Quantum Wells, Tunnels and Swings

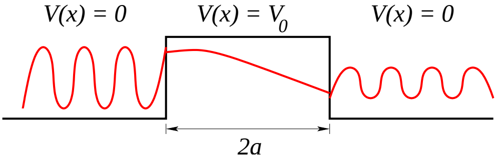
UP201

IISc Bangalore

Of course, the questions..

1. How does an alpha particle escape a nucleus?
2. Whats with STM? (Scanning tunneling microscope)
3. And quantum wells?
4. Ramsauer effect – alpha particles incident on inert gas atoms show "resonances" in transmission!
5. Bound states? Metal-insulator transitions!

The Great Barrier



- Model (What do you expect classically?)
- Scrödinger Recipe: Say energy state is E

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi, \quad |x| \geq a; \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V_0\psi = E\psi, \quad |x| \leq a$$

- Is $E < V_0$ possible? What happens?
- Two length scales (a and $\sqrt{\frac{\hbar^2}{2mV_0}}$)!!

Barrier Tunneling

- Think of a state when electron is incident from left
- State to the left of the barrier $x < -a$: superposition of plane wave "traveling" to right and a *"reflected wave"*
  $\psi_l(x) = e^{ikx} + Re^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$
- To the right of the barrier a wave traveling to right $\psi_r(x) = Te^{ikx}$
- Restrict to case when $E < V_0$
- The state in the barrier is $\psi_b(x) = Ae^{qx} + Be^{-qx}$ $(q = \sqrt{\frac{2m(V_0-E)}{\hbar^2}})$ – does *not* correspond to a wavelike state

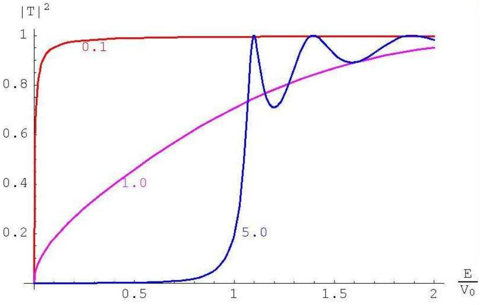
Barrier Tunneling

- How to determine R, T, A, B? Of interest: T!
- Use conditions

$$\psi_l(-a) = \psi_b(-a), \qquad \psi_l'(-a) = \psi_b'(-a)$$
$$\psi_b(a) = \psi_r(a), \qquad \psi_b'(a) = \psi_r'(a)$$

  four equations for four unknowns! All OK!
- Solution $T = \frac{4ie^{2a(-ik+q)}kq}{(1-e^{4aq})q^2+2i(1+e^{4aq})kq-(1-e^{4aq})k^2}$
- The quantity $|T|^2$ is probability of transmission...upshot $|T|^2 \sim e^{-4aq}$!
- For a given V_0, how does $|T|^2$ depend on E, for various values of $a/\sqrt{\frac{\hbar^2}{2mV_0}}$?

Barrier Tunneling



Curves for various $a/\sqrt{\frac{\hbar^2}{2mV_0}}$ indicated

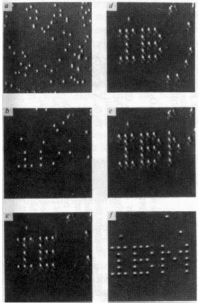
- For small a the electron does not feel the barrier, for large a there is very little transmission
- Note "resonances" for large values of a, when $E > V_0$ (not considered, so far)

Tunneling in Real Life

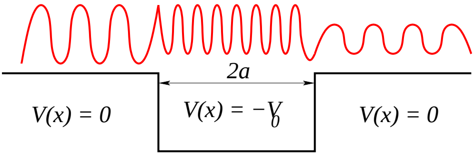
- Alpha particles: Held to nucleus by *very strong* nuclear forces. Barrier height can be of many eVs!! Very high kinetic energy (confinement in 10^{-15}m)!! $|T|^2$ is quite small (in fact, can be shown to be $\sim e^{-90}$(!!!!!)), the number of "attempts" to jump out are large (of the order of 10^{21} per second)...probaility of decay is 10^{-11} per year!!
- Ohmic contacts between metals and semiconductors: Need to have linear $I - V$ characteristics for contacts...problem...contact barrier! Solution: Try to make a as small as possible by heavily doping semiconductor near contact...depletion zone size comes down and electrons tunnel across!

Tunneling in Real Life

- Field emission devices...pull out electrons using voltage–flat panel displays
- STM...maintain a constant tunneling current (at constant voltage) by adjusting distance...maps out topography of surface!



Well, What Now?...



- Model (What do you expect classically?)
- Scrödinger Recipe: Say energy state is E

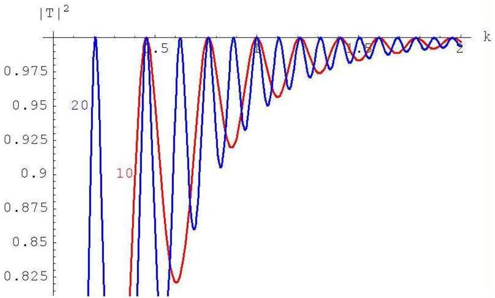
$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi, \quad |x| \geq a; \qquad -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} - V_0\psi = E\psi, \quad |x| \leq a$$

- What happens when $E > 0$? Is $E < 0$ possible?

Quantum Well

- Think of a state when electron is incident from left
- State to the left of the well $x < -a$: superposition of plane wave "traveling" to right and a *"reflected wave"*
  $\psi_l(x) = e^{ikx} + Re^{-ikx}, \quad k = \sqrt{\frac{2mE}{\hbar^2}}$
- To the right of the well a wave traveling to right $\psi_r(x) = Te^{ikx}$
- Restrict to case when $E > 0$
- The state in the well is $\psi_w(x) = Ae^{iqx} + Be^{-iqx}$ ($q = \sqrt{\frac{2m(E+V_0)}{\hbar^2}}$) – *does* correspond to a wavelike state of shorter wavelength!
- Solve for T in exactly the same way as the barrier problem!

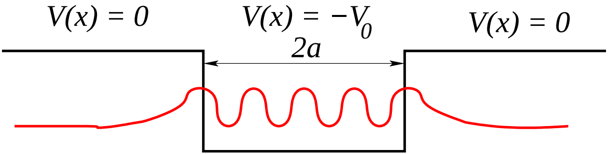
Quantum Well



Curves for various $a/\sqrt{\frac{\hbar^2}{2mV_0}}$ indicated

- There are particular values of k at which $T = 1$..."Resonances"...Why?
- Roughly explains the Ramsauer effect!
- What happens if $E < 0$?

Quantum Well – Bound States



- States with $-V_0 < E < 0$ *are possible*! "Bound states"!
- Wavefunction ($q = \sqrt{\frac{2m|E|}{\hbar^2}}, k = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}$)

$$\psi_l(x) = Ae^{qx}, \quad \psi_w(x) = Be^{ikx} + Ce^{-ikx}, \quad \psi_r(x) = De^{-qx}$$

- Main idea: Wavefunction decay exponentially outside the box!
- How to determine allowed Es?

Quantum Well – Bound States

- Use exactly same ideas as before

$$\psi_l(-a) = \psi_w(-a), \qquad \psi_l'(-a) = \psi_w'(-a)$$
$$\psi_w(a) = \psi_r(a), \qquad \psi_w'(a) = \psi_r'(a)$$

- Main point: *Homogeneous equations for* A, B, C, D
- Condition of non-triviality gives possible energy states

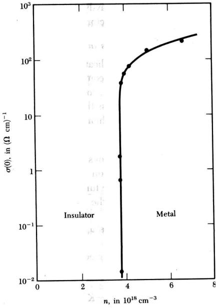
$$\sqrt{\frac{|E|}{V_0 - |E|}} = \tan\left(\sqrt{\frac{2m(V_0 - |E|)a^2}{\hbar^2}}\right) \quad n \text{ even}$$
$$\sqrt{\frac{|E|}{V_0 - |E|}} = -\cot\left(\sqrt{\frac{2m(V_0 - |E|)a^2}{\hbar^2}}\right) \quad n \text{ odd}$$

Bound States...Big Deal?

- Whats the big deal?
- The “simplest” model of an atom!!
- Bound state are always possible in 1D (and 2D..I am not sure about this) for “attractive” potentials
- Quantum wells are used for many purposes... Infrared sensor, lasers etc. etc..

Bound States...Big Deal?

- In 3D there are attractive potentials for which there are no bound states!For example, $V(r) \sim \frac{e^{-\xi r}}{r}$, there is no bound state for $\xi > \xi_c$...crucial to understand metal-insulator transitions (Mott)



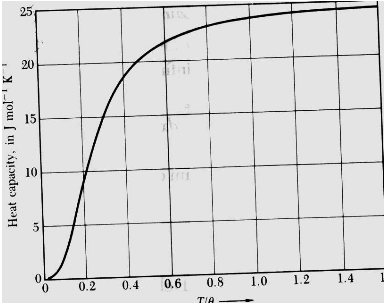
P in Si

Summary

- Tunneling : Transmission probability goes as $e^{-2\ell q}$ where ℓ is the size scale of the barrier
- Quantum wells: “Resonances”
- Bound states: Again useful for many things!

Why Harmonic Oscillator?

- What is with specific heat of solids?



- Molecular vibrations?
- Light itself...really?

1D Harmonic Oscillator

- Hamiltonian (ω – "natural frequency")

$$H = \frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2$$

- What are the energy eigenvalues and eigenstates? Need to solve

$$H\psi = E\psi$$

- Are there bound states? Extended states? Both?

1D Harmonic Oscillator

- What can we say without solving anything?
- Well, what do you expect classically? Any energy E is possible. Particle will be confined to $|x| \leq \sqrt{\frac{2E}{m\omega^2}}$
- Looks like we will have only bound states!
- Clearly, $\langle X \rangle = 0$!

1D Harmonic Oscillator

- Since, $\langle X \rangle = 0$, $\langle V(X) \rangle = \frac{1}{2} m\omega^2 \Delta x^2$
- Since bound state, $\langle P \rangle = 0$ and $\langle \frac{P^2}{2m} \rangle = \frac{\Delta p^2}{2m}$
- From uncertainty relation $\Delta p = \frac{\hbar}{\Delta x}$
- Total energy $E = \frac{\hbar^2}{2m\Delta x^2} + \frac{1}{2} m\omega^2 \Delta x^2$
- We can show this energy is minimum if $\Delta x = \sqrt{\frac{\hbar}{m\omega}}$, for this value of Δx, $E \approx \hbar\omega$!
- Thus, uncertainty principle tells us that the minimum energy level of the harmonic oscillator must have energy of the order of $\hbar\omega$!
- Contrast this with classical result!

Solution of Quantum Swing

- Solution of $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi$ is a bit technical
- Allowed energy levels $E_n = (n + \frac{1}{2})\hbar\omega, \quad n = 0, 1, 2...$
- Lowest energy level $\frac{1}{2}\hbar\omega$! Very close to our estimate!
- Levels are equally spaced
- Energy eigenstates $\psi_n(x) = C_n H_n(\alpha x)e^{-\frac{1}{2}\alpha^2x^2}$ with $\alpha = \sqrt{\frac{m\omega}{\hbar}}$, $C_n = \sqrt{\frac{\alpha}{\sqrt{\pi}2^n n!}}$
- $H_n(\xi)$ are the Hermite polynomials which satisfy the differential equation $H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n = 0$

Hermite Polynomials...What?

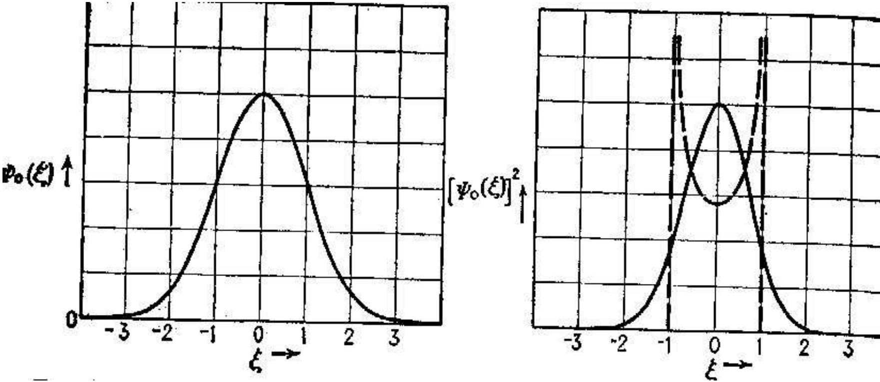
- $H_n(\xi)$ are the Hermite polynomials which satisfy the differential equation $H_n''(\xi) - 2\xi H_n'(\xi) + 2nH_n = 0$

$$
\begin{aligned}
H_0(\xi) &= 1 \\
H_1(\xi) &= 2\xi \\
H_2(\xi) &= 4\xi^2 - 2 \\
H_3(\xi) &= 8\xi^3 - 12\xi \\
H_4(\xi) &= 16\xi^4 - 48\xi^2 + 12 \\
H_5(\xi) &= 32\xi^5 - 160\xi^3 + 120\xi \\
H_6(\xi) &= 64\xi^6 - 480\xi^4 + 720\xi^2 - 120 \\
H_7(\xi) &= 128\xi^7 - 1344\xi^5 + 3360\xi^3 - 1680\xi \\
H_8(\xi) &= 256\xi^8 - 3584\xi^6 + 13440\xi^4 - 13440\xi^2 + 1680 \\
H_9(\xi) &= 512\xi^9 - 9216\xi^7 + 48384\xi^5 - 80640\xi^3 + 30240\xi
\end{aligned}
$$

(Pauling and Wilson)

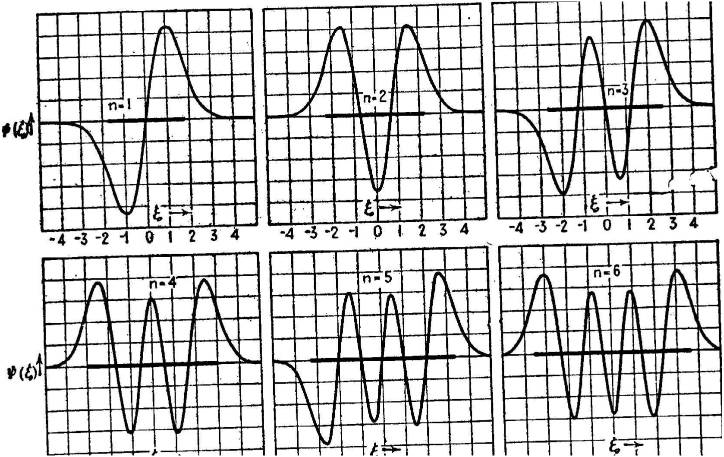
What does the ground state look like?

- $\psi_0(x) \sim e^{-\frac{1}{2}\alpha^2 x^2}$



(Pauling and Wilson)

What do other states look like?



(Pauling and Wilson)

(Extra) Playing God with Quantum Swing!

- Much cleaner way to derive energy levels...play God with Driac notation!
- Intrinsic length scale $x_o = \sqrt{\frac{\hbar}{m\omega}}$, momentum scale $p_o = \sqrt{\hbar m\omega}$
- Define *nondimensional operators* $\hat{X} = \frac{X}{x_o}$ and $\hat{P} = \frac{P}{p_o}$
- Hamiltonian $H = \hbar\omega\left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2\right)$
- Commutation relation $[\hat{X}, \hat{P}] = i$

(Extra) Playing God with Quantum Swing!

- *Define* annihilation operator $a = \frac{\hat{X}+i\hat{P}}{\sqrt{2}}$
- Creation operator: Hermitian conjugate $a^\dagger = \frac{\hat{X}-i\hat{P}}{\sqrt{2}}$
- Clearly $\hat{X} = \frac{a^\dagger + a}{\sqrt{2}}$ and $\hat{P} = \frac{a - a^\dagger}{\sqrt{2}i}$
- Commutation relation $[\hat{X}, \hat{P}] = i$ implies $[a, a^\dagger] = 1$
- Hamiltonian $H = \hbar\omega \left(\frac{1}{2}\hat{P}^2 + \frac{1}{2}\hat{X}^2\right) = \hbar\omega \left(a^\dagger a + \frac{1}{2}\right)$!!
- Clearly, H and $a^\dagger a$ have the same eigenvectors! Thus, if $a^\dagger a|\alpha\rangle = \alpha|\alpha\rangle$, $H|\alpha\rangle = \hbar\omega(\alpha + \frac{1}{2})|\alpha\rangle$
- Anticipating, lets us call $a^\dagger a = N$, a Hermitian operator

(Extra) Playing God with Quantum Swing!

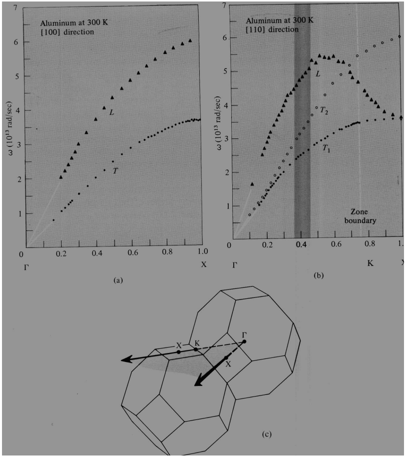
- Suppose, $N|\alpha\rangle = \alpha|\alpha\rangle$, what is $a|\alpha\rangle$?
- $Na|\alpha\rangle = a^\dagger aa|\alpha\rangle = (aa^\dagger - 1)a|\alpha\rangle = (\alpha - 1)a|\alpha\rangle$! This implies $a|\alpha\rangle = C|\alpha - 1\rangle$, with $C = \sqrt{\alpha}$! Annihilation operator!
- Similarly, $a^\dagger|\alpha\rangle = \sqrt{\alpha + 1}|\alpha + 1\rangle$! Creation operator!
- "Clearly": $a^m|\alpha\rangle = \sqrt{\alpha(\alpha - 1)(\alpha - 2)...(\alpha - (m - 1)}|\alpha - m\rangle$...this necessarily implies that α has to be a nonnegative integer! Thus $\alpha = 0, 1, 2$...etc. We have shown that the eigenvalues of N are nonnegative integers i. e., $N|n\rangle = n|n\rangle$!

(Extra) Playing God with Quantum Swing!

- $H = \hbar\omega\left(N + \frac{1}{2}\right), H|n\rangle = \underbrace{\hbar\omega\left(n + \frac{1}{2}\right)}_{E_n}|n\rangle$
- The ground state is $|0\rangle$...called "vacuum" state
- Any higher state can be generated from the ground state $|n\rangle = \frac{(a^\dagger)^n}{\sqrt{n!}}|0\rangle$
- Modern theory of solids is formulated using creation and annihilation operators, the number n being interpreted as the "number of particles"
- The above are called Bose operators (applicable to phonons); for electrons there are Fermi operators which satisfy *anti-commutation relations*!

Phonons in solids

- Quantized lattice vibrations! Phonon frequency depends on wavelength



Ashcroft and Mermin

Phonons, and other things

- Quantum mechanics explains specific heat anomaly (if $k_bT \ll \hbar\omega, C_v \sim e^{-\hbar\omega/k_bT}$, if $k_bT \gg \hbar\omega, C_v \sim k_b$ (Dulong-Petit)) Quantum alacrity!
- Can be used to understand molecular vibrations
- Quantum theory of light is developed in "exact analogy" with the theory of phonons...can show that light of frequency has energy levels $\hbar\omega(n+\frac{1}{2})$ where n is the number of photons...if you have large n you will have very intense light
- More interestingly this will tell you that "vacuum" in quantum mechanics is a VERY BUSY place!

Summary – Quantum Swing

- Energy levels go as $\left(n + \frac{1}{2}\right) \hbar\omega$
- There is a very nice way to do this using creation and annihilation operators
- Explains many things about materials – example specific heat anomaly
- Quantum swing is a very basic problem in physics, it will arise in one form or other in *many* problems