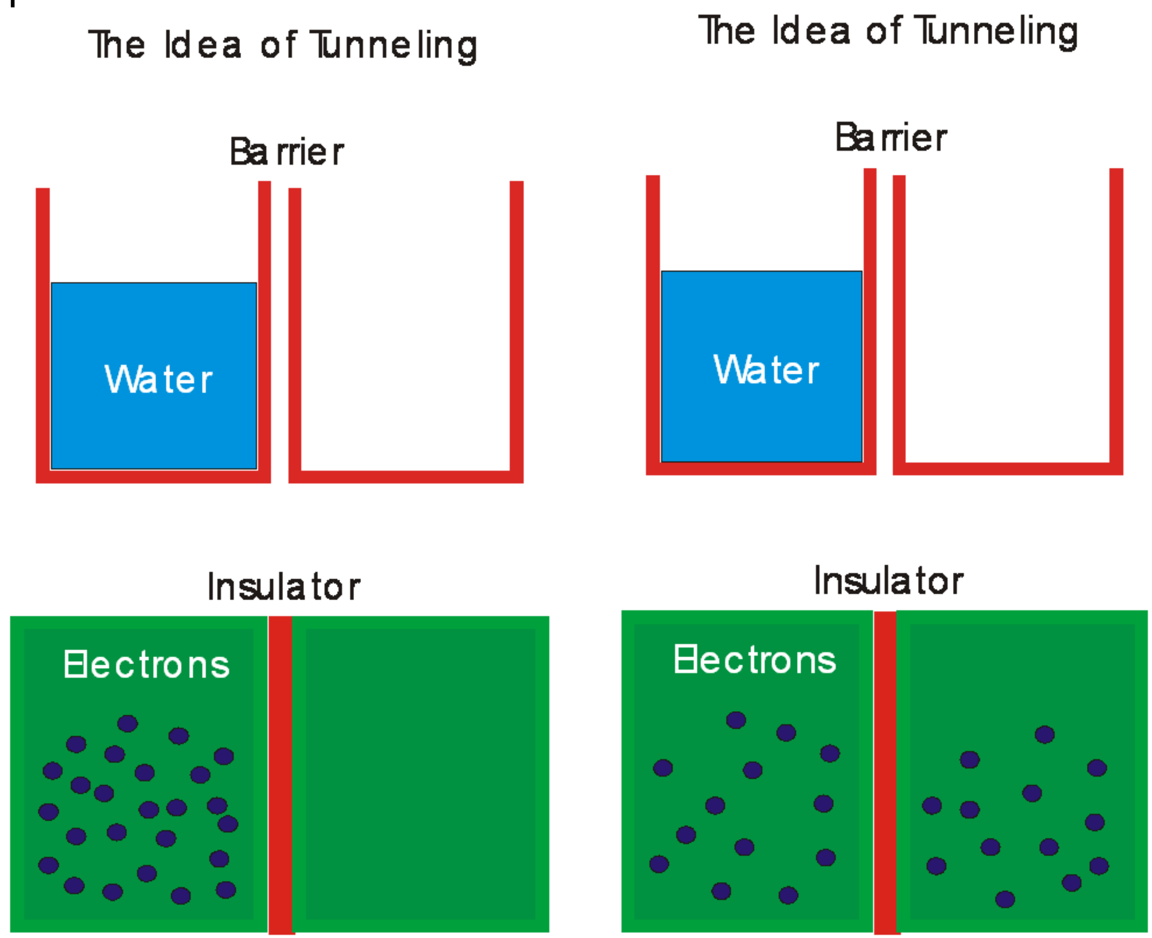
- Discrete $E_n = (n + 1/2)\hbar\omega_0$
- **In regions where $E < U(x)$, $\psi(x)$ is nonzero,** although it decays rapidly away from the center. It is possible to find the particle in classically forbidden regions.
- One can roughly think of the spatial oscillations as the interference of left and right-propagating waves. The higher energy states have smaller periods and larger momenta ($\hbar k$).

Important Generic Features of Quantum Bound States

- **Discrete Energy**: Standing-wave solutions exist only for discrete energies.
- **Energy Must be Below the Maximum Potential Energy**: If $U_{\min} \leq U(x) \leq U_{\max}$, a bound state must have energy $U_{\min} \leq E \leq U_{\max}$. This is to ensure propagating waves inside the potential well and evanescent waves outside the well.
- **Evanescent Waves**: As long as $U(x)$ is not infinite, it is possible for the wavefunction to be nonzero where $U(x) > E$, although it decays rapidly away from the potential well.
- **Zero-Point Energy**: The lowest bound-state energy is always above $U_{\min}$. *This is because the wavefunction always has nonzero derivatives somewhere, implying nonzero kinetic energy.
- **Note, however,** that the following features depend on the specific potential:
  - The specific energy levels and the spacings between them.
  - The evanescent waves may decay in different ways depending on the potential (exponential for flat potential outside well, Gaussian for harmonic oscillator).

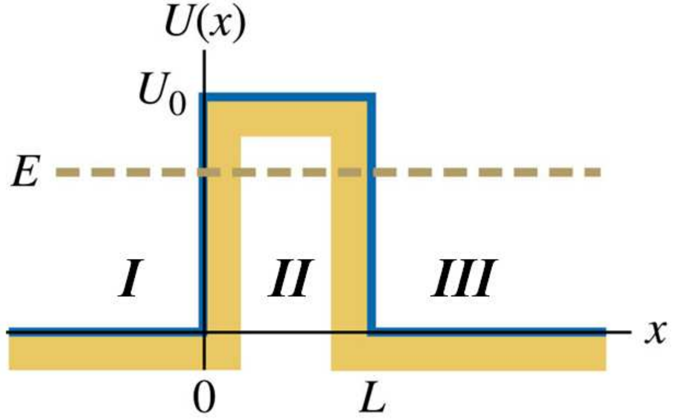
Tunneling

- The fact that a wavefunction can be nonzero where its energy is below the potential has incredible consequences.



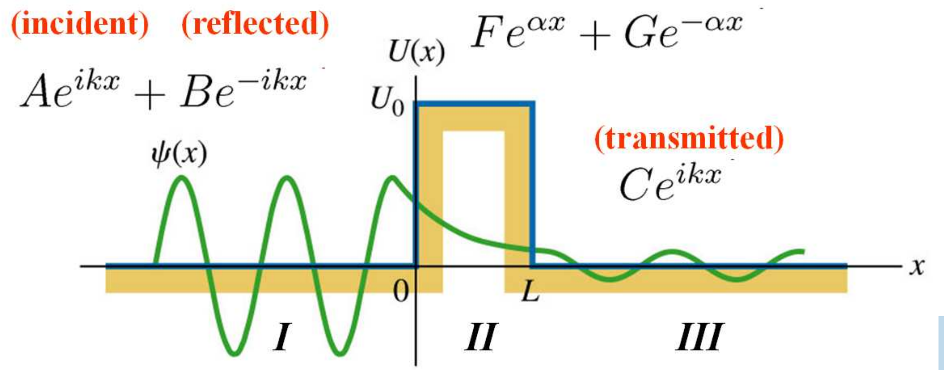
- It is possible for a quantum particle to leak past a potential barrier higher than its energy into another lower-potential region.
- We will study this by way of a simple example, but note that tunneling can occur whenever there is a potential barrier higher than energy of the wave.

$$\boxed{U(x) = \begin{cases} 0 & : \quad x < 0 & : \quad I \\ U_0 & : \quad 0 \leq x \leq L & : \quad II \\ 0 & : \quad x > L & : \quad III \end{cases}}$$



- Consider $0 \leq E \leq U_0$. Propagating solutions in regions I and III (think of them as a stream of quantum particles), real exponential solutions in region II:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & : \quad I \\ Fe^{\alpha x} + Ge^{-\alpha x} & : \quad II \\ Ce^{ikx} & : \quad III \end{cases}$$



- Given E, we can get k and α via

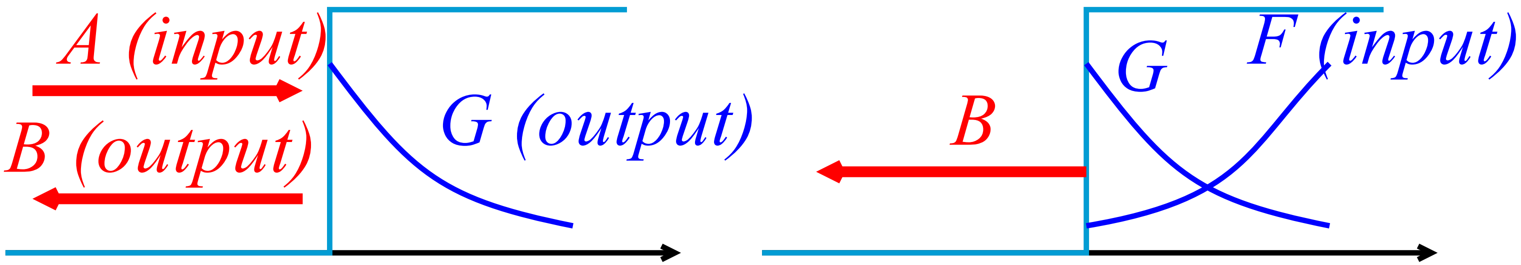
$$E = \frac{\hbar^2 k^2}{2m} = U_0 - \frac{\hbar^2 \alpha^2}{2m}. \tag{16}$$

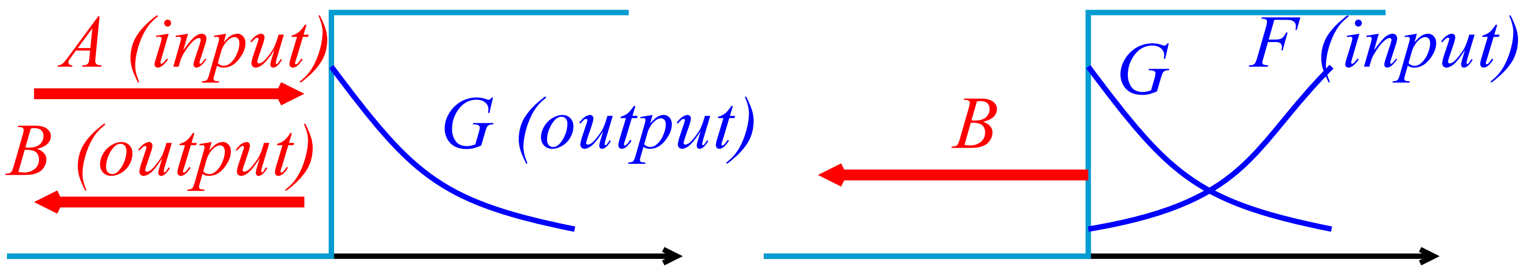
- At the $x = 0$ interface, matching boundary conditions ($\psi_I(0) = \psi_{II}(0)$ and $\psi'_I(0) = \psi'_{II}(0)$) gives

$$A + B = F + G, \qquad ikA - ikB = \alpha F - \alpha G. \tag{17}$$

Rearranging in terms of inputs (A and F) and outputs (B and G),

$$B - G = -A + F, \qquad ikB - \alpha G = ikA - \alpha F. \tag{18}$$





- In matrix form,

$$\begin{pmatrix} 1 & -1 \\ ik & -\alpha \end{pmatrix}\begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} -1 & 1 \\ ik & -\alpha \end{pmatrix}\begin{pmatrix} A \\ F \end{pmatrix}, \tag{19}$$

$$\begin{pmatrix} B \\ G \end{pmatrix} = \begin{pmatrix} 1 & -1 \\ ik & -\alpha \end{pmatrix}^{-1}\begin{pmatrix} -1 & 1 \\ ik & -\alpha \end{pmatrix}\begin{pmatrix} A \\ F \end{pmatrix} \tag{20}$$

$$\equiv \begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix}\begin{pmatrix} A \\ F \end{pmatrix}. \tag{21}$$

The result is

$$\begin{pmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{pmatrix} = \begin{pmatrix} \frac{ik+\alpha}{ik-\alpha} & \frac{-2\alpha}{ik-\alpha} \\ \frac{2ik}{ik-\alpha} & \frac{-ik-\alpha}{ik-\alpha} \end{pmatrix}. \tag{22}$$

Note $|s_{11}|^2 = 1$ (total internal reflection).

Transmission and Reflection

- Similarly, matching the boundary conditions at the second interface,

$$Fe^{\alpha L} + Ge^{-\alpha L} = Ce^{ikL} + De^{-ikL}, \qquad \alpha Fe^{\alpha L} - \alpha Ge^{-\alpha L} = ikCe^{ikL} - ikDe^{-ikL}, \tag{23}$$

$$Fe^{\alpha L} - Ce^{ikL} = -Ge^{-\alpha L} + De^{-ikL}, \qquad \alpha Fe^{\alpha L} - ikCe^{ikL} = \alpha Ge^{-\alpha L} - ikDe^{-ikL}. \tag{24}$$

After some algebra,

$$\begin{pmatrix} Fe^{\alpha L} \\ Ce^{ikL} \end{pmatrix} = \begin{pmatrix} s_{22} & s_{21} \\ s_{12} & s_{11} \end{pmatrix} \begin{pmatrix} Ge^{-\alpha L} \\ De^{-ikL} \end{pmatrix}, \tag{25}$$

where the scattering matrix here is just the same as the first one with the elements re-arranged.
- I can now use the same partial-wave method as before to compute the amplitude transmission and reflection coefficients:

$$\frac{Ce^{ikL}}{A} = \frac{s_{12}e^{-\alpha L}s_{21}}{1 - s_{22}^2 e^{-2\alpha L}}, \qquad \frac{B}{A} = s_{11} + \frac{s_{12}s_{22}s_{21}e^{-2\alpha L}}{1 - s_{22}^2 e^{-2\alpha L}}. \tag{26}$$

- Unlike the Fabry-Perot case, $e^{-2\alpha L}$ is real here, and there is no resonance behavior, that is, the transmission is always less than 100%.
- The important point here is that transmission through a potential barrier higher than the wave energy is possible. This is because of the evanescent waves inside the barrier.

Tunneling Probability

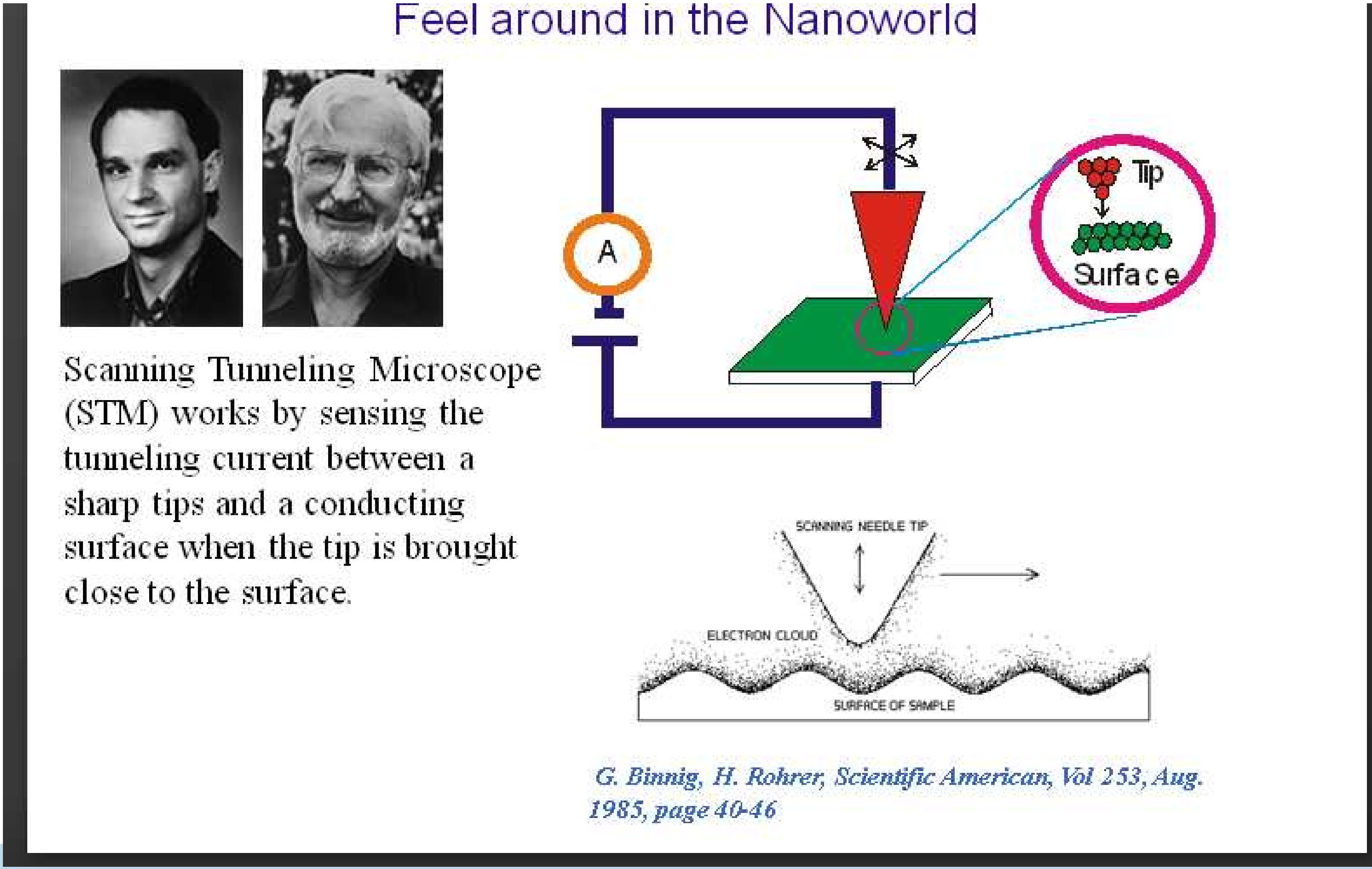
- Probability transmission coefficient:

$$T = \frac{|C|^2}{|A|^2} = \frac{|s_{12}s_{21}|^2 e^{-2\alpha L}}{|1 - s_{22}^2 e^{-2\alpha L}|^2}. \tag{27}$$

- Roughly speaking, this is the probability that a particle with energy E can tunnel through the barrier (remember that α, k depend on $E = \hbar^2 k^2/(2m) = U_0 - \hbar^2\alpha^2/(2m)$, and the s matrix depends on α and k).
- If the decay of exponential wave is severe such that $s_{22}^2 e^{-2\alpha L} \ll 1$, the partial waves with multiple round trips are very small, and we can assume only the lowest-order partial wave:

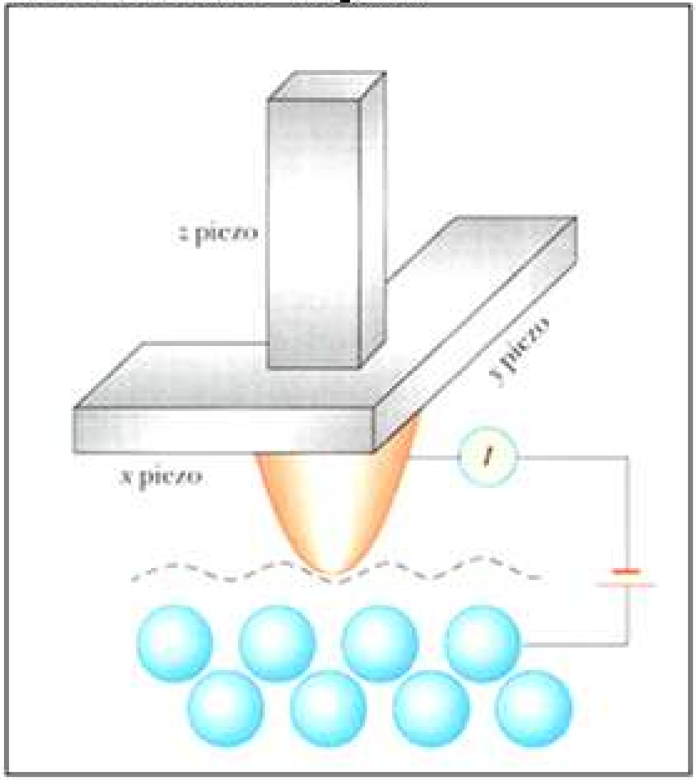
$$T \approx |s_{12}s_{21}|^2 e^{-2\alpha L} = \frac{16\alpha^2 k^2}{(k^2+\alpha^2)^2} e^{-2\alpha L} = 16\frac{E}{U_0}\left(1 - \frac{E}{U_0}\right) e^{-2\alpha L}, \quad \alpha \quad = \sqrt{\frac{2m}{\hbar^2}(U_0 - E)}. \tag{28}$$

- PhET/sims/quantum-tunneling
- For $E \ll U_0$, the transmission is very low, as $\alpha \approx \sqrt{2mU_0/\hbar^2}$, $E/U_0 \ll 1$, and $T \ll 1$, as one would expect.


Feel around in the Nanoworld
A
Tip
Surface
Scanning Tunneling Microscope (STM) works by sensing the tunneling current between a sharp tips and a conducting surface when the tip is brought close to the surface.
SCANNING NEEDLE TIP
ELECTRON CLOUD
SURFACE OF SAMPLE
G. Binnig, H. Rohrer, Scientific American, Vol 253, Aug. 1985, page 40-46

Application: Scanning Tunneling Microscope (STM)

STM schematic diagram.



•A conducting **very sharp tip** (< 1 nm) is positioned very close to the surface of a specimen (about a nanometre). Electrons will tunnel through the barrier with an exponential probability with surface/tip distance.

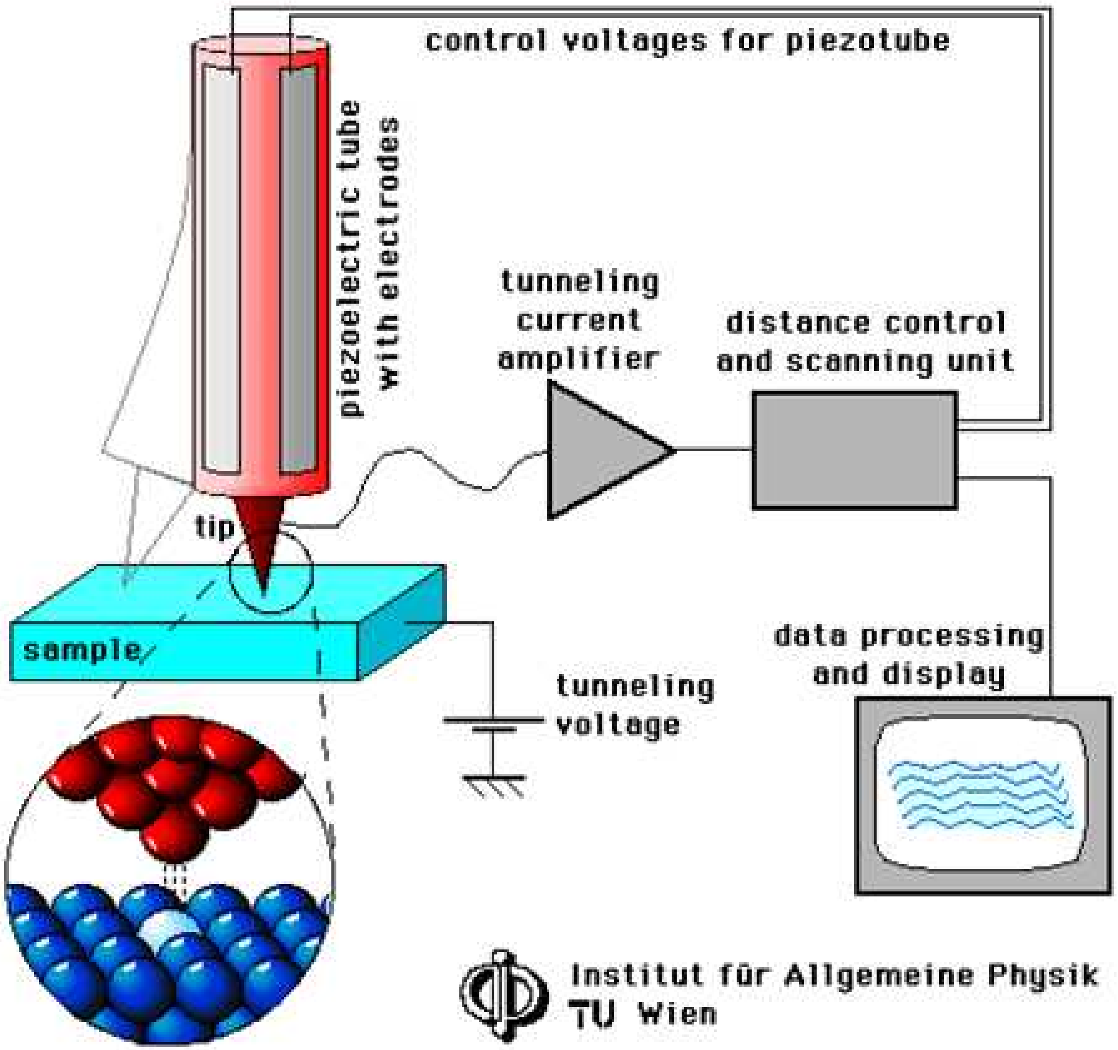
• If the XYZ piezoelectric drivers receive a feedback signal to keep the tip current constant, then the distance will also be constant.

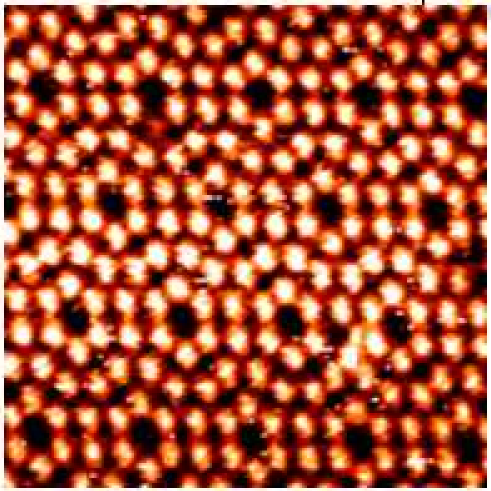
• If the tip is raster scanned across the surface, keeping the tip current constant, then tip will follow the surface atom profile.

• **The tip can be accurately positioned because of the exponential current change with the tip-surface distance.**

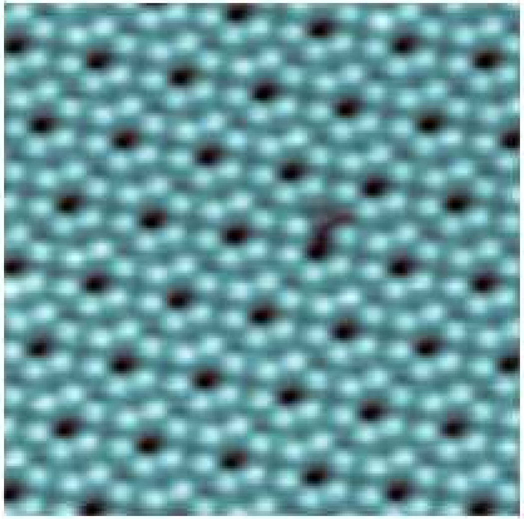
• **The STM can measure the height of surface features to within 0.001 nm, approximately 1/100 of an atomic diameter.**

Application: Scanning Tunneling Microscope (STM)





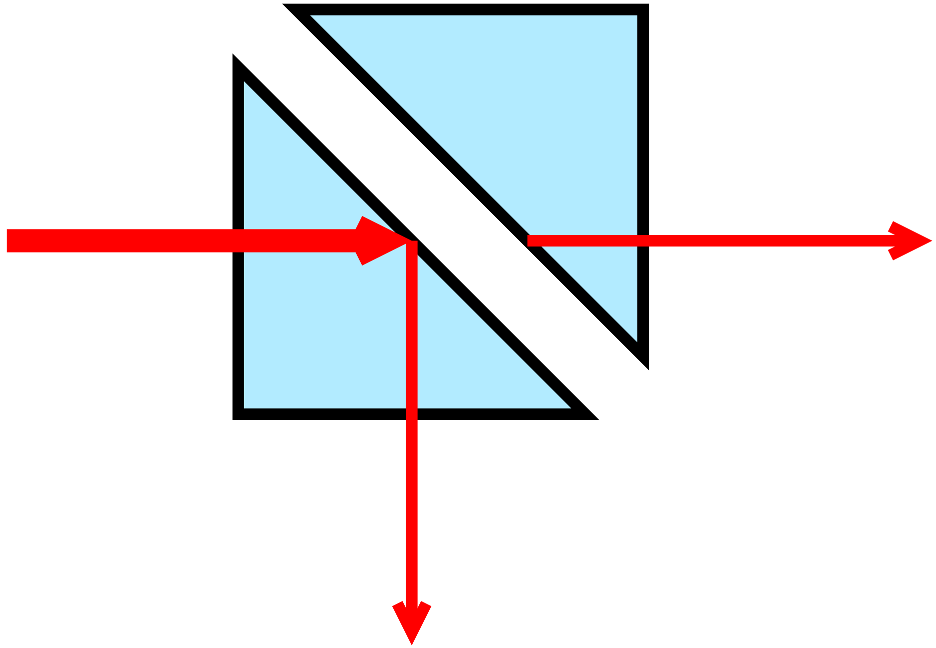
Andrew Wee et al NUS



Prof. Randall Feenstra
Carnegie Mellon

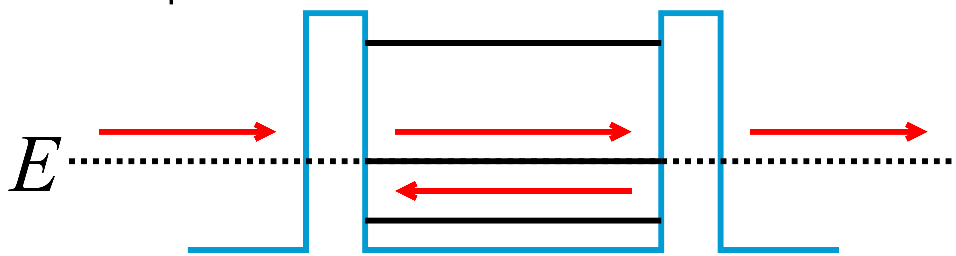
Optical Tunneling

- As you might have guessed, the same tunneling effect can happen in optics.
- For oblique incidence from glass to air, total internal reflection can occur.
- There is evanescent wave in air. If another piece of glass is close, it can pick up the evanescent wave and leak optical power to the other side (this is called frustrated total internal reflection).

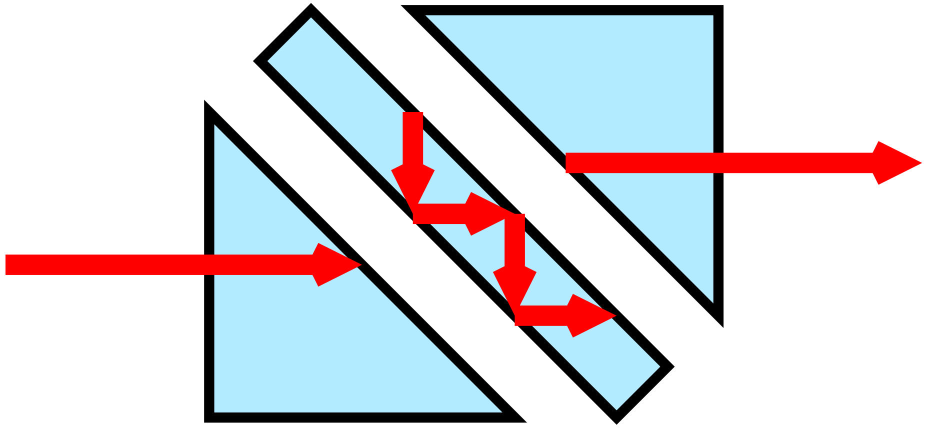


*Resonant Tunneling

- Can I get 100% transmission through tunneling?
- Not with one barrier, but it's possible with two!



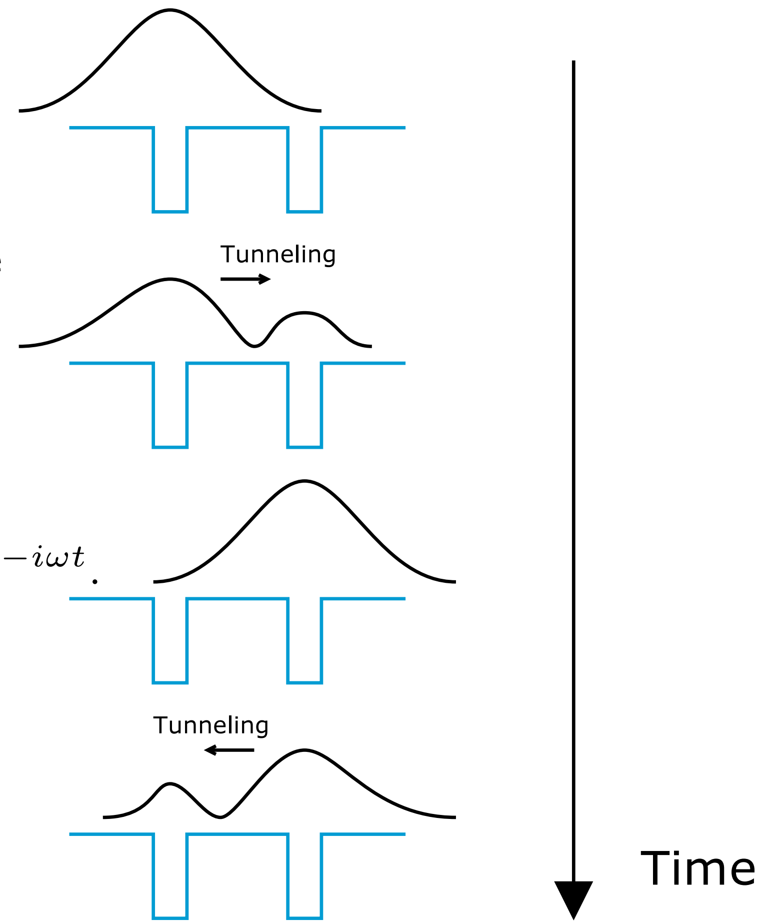
- It's the same as the Fabry-Perot effect. There is maximum transmission if the energy/frequency of the incoming wave matches the resonant frequency of the center cavity.
- When the barriers are high, the incoming frequency/energy must be very precise for resonant tunneling to occur.
- Same effect in optics: maximum transmission when the incidence wave is on resonance with the film.



Tunneling of Bound States

- Consider now two identical potential wells nearby.
- The time-independent solution for one well ($\tilde{\psi}(x+\frac{d}{2})$) is not the time-independent solution for two wells.
- Consider the time-dependent case, and assume $\tilde{\psi}(x+\frac{d}{2})$ as the initial condition.
- In time, the wavefunction will leak into the other well via tunneling.
- General solution is possible, but I'll just tell you what happens: the wave keeps tunneling back and forth between the two wells at a certain frequency $\Delta\omega$ depending on the geometry.
- When the wells are farther away, tunneling is slower, and $\Delta\omega$ is smaller.
- The solution will look like

$$\psi(x,t) \propto \left[\tilde{\psi}(x+\frac{d}{2})\cos(\Delta\omega t) + i\tilde{\psi}(x-\frac{d}{2})\sin(\Delta\omega t)\right] e^{-i\omega t}. \tag{29}$$



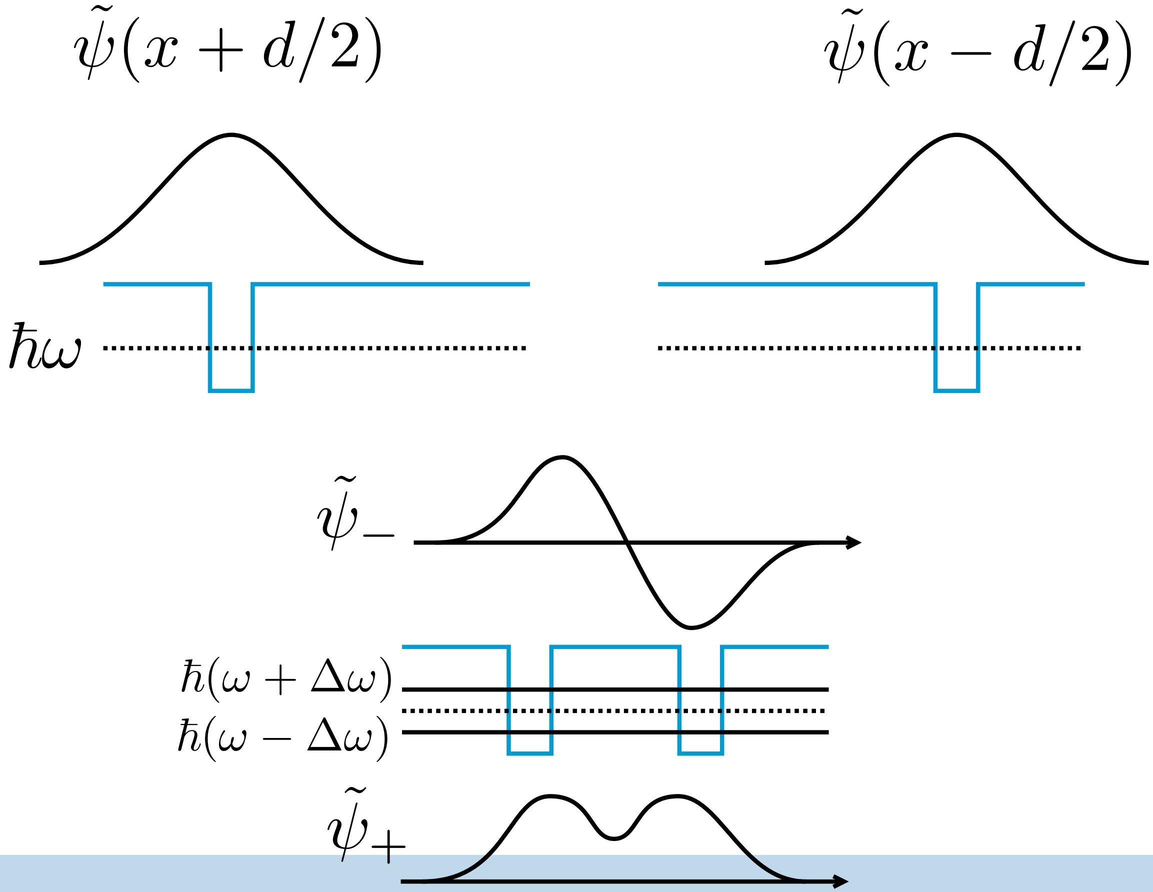
I can rewrite it as

$$\psi(x,t) \propto \left[\tilde{\psi}_+(x)e^{i\Delta\omega t} + \tilde{\psi}_-(x)e^{-i\Delta\omega t}\right] e^{-i\omega t}, \tag{30}$$

$$\tilde{\psi}_+(x) \equiv \frac{1}{2}\left[\tilde{\psi}(x+d/2) + \tilde{\psi}(x-d/2)\right], \tag{31}$$

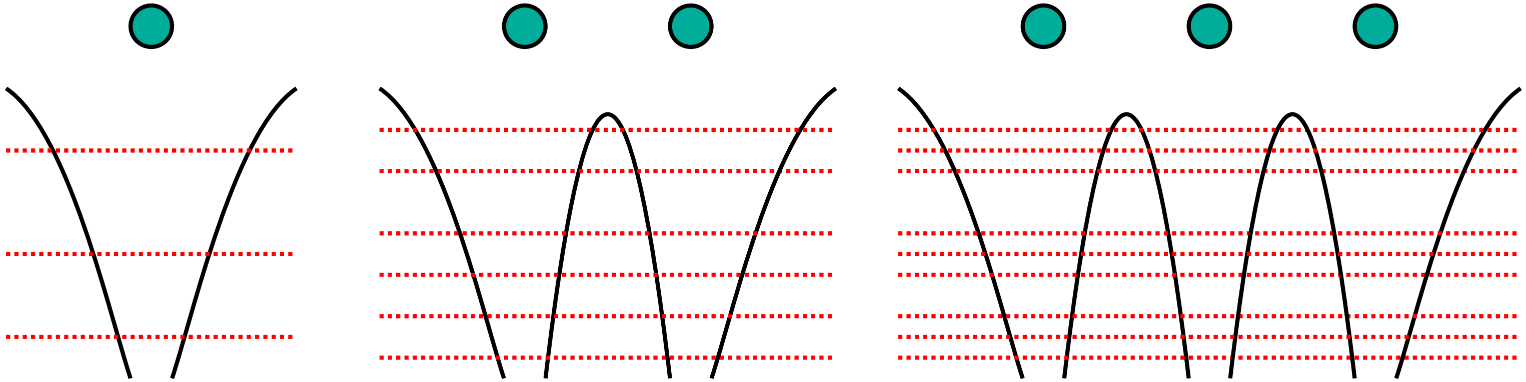
$$\tilde{\psi}_-(x) \equiv \frac{1}{2}\left[\tilde{\psi}(x+d/2) - \tilde{\psi}(x-d/2)\right]. \tag{32}$$

- Since the $\tilde{\psi}_+(x)$ part oscillates at single frequency $\omega - \Delta\omega$, it is a solution of the time-independent Schrödinger equation with two wells, with energy $\hbar(\omega - \Delta\omega)$.
- Similarly, the $\tilde{\psi}_-(x)$ part oscillates at frequency $\omega + \Delta\omega$, it is also a solution of the time-independent Schrödinger equation with two wells with energy $\hbar(\omega + \Delta\omega)$.
- The bound-state energy for each potential will split into two for two identical potentials.
- This will be important for covalent bonds, solids, etc.

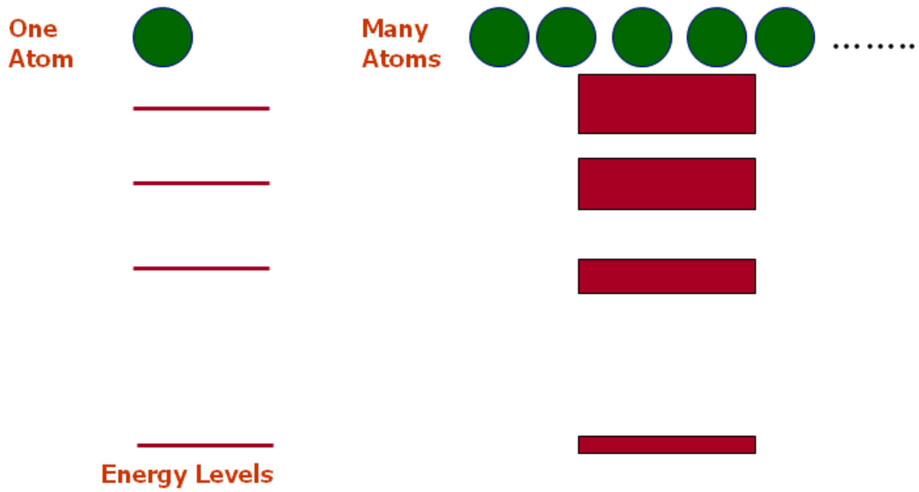


From Energy Splitting to Energy Bands

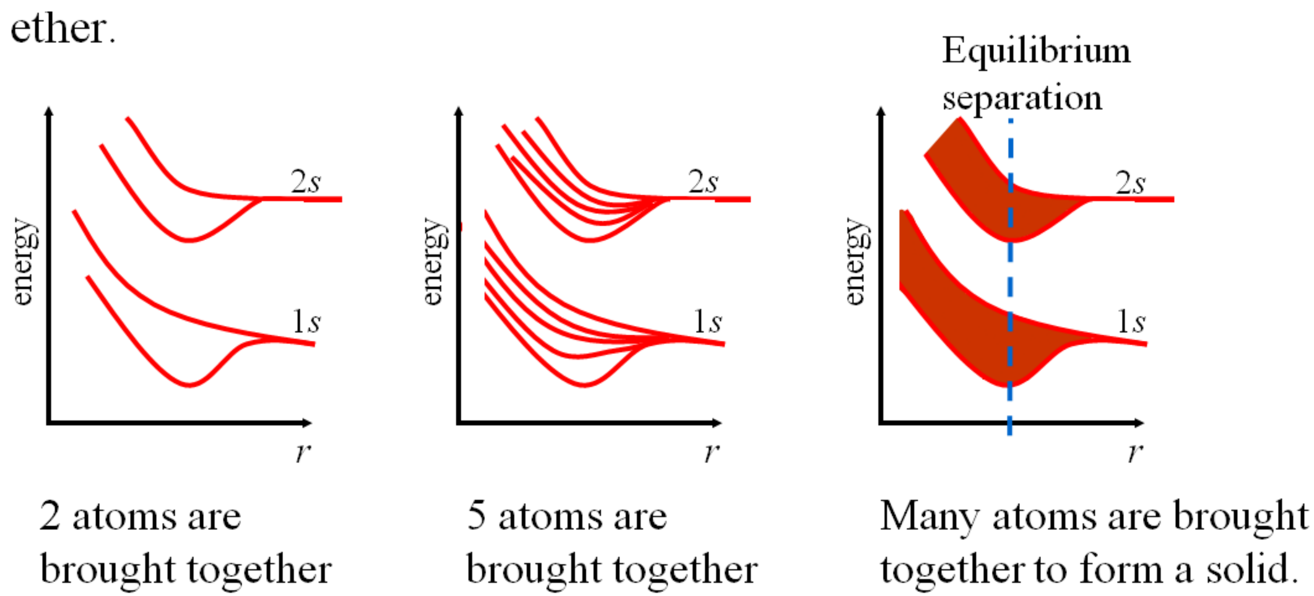
- An atom consists of a positively nucleus that acts as a potential for electrons.
- For two nearby atoms, each electron energy level splits into two due to tunneling. For N atoms, there are N energy splits.

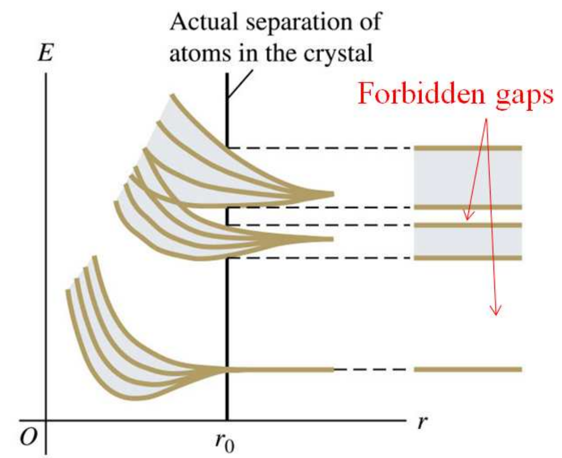


- When there are many atoms, e.g., in a solid, where there are $\sim 10^{24}$ atoms, the huge amount of energy levels become effectively a continuous band of energy.



Energy Bands and Bandgaps





Suggested Problems

- Quantum Harmonic Oscillator: plug the ground-state solution into right-hand side of Schrödinger equation and verify that it is indeed a solution with the right energy. Calculate the normalization constant A_0.
- Consider a classical harmonic oscillator with $E \approx 1$ J and $\omega_0 \approx 1$ rad/s (typical everyday-life values). Compute the approximate number of quanta n in the quantum case. Now do the same for $E \approx 1$ eV (typical semiconductor bandgap) and $\omega_0 \approx 10^{15}$ rad/s (typical optical frequency).
- Quantum harmonic oscillator: Given the ground state solution $\psi_0(x)$, show that

$$\psi_1(x) \propto \frac{1}{\sqrt{2\hbar m\omega_0}} \left(-\hbar \frac{\partial}{\partial x} + m\omega_0 x \right) \psi_0(x) \tag{33}$$

  is also a solution. Show that $\psi_1(x)$ is proportional to the solution with energy $(n + 1/2)\hbar\omega_0$, $n = 1$. $a_+ \equiv \frac{1}{\sqrt{2\hbar m\omega_0}} \left(-\hbar \frac{\partial}{\partial x} + m\omega_0 x \right)$ is called a raising operator.
  Show that

$$\frac{1}{\sqrt{2\hbar m\omega_0}} \left(\hbar \frac{\partial}{\partial x} + m\omega_0 x \right) \psi_1(x) \propto \psi_0(x). \tag{34}$$

  $a_- \equiv \frac{1}{\sqrt{2\hbar m\omega_0}} \left(\hbar \frac{\partial}{\partial x} + m\omega_0 x \right)$ is called a lowering operator. These operators are very useful for generating solutions for quantum harmonic oscillators.
- Tunneling: A 2.0-eV electron encounters a barrier with height 5.0 eV. What is the probability that it will tunnel through the barrier if the barrier width is (a) 1.00 nm, and (b) 0.50 nm, roughly 10 and 5 atomic diameters respectively? Use the approximate formula for low transmission.
- *Resonant tunneling: use input-output analysis to compute transmission and reflection coefficients. When is transmission maximum?