Nanophysics

(II - MSc PHYSICS - 3rd Semester)

Quantum Confinement

(Unit-I)

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Physics of Quantum Confinement

History: In 1970 Esaki & Tsu proposed fabrication of an artificial structure, consisting of alternating layers of 2 different semiconductors

Layer Thickness

$\approx$ 1 nm = 10 Å = 10^{-9} m $\equiv$ *SUPERLATTICE*

- ***PHYSICS:*** The ***main idea*** was that introduction of an ***artificial periodicity*** will "fold" the Brillouin Zones into smaller BZ's **$\equiv$ "mini-zones".**

$\Rightarrow$ The idea was that this would **raise the conduction band minima**, which is needed to observe novel physics and can be employed for some quantum and nano device applications.

- **Modern growth techniques** (starting in the 1980's), especially **MBE** & **MOCVD**, make fabrication of such structures possible!
- For the same reason, it is also possible to fabricate **many other kinds** of artificial structures on the scale of nm

(**nanometers**) ≡ **"Nanostructures"**

Superlattices = **"2 dimensional"** structures
Quantum Wells = **"2 dimensional"** structures
Quantum Wires = **"1 dimensional"** structures
Quantum Dots = ***"0 dimensional"*** structures!!

- Clearly, it is not only the electronic properties of materials which can be drastically altered in this way. Also, vibrational properties (phonons). Here, only electronic properties & only an overview!
- For many years, quantum confinement has been a fast growing field in both theory & experiment! It is at the forefront of current research!
- Note that I am not an expert on it!

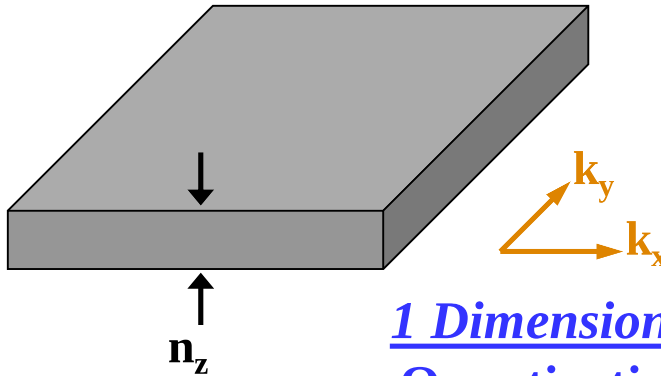
Quantum Confinement in Nanostructures: Overview

Electrons *Confined in 1 Direction*:

Quantum Wells (thin films):

⇒ **Electrons** can easily move in

***2 Dimensions*!**



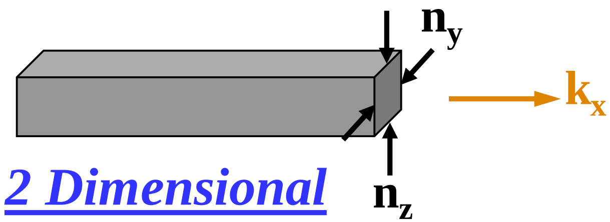
1 Dimensional
Quantization!

Electrons *Confined in 2 Directions*:

Quantum Wires:

⇒ **Electrons** can easily move in

***1 Dimension*!**



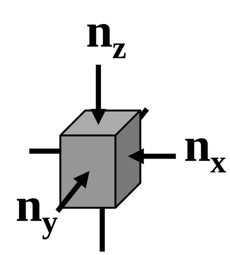
2 Dimensional
Quantization!

Electrons *Confined in 3 Directions*:

Quantum Dots:

⇒ **Electrons** can easily move in

***0 Dimensions*!**



3 Dimensional
Quantization!

Each further confinement direction changes a continuous k component to a discrete component characterized by a quantum number n.

- **PHYSICS:** Revisit the band structure
  - Consider the 1st Brillouin Zone for the infinite crystal. The maximum wave vectors are of the order

$$k_m \approx (\pi/a)$$

a = lattice constant. The potential **V** is periodic with period **a**. In the almost free e^- approximation, the bands are free e^- like except near the Brillouin Zone edge. That is, they are of the form:

$$E \approx (\hbar k)^2/(2m_o)$$

So, the **energy at the Brillouin Zone edge** has the form:

$$E_m \approx (\hbar k_m)^2/(2m_o)$$

or

$$E_m \approx (\hbar \pi)^2/(2m_o a^2)$$

PHYSICS

- ***SUPERLATTICES*** $\equiv$ Alternating layers of material. Periodic, with periodicity **L** (layer thickness). Let $\mathbf{k_z}$ = wavevector perpendicular to the layers.
- In a superlattice, the potential **V** has a ***new periodicity*** in the **z** direction with periodicity **L >> a**

$\Rightarrow$ In the **z** direction, the Brillouin Zone is much smaller than that for an infinite crystal. The maximum wavevectors are of the order: $\mathbf{k_s \approx (\pi/L)}$

$\Rightarrow$ At the BZ edge in the **z** direction, the energy has the form:

$$E_s \approx (\hbar\pi)^2/(2m_oL^2) + E_2(k)$$

$\mathbf{E_2(k)}$ = the 2 dimensional energy for **k** in the **x,y** plane.

Note that: $(\hbar\pi)^2/(2m_oL^2) << (\hbar\pi)^2/(2m_oa^2)$

Primary Qualitative Effects of Quantum Confinement

- Consider ***electrons confined along 1 direction*** (say, **z**) to a layer of width **L:**

Energies

- The ***energy bands are quantized*** (instead of continuous) in k_z & shifted **upward.** So **k_z is quantized:**

$$k_z = k_n = [(n\pi)/L],\ n = 1, 2, 3$$

- So, in the effective mass approximation (**m***)**,** ***the bottom of the conduction band is quantized*** (like a particle in a **1 d** box) & shifted:

$$E_n = (n\hbar\pi)^2/(2m^*L^2)$$

- ***Energies are quantized!*** Also, the ***wavefunctions are 2 dimensional Bloch functions*** (***traveling waves***) for **k** in the **x,y** plane & ***standing waves in the z direction*****.**

Quantum Confinement Terminology

Quantum Well ≡ QW

= A single layer of material **A** (layer thickness **L**), sandwiched between 2 **macroscopically large layers** of material **B**. Usually, the bandgaps satisfy:

$$E_{gA} < E_{gB}$$

Multiple Quantum Well ≡ MQW

= Alternating layers of materials **A** (thickness **L**) & **B** (thickness **L′**). In this case:

$$L' >> L$$

So, the e^- & e^+ in one **A** layer are independent of those in other **A** layers.

Superlattice ≡ SL

= Alternating layers of materials **A** & **B** with similar layer thicknesses.

Brief Elementary Quantum Mechanics & Solid State Physics Review

- **Quantum Mechanics of a Free Electron:**
  - The **energies are continuous**: $E = (\hbar k)^2/(2m_o)$ (1d, 2d, or 3d)
  - The **wavefunctions are traveling waves**:

$$\psi_k(x) = A\, e^{ikx} \quad \text{(1d)} \qquad\qquad \psi_k(\mathbf{r}) = A\, e^{i\mathbf{k}\bullet\mathbf{r}} \quad \text{(2d or 3d)}$$

- **Solid State Physics: Quantum Mechanics of an Electron in a Periodic Potential in an infinite crystal :**
  - The **energy bands are (approximately) continuous**: $E = E_{nk}$
  - At the bottom of the conduction band or the top of the valence band, in the effective mass approximation, **the bands can be written:**

$$E_{nk} \cong (\hbar k)^2/(2m^*)$$

  - The **wavefunctions are Bloch Functions = *traveling waves***:

$$\Psi_{nk}(\mathbf{r}) = e^{i\mathbf{k}\bullet\mathbf{r}}\, u_{nk}(\mathbf{r});\quad u_{nk}(\mathbf{r}) = u_{nk}(\mathbf{r}+\mathbf{R})$$

Some Basic Physics

- **Density of states** (DoS)

$$DoS = \frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE}$$

in 3D:

$$N(k) = \frac{\text{k space vol}}{\text{vol per state}}$$

$$= \frac{4/3\,\pi k^3}{(2\pi)^3/V}$$

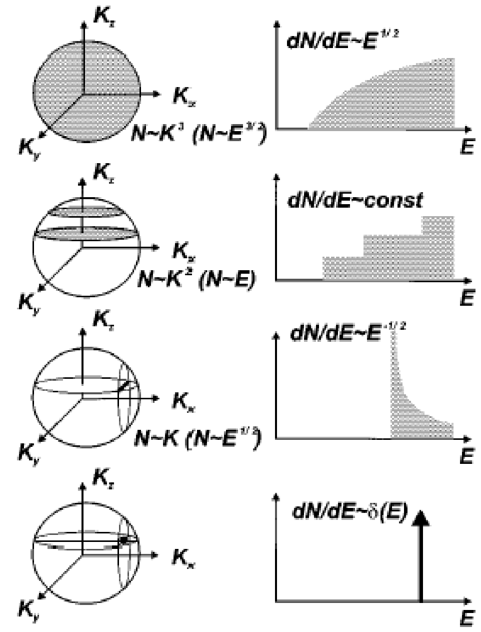


Fig. 1. Density of states for charge carriers in structures with different dimensionalities.

Structure	Degree of Confinement	$\frac{dN}{dE}$
Bulk Material	0D	$\sqrt{E}$
Quantum Well	1D	1
Quantum Wire	2D	$1/\sqrt{E}$
Quantum Dot	**3D**	**$\delta(E)$**

QM Review: The 1D (infinite) Potential Well
("particle in a box")

- We want to solve the **Schrödinger Equation for:**

  $x < 0,\ V \to \infty\ ;\ 0 < x < L,\ V = 0;\ x > L,\ V \to \infty$

  $$\Rightarrow -[\hbar^2/(2m_o)](d^2\psi/dx^2) = E\psi$$

- Boundary Conditions:

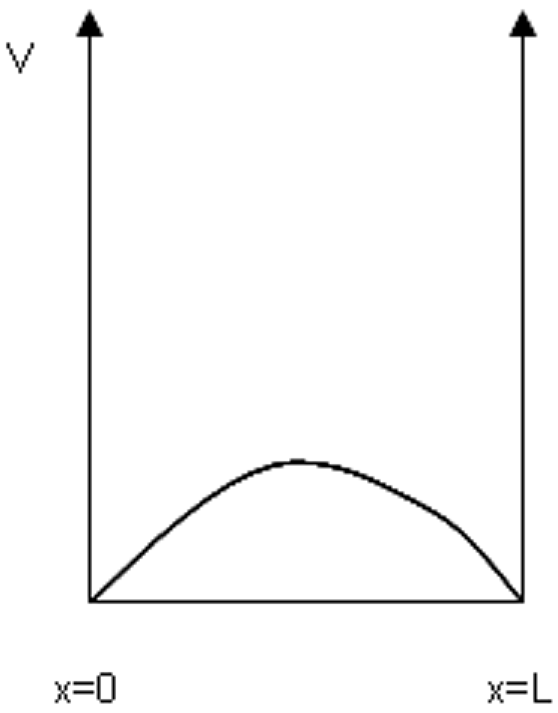
  $\psi = 0$ at $x = 0$ & $x = L$ ($V \to \infty$ there)

- Energies:

  $$E_n = (\hbar n\pi)^2/(2m_oL^2), \quad n = 1,2,3$$

  Wavefunctions:

  $$\psi_n(x) = (2/L)^{1/2}\sin(n\pi x/L)$$ (a standing wave!)



Qualitative Effects of Quantum Confinement:

Energies are quantized & ψ changes from a traveling wave to a **standing wave**.

In 3Dimensions…

- For the **3D infinite potential well**:

$$\Psi(x, y, z) \sim \sin(\frac{n\pi x}{L_x})\sin(\frac{m\pi y}{L_y})\sin(\frac{q\pi z}{L_z}),\ \text{n, m, q} = \text{integer}$$

$$\text{Energy levels} = \frac{n^2h^2}{8mL_x^{\ 2}} + \frac{m^2h^2}{8mL_y^{\ 2}} + \frac{q^2h^2}{8mL_z^{\ 2}}$$

Real Quantum Structures aren't this simple!!

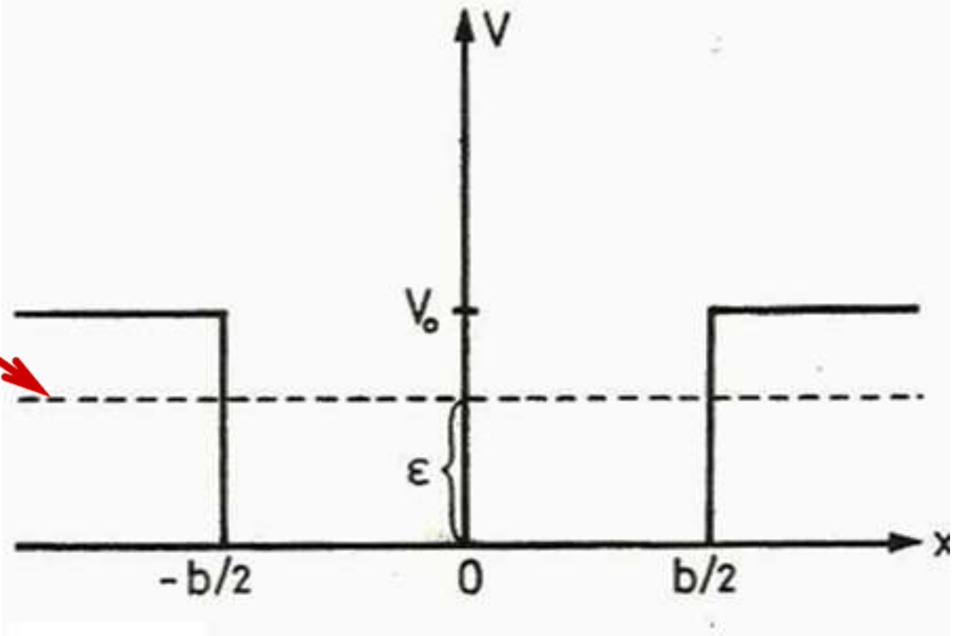
- In **Superlattices & Quantum Wells,** the potential barrier is obviously not infinite!
- In **Quantum Dots**, there is usually ~ **spherical confinement**, not rectangular.
- The simple problem only considers a single electron. But, in **real structures, there are many electrons** & also **holes!**
- Also, there is often **an effective mass mismatch** at the boundaries. That is ***the boundary conditions we've used are too simple***!

QM Review: The 1d (finite) Rectangular Potential Well

In most QM texts!! Analogous to a Quantum Well

- We want to solve the Schrödinger Equation for:

We want bound states: **$\varepsilon < V_o$**



Rectangular potential well

$$[-\{\hbar^2/(2m_o)\}(d^2/dx^2) + V]\psi = \varepsilon\psi \quad (\varepsilon \equiv E)$$

$$V = 0,\ -(b/2) < x < (b/2); \qquad V = V_o \text{ otherwise}$$

Solve the Schrödinger Equation:

$$[-\{\hbar^2/(2m_o)\}(d^2/dx^2) + V]\psi = \varepsilon\psi$$

$(\varepsilon \equiv E)$ $V = 0$, $-(b/2) < x < (b/2)$

$V = V_o$ **otherwise**

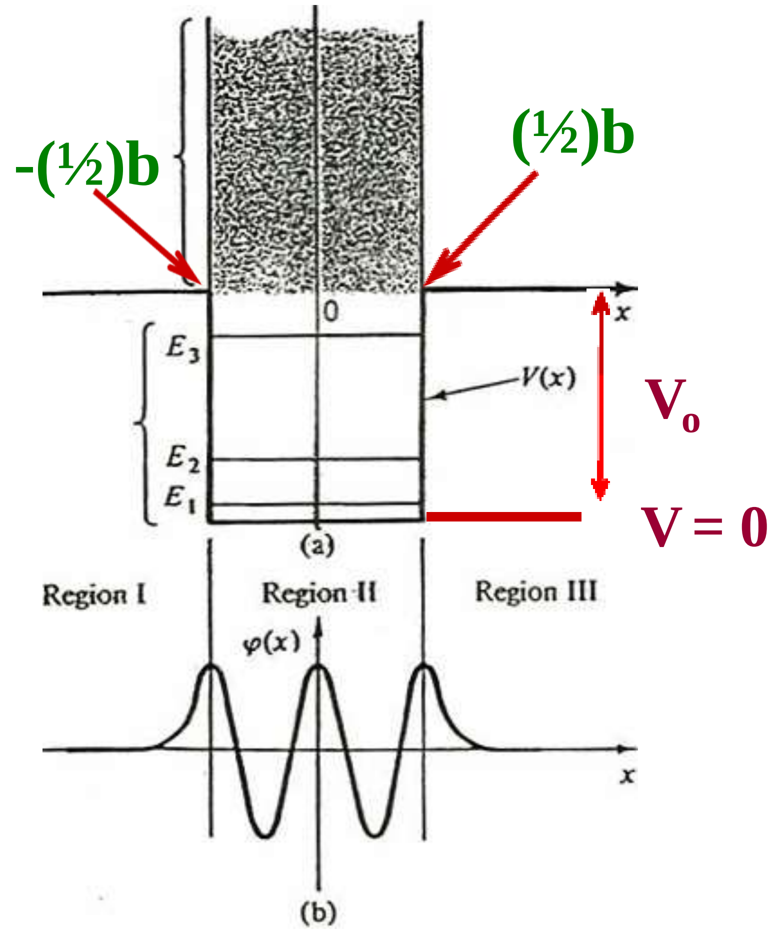
Bound states are in Region II

Region II:

$\psi(x)$ **is *oscillatory***

Regions I & III:

$\psi(x)$ **is *decaying***



Finite rectangular potential well. (a) The potential function $V(x)$ and energy spectrum. (b) Typical structure of a bound eigenstate. Function oscillates in region II where kinetic energy is positive and decays in regions I and III, where kinetic energy is negative.

The 1d (finite) rectangular potential well

A brief math summary!

Define: $\alpha^2 \equiv (2m_o\varepsilon)/(\hbar^2)$; $\beta^2 \equiv [2m_o(\varepsilon - V_o)]/(\hbar^2)$

The Schrödinger Equation becomes:

$$(d^2/dx^2)\,\psi + \alpha^2\psi = 0, \quad -(\tfrac{1}{2})b < x < (\tfrac{1}{2})b$$

$$(d^2/dx^2)\,\psi - \beta^2\psi = 0, \quad \text{otherwise.}$$

⇒ **Solutions:**

$\psi = C\exp(i\alpha x) + D\exp(-i\alpha x)$, $\quad -(\tfrac{1}{2})b < x < (\tfrac{1}{2})b$

$\psi = A\exp(\beta x)$, $\quad x < -(\tfrac{1}{2})b$

$\psi = A\exp(-\beta x)$, $\quad x > (\tfrac{1}{2})b$

Boundary Conditions:

⇒ ψ & $d\psi/dx$ are continuous **SO:**

- Algebra (2 pages!) leads to:

$$(\varepsilon/V_o) = (\hbar^2\alpha^2)/(2m_oV_o)$$

ε, α, β are related to each other by transcendental equations. For example:

$$\tan(\alpha b) = (2\alpha\beta)/(\alpha^2 - \beta^2)$$

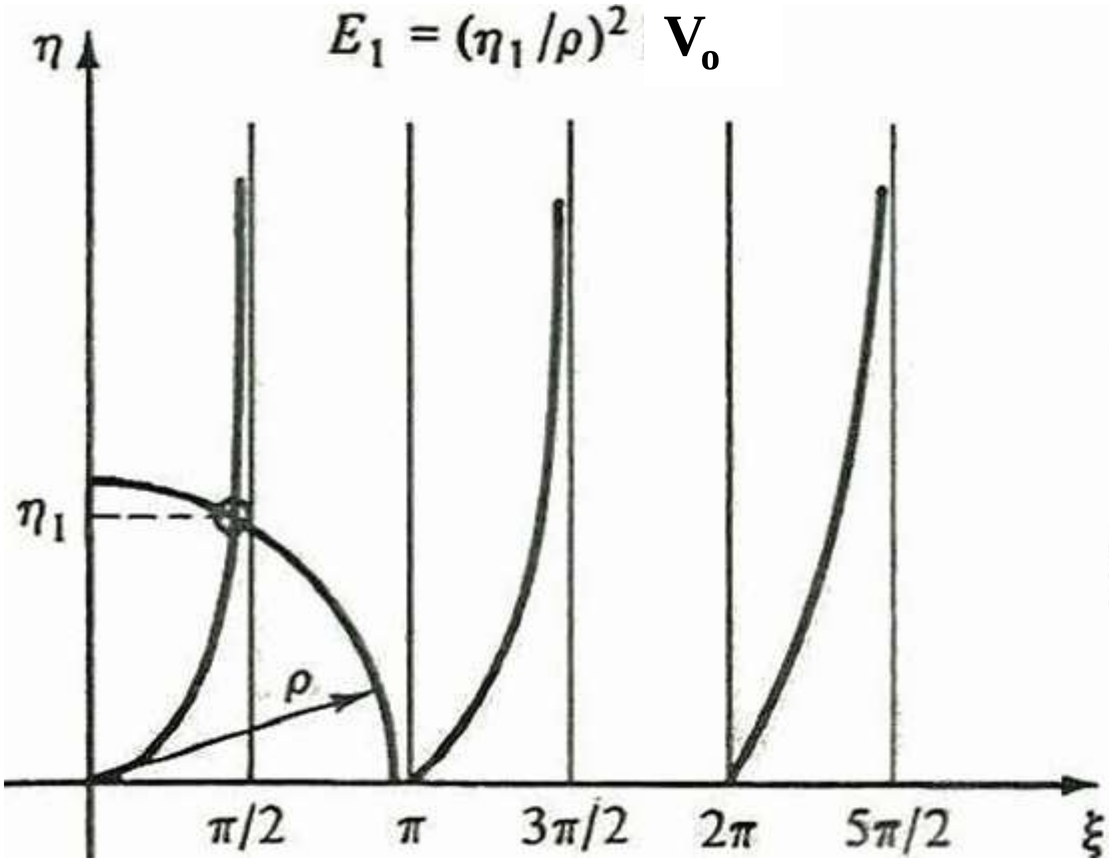
- Solve graphically or numerically.

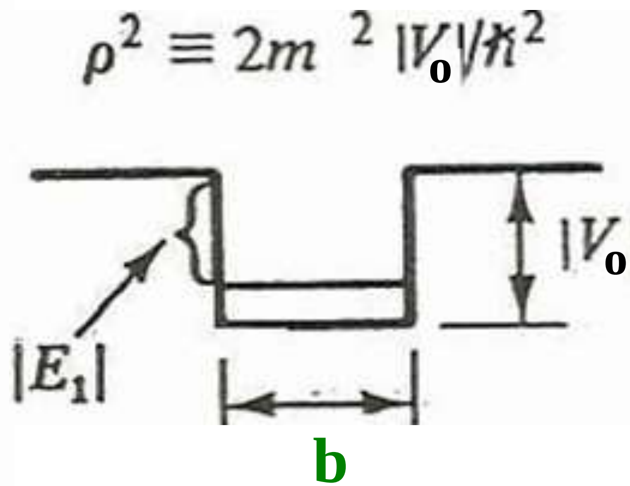
- **Get:** ***Discrete Energy Levels*** in the well

  (a finite number of finite well levels!)

- **Even eigenfunction** solutions (a finite number):

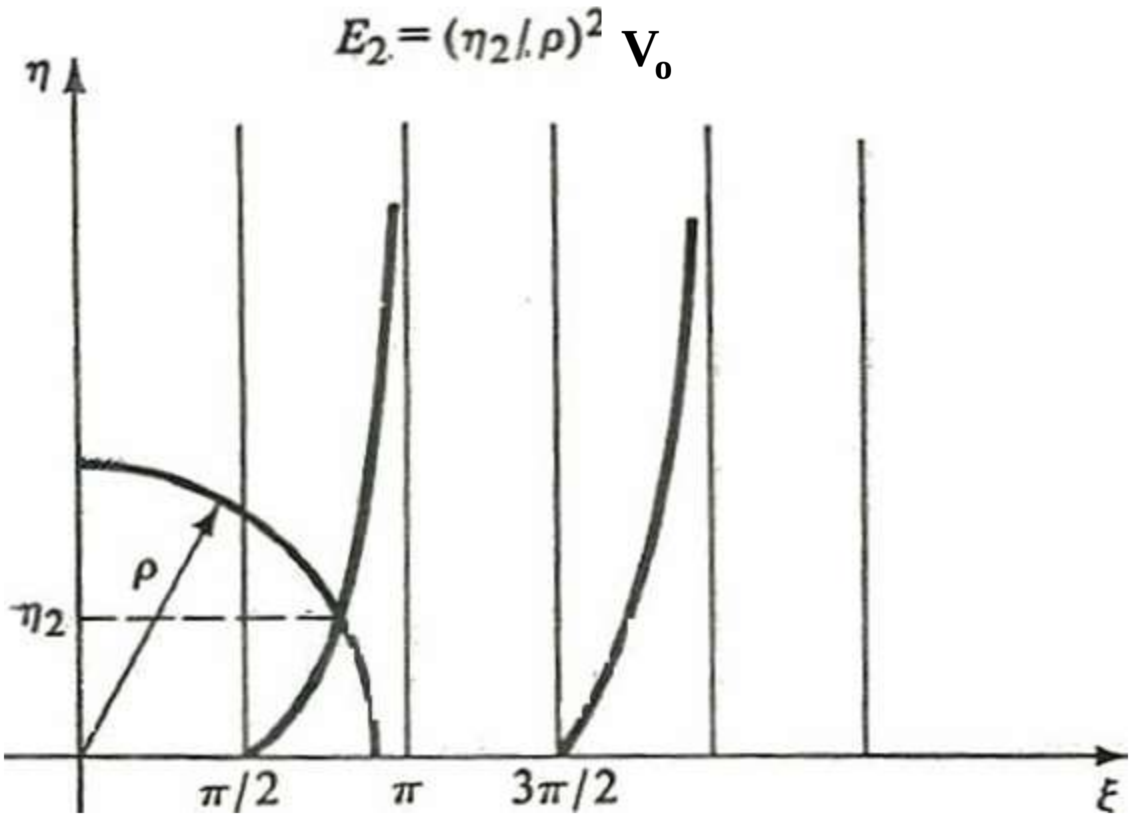
Circle, $\xi^2 + \eta^2 = \rho^2$, **crosses** $\eta = \xi \tan(\xi)$

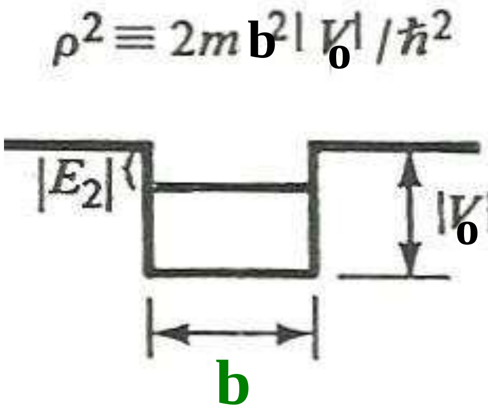




- **Odd eigenfunction** solutions:

Circle, $\xi^2 + \eta^2 = \rho^2$, crosses $\eta = -\xi \cot(\xi)$





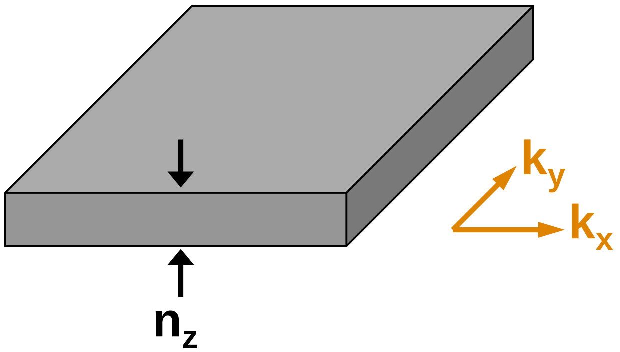
$$|E_2| < |E_1|$$

Quantum Confinement in Nanostructures

Confined in:

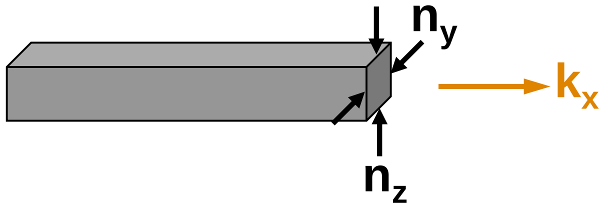
1 Direction: Quantum well (thin film)

Two-dimensional electrons



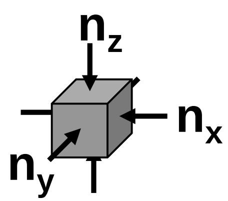
2 Directions: Quantum wire

One-dimensional electrons



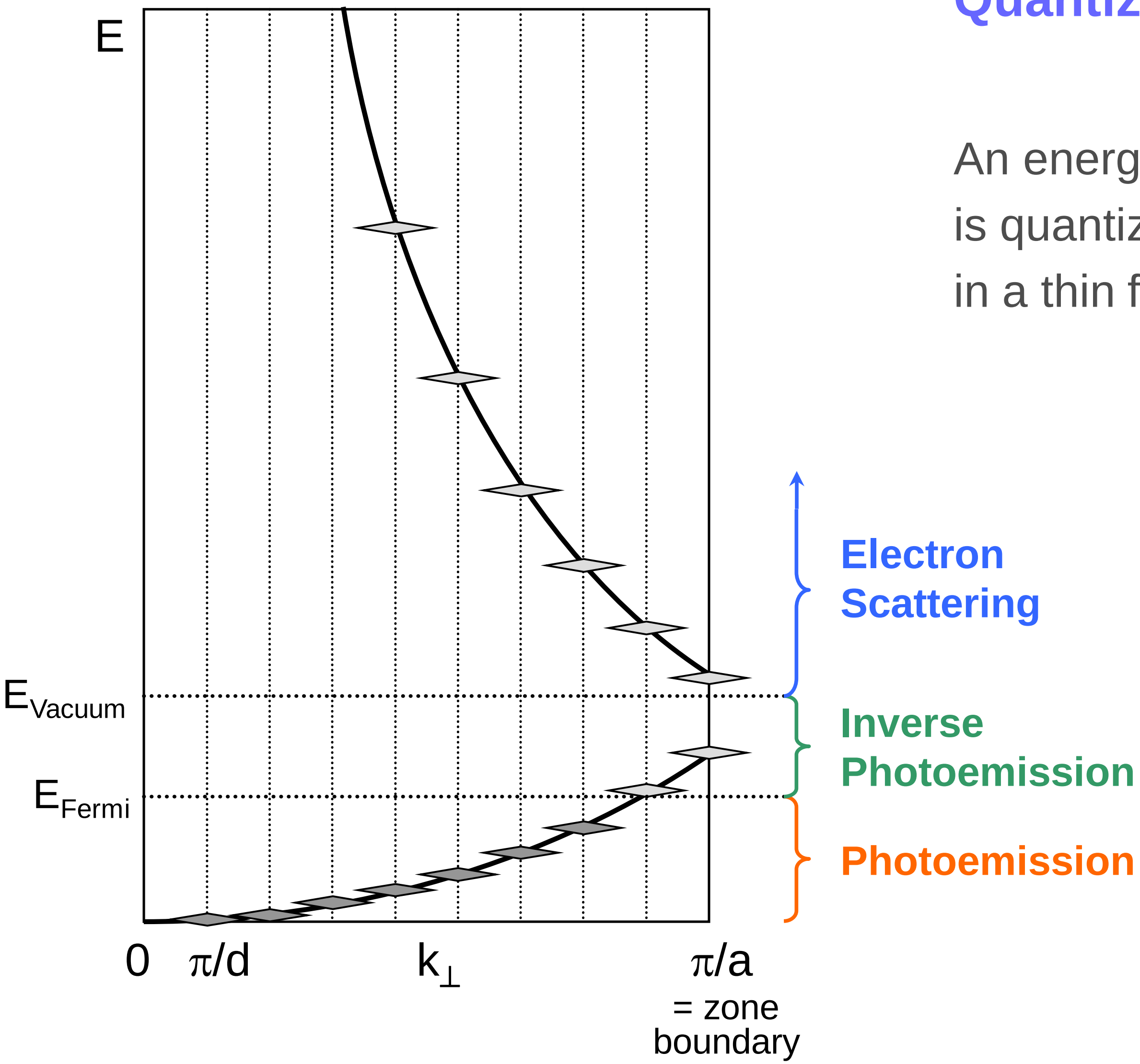
3 Directions: Quantum dot

Zero-dimensional electrons

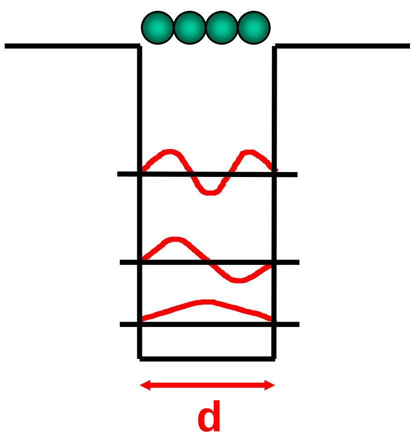


Each confinement direction converts a continuous k in a discrete quantum number n.

Quantization in a Thin Crystal



An energy band with continuous k is quantized into N discrete points k_n in a thin film with N atomic layers.



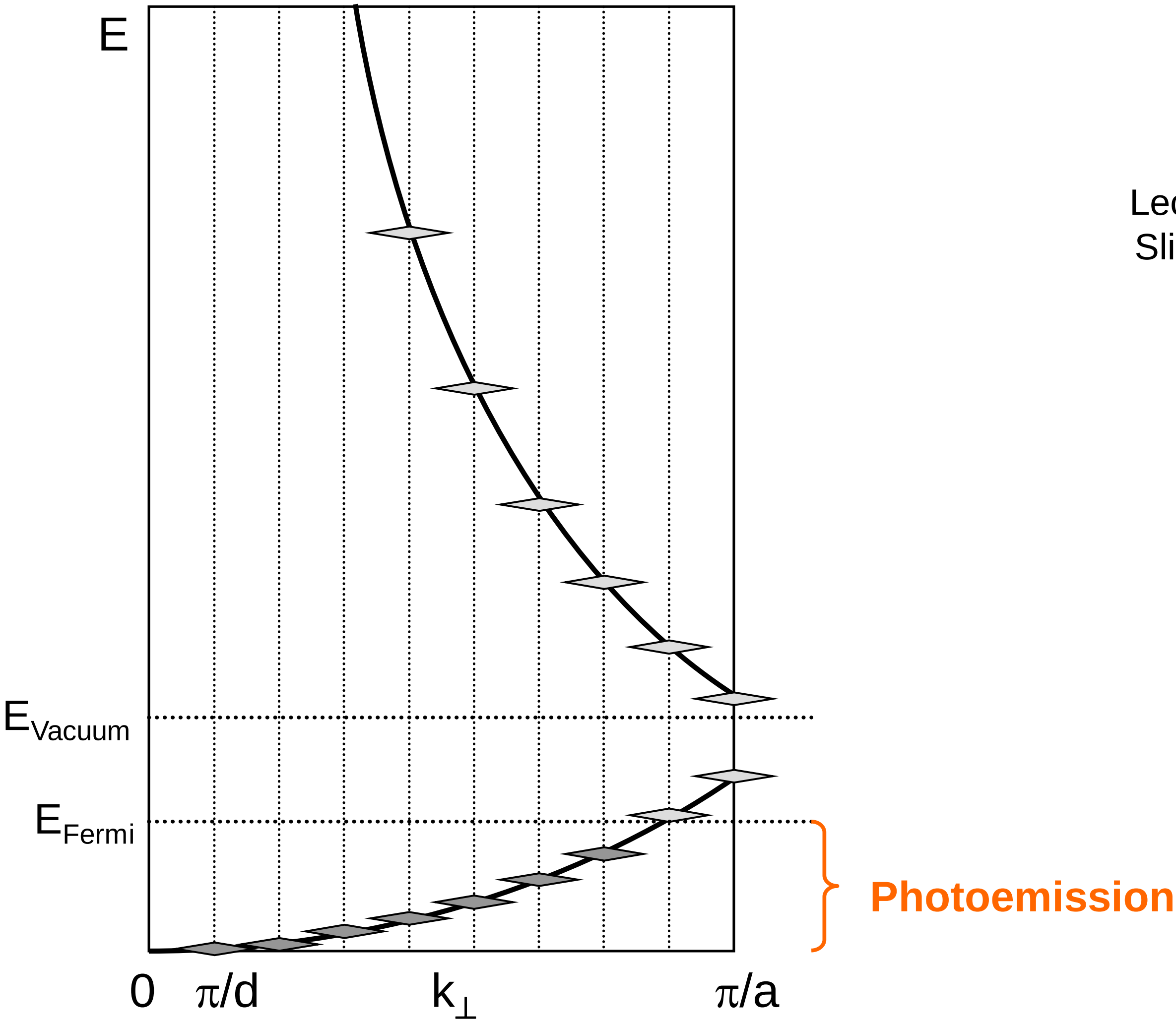
N atomic layers with the spacing $a = d/n$

N quantized states with $k_n \approx n \cdot \pi/d \quad (n = 1,\ldots,N)$

$$\lambda_n = 2d / n$$

$$k_n = 2\pi / \lambda_n = n \cdot \pi/d$$

Quantization in Thin Graphite Films



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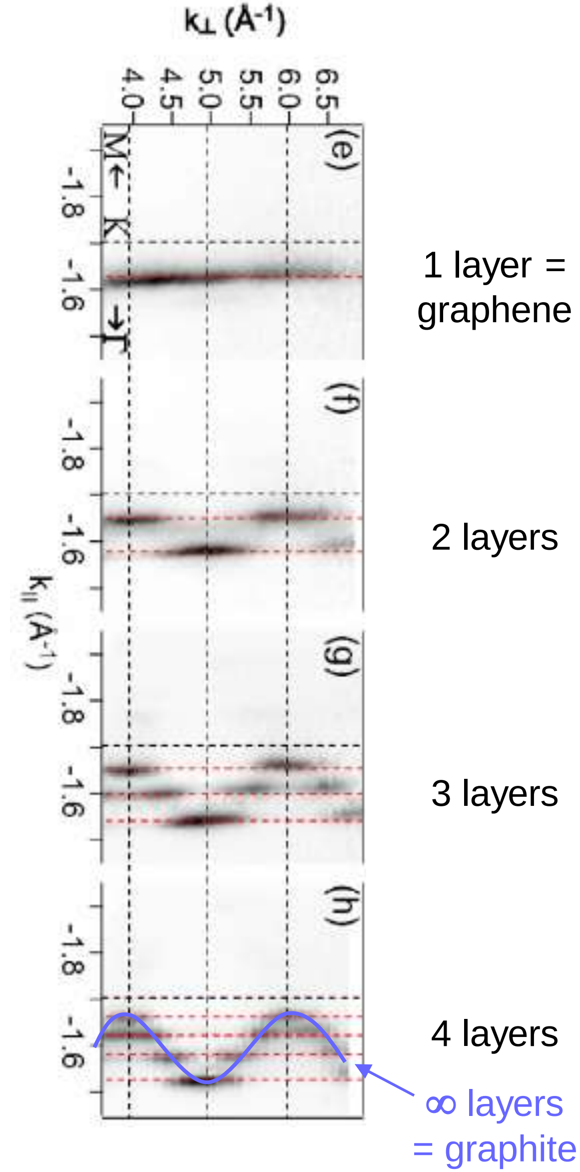

N atomic layers with spacing a = d/n :

$\Rightarrow$ N quantized states with $k_n \approx N \cdot \pi/d$

The Important Electrons in a Metal

Energy $\approx$ E_{Fermi}

Energy Spread $\approx$ 3.5 $k_B T$

Transport (conductivity, magnetoresistance, screening length, ...)

Width of the Fermi function:

FWHM $\approx$ 3.5 $k_B T$

Phase transitions (superconductivity, magnetism, ...)

Superconducting gap:

$E_g \approx 3.5\, k_B T_c$ (T_c= critical temperature)