The Bandstructure Problem

A One-Dimensional Model ("easily generalized" to 3D!)

Bandstructure Problem:

A One Dimensional Model

- **One e^- Hamiltonian:** $H = (p)^2/(2m_o) + V(x)$

$p \equiv -i\hbar(\partial/\partial x)$, $V(x) \equiv V(x + a) \equiv$ **Effective Potential**.

- **V** has translational symmetry with repeat distance = **a**.
- ***GOAL: Solve the Schrödinger Equation:***

$H\psi_k(x) = E_k\psi_k(x)$, **k** ≡ Eigenvalue Label

E_k = **Electronic Energy** of the e^- in state **k**

$\psi_k(x)$ = **Wavefunction** of the e^- in state **k**

- Define a ***Translation operator*** ≡ **T**.

T is defined, for any function **f(x)**, as

$$T\,f(x) \equiv f(x + a)$$

- Now consider the ***Translation Operator*** **T** for this one dimensional solid: $\mathbf{T}\, f(x) \equiv f(x+a)$
- Take the **special case** for which $f(x) = \psi_k(x)$
  - That is, for $f(x)$ = an eigenfunction solution of the Schrödinger Equation
- Definition of **T**: $\mathbf{T}\,\psi_k(x) = \psi_k(x+a)$ (1)
- Look for the eigenvalues of **T**:

$$\mathbf{T}\,\psi_k(x) \equiv \lambda_k \psi_k(x) \qquad (2)$$

$\lambda_k \equiv$ Eigenvalue of **T**. It can be shown using (1) & (2) that:

$$\lambda_k \equiv e^{ika} \textit{ and } \psi_k(x) \equiv e^{ikx}\, u_k(x)$$

With $u_k(x) \equiv u_k(x+a)$

(see Kittel's book for proof)

- **This Shows:** The translation operator applied to an eigenfunction of the Schrödinger Equation (or of Hamiltonian **H**, with a periodic potential) gives:

$$T\psi_k(x) = e^{ika}\,\psi_k(x)$$

$$\Rightarrow \psi_k(x) \textit{ is also an eigenfunction of the translation operator } T!$$

- **This also shows** that the general form of $\psi_k(x)$ is

$$\psi_k(x) = e^{ikx}\,u_k(x), \text{ where } u_k(x) = u_k(x+a)$$

$$u_k(x) = \textit{a periodic function with the same period as the potential!}$$

- ***In other words*:** For a periodic potential **V(x)**, with period **a**, $\psi_k(x)$ **is *a simultaneous eigenfunction* of the translation operator T *and* the Hamiltonian H.**
- **The Commutator Theorem** of QM tells us that this is equivalent to **[T,H] = 0.** The commutator of **T** & **H** vanishes; they commute!

$\Rightarrow$ ***They share a set of eigenfunctions*.**

- ***In other words*:** The eigenfunction (electron wavefunction!) in a periodic crystal has the form:

$$\psi_k(x) = e^{ikx}\, u_k(x) \text{ with } u_k(x) = u_k(x+a)$$

$\equiv$ "*Bloch's Theorem*"

Bloch's Theorem:

From Translational Symmetry

- For a periodic potential **V(x)**, the eigenfunctions of **H** (wavefunctions of the e^-) have the form:

$$\psi_k(x) = e^{ikx}\, u_k(x) \text{ with } u_k(x) = u_k(x+a)$$

$$\equiv \text{“}\textit{Bloch Functions}\text{”}$$

- ***Recall***, for a free e^-, the wavefunctions have the form:

$$\psi^f_k(x) = e^{ikx} \quad \text{(a plane wave)}$$

$\Rightarrow$ A ***Bloch Function*** is the generalization of a plane wave for an e^- in periodic potential. It is a plane wave modulated by a periodic function $u_k(x)$ (with the same period as $V(x)$).

Bandstructure: A One Dimensional Model

- So, the wavefunctions of the e^- in a perfect, periodic crystal ***MUST*** have the ***Bloch Function*** form:

$$\psi_k(x) = e^{ikx}u_k(x), \quad u_k(x) = u_k(x + a) \qquad (1)$$

- This is easily generalized to & proven in 3 D!!
- Label the eigenfunctions & eigenvalues (E_k) by the wavenumber **k:**

$p = \hbar k \equiv$ the e^- **"Quasi-Momentum"** or **"Crystal Momentum".**

Bandstructure: A One Dimensional Model

- The e^- wavefunctions in a perfect, periodic crystal are ***Bloch Functions***:

$$\psi_k(x) = e^{ikx}u_k(x),\ u_k(x) = u_k(x+a) \quad (1)$$

$p = \hbar k \equiv e^-$ "Quasi-Momentum"

or **"Crystal Momentum".**

$p = \hbar k =$ Electron Momentum

for ***FREE*** e^-s ***ONLY!***

Bandstructure: A One Dimensional Model

- Free e^- wavefunctions are plane waves: $\psi^f_k(x) = e^{ikx}$ which are also eigenfunctions of the momentum operator $p \equiv -i\hbar(\partial/\partial x)$ with eigenvalue $\hbar k$.
- By contrast, the wavefunctions for e^- 's in bands are ***Bloch Functions*** (see (1) on previous slide!) which are ***NOT*** eigenfunctions of the momentum operator.
- The e^- momentum for a **Bloch Electron** state $\psi_k(x)$ is the QM expectation value of the momentum operator in that state:

$$\langle p \rangle = \langle \psi_k(x) | p | \psi_k(x) \rangle \equiv \textit{Integral of } [\{\psi_k(x)\}^* p\{\psi_k(x)\}] \textit{ over all } x \neq \hbar k$$

- **The Schrödinger Equation** for an electron in a periodic potential is:

$$H\psi_k(x) = E_k\psi_k(x)$$

$\psi_k(x)$ must have the ***Bloch Function*** form:

$$\psi_k(x) = e^{ikx}u_k(x), \quad u_k(x) = u_k(x + a)$$

$E_k \equiv$ ***The Electronic "Bandstructure".***

- One way to plot E_k is in

The "Extended Zone Scheme"

$\equiv$ A plot of E_k with no restriction on **k**

$E_k \equiv$ *The Electronic "Bandstructure"*

- The wavefunctions $\psi_k(x)$ must be

Bloch Functions:

$$\psi_k(x) = e^{ikx}u_k(x), \quad u_k(x) = u_k(x + a) \quad (1)$$

- Another way to plot E_k is to first consider the **Bloch Function** in **(1)** & look at the identity:

$$\exp[i\{k + (2\pi n/a)\}a] \equiv \exp[ika] \text{ (integer } n\text{)}$$

$\Rightarrow$ The label **k** & the label **[k + (2πn/a)]**

give the same $\psi_k(x)$ (& the ***same energy***)!

$E_k \equiv$ ***The Electronic "Bandstructure"***

- In other words,

Translational symmetry in the lattice

$\Rightarrow$ ***Translational symmetry in the Reciprocal Lattice!***

- So, we can plot E_k **vs.** **k** & restrict **k** to the range

$$-(\pi/a) < k < (\pi/a) \equiv$$

"The First Brillouin Zone" **(BZ)**

(**k** outside this range gives redundant information!)

≡ The *"Reduced Zone Scheme"*

Bandstructure: E versus k

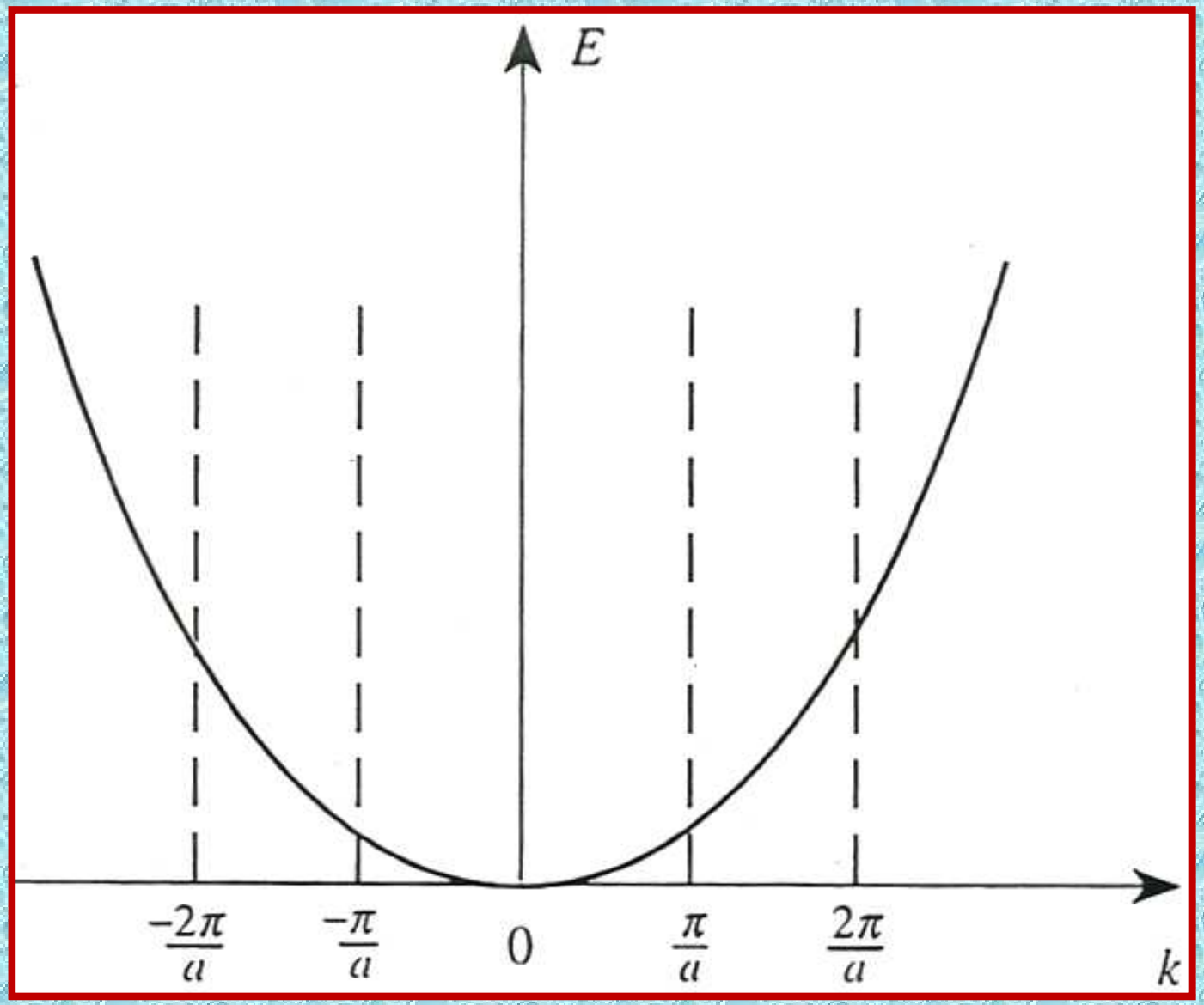
Example Illustration

- The **Extended & Reduced Zone Schemes** in 1d with the free electron energy:

$$E_k = (\hbar^2 k^2)/(2m_o)$$

- **Note:** Obviously, for free e^-'s there are ***no bands***! In what follows, the 1d lattice symmetry (with period **a**) is imposed onto the free e^- parabola.

Free e^- "bandstructure" in the 1d ***Extended Zone*** scheme: $E_k = (\hbar^2 k^2)/(2m_o)$



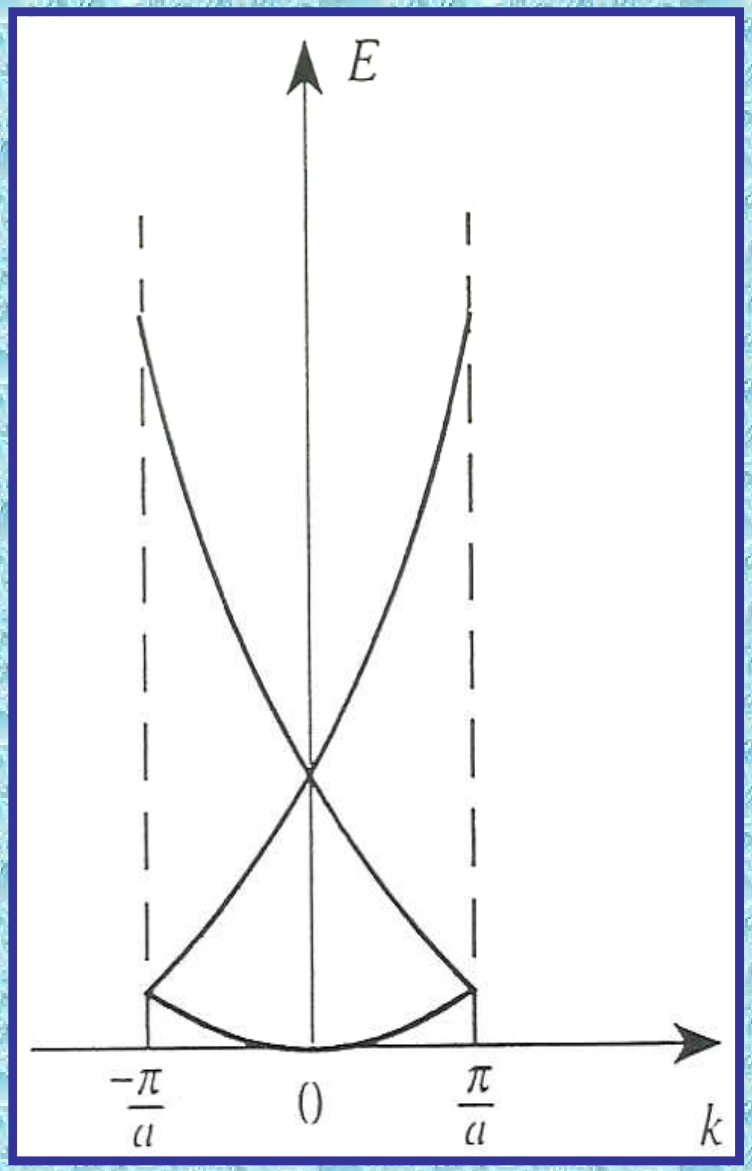
Free e^- "bandstructure" in the 1d ***Reduced Zone*** scheme: $E_k = (\hbar^2 k^2)/(2m_o)$

- For **k** outside the 1st BZ, take E_k & translate it into the 1st BZ by adding a reciprocal lattice Vector:

  $\pm(\pi n/a)$ to **k**

- That is, use the translational symmetry in **k**-space just discussed.

$\pm(\pi n/a) \equiv$ ***"Reciprocal Lattice Vector"***



Bandstructure: Now, illustrate these concepts with an ***EXACT*** 1d model calculation (Kittel Ch. 7)

The Krönig-Penney Model

Developed in the 1930's.

- Discussed in detail in ***MANY*** Solid State Physics & Quantum Mechanics books.

Why do this simple model?

- It's solution contains ***MANY*** features of real, 3d bandstructures! The results are "easily" understood. The math can be done exactly. We won't do this in class. It is in many books, including Kittel!

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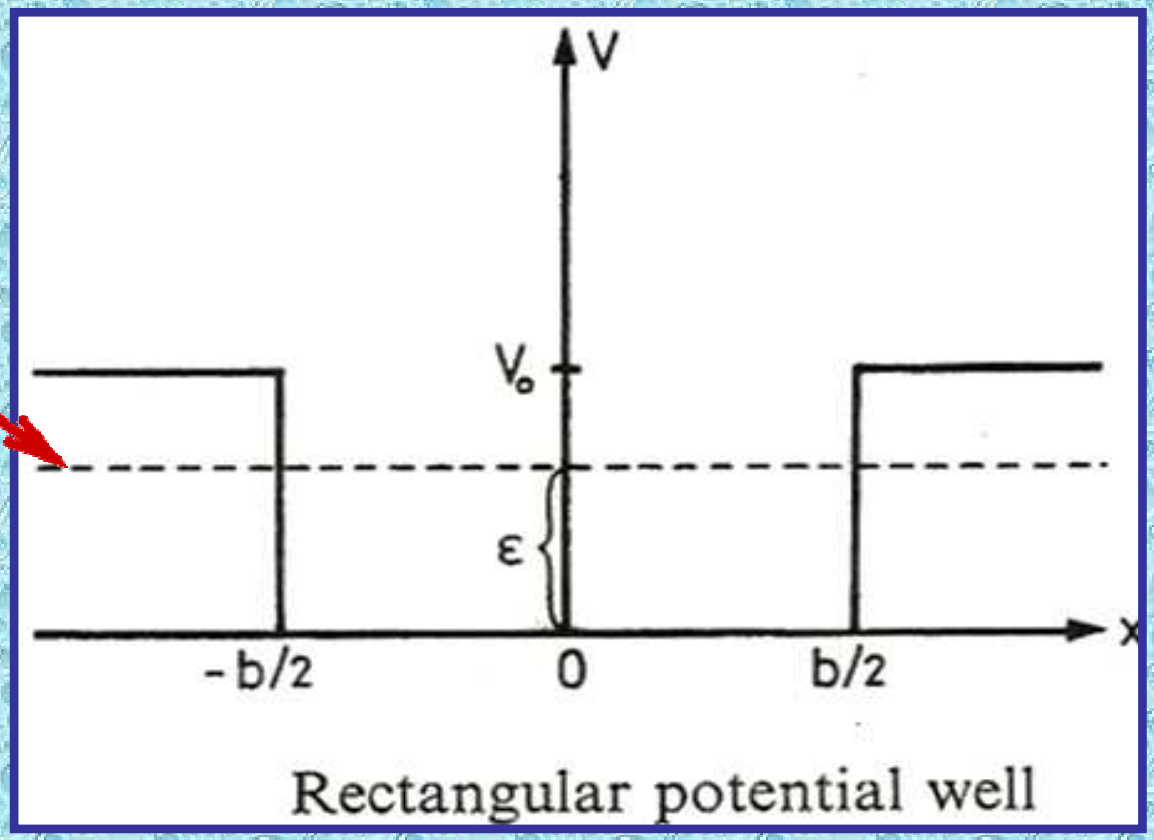
21st Century Reason to do this simple model!

It can be used as a prototype for the understanding of artificial semiconductor structures called Superlattices!

First, a QM Review: The 1d (finite) Rectangular Potential Well. Discussed in most QM texts!!

- We want to solve the Schrödinger Equation for:

We want bound states: $\varepsilon < V_o$



Rectangular potential well

The Schrödinger Equation

↓

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

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

Solve the Schrödinger Equation:

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

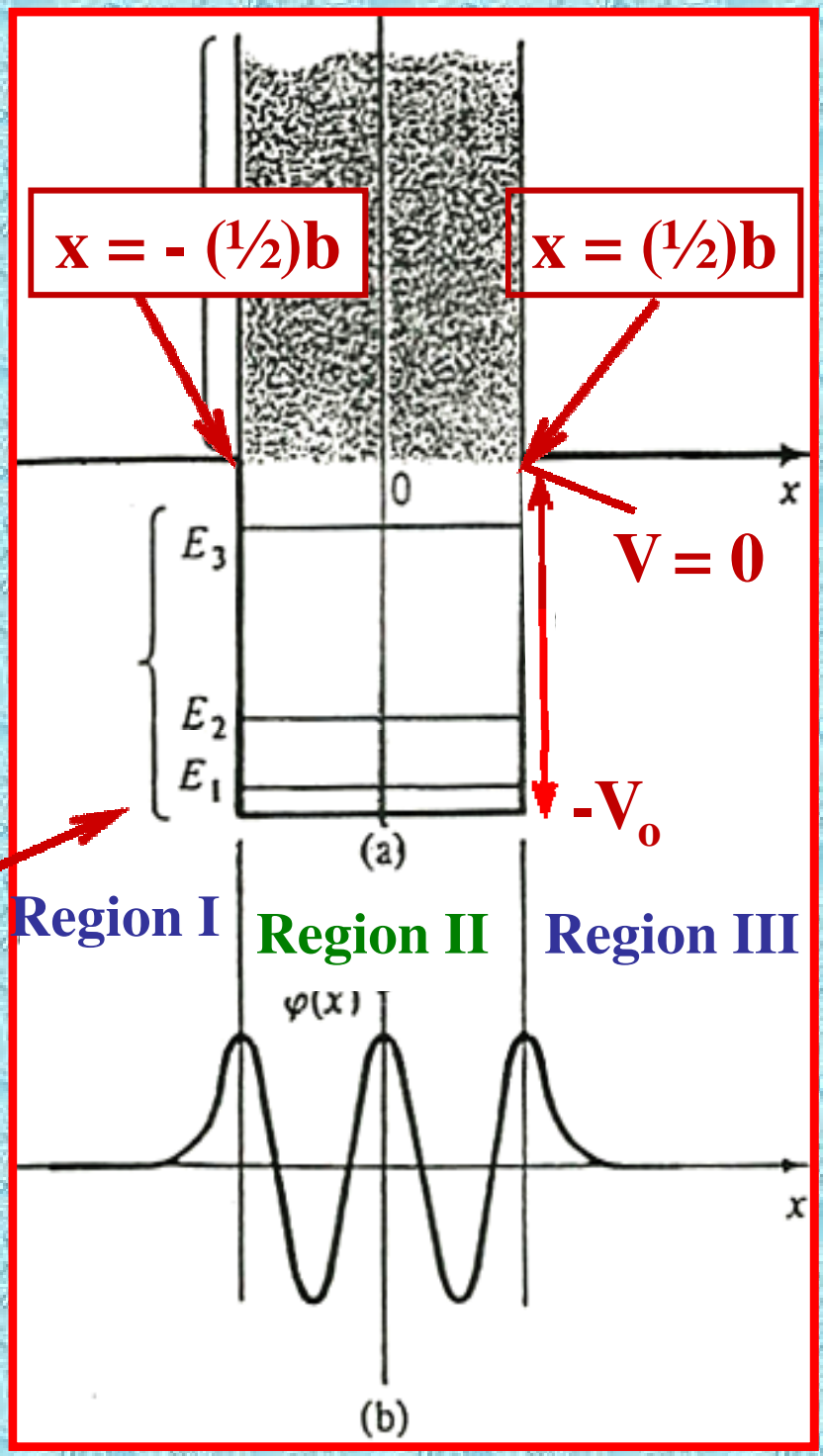
$(\varepsilon \equiv E)$ $V = 0$, $-(b/2) < x < (b/2)$

$V = V_o$ otherwise

Bound States 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:**

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

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

- **Solutions:**

$$\psi = Ce^{(i\alpha x)} + De^{(-i\alpha x)}, \quad -(1/2)b < x < (1/2)b$$

$$\psi = Ae^{(\beta x)}, \quad x < -(1/2)b$$

$$\psi = Ae^{(-\beta x)}, \quad x > (1/2)b$$

Boundary Conditions:

$\Rightarrow \psi$ & $d\psi/dx$ are continuous. So:

- **Algebra** (2 pages!) leads to:

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

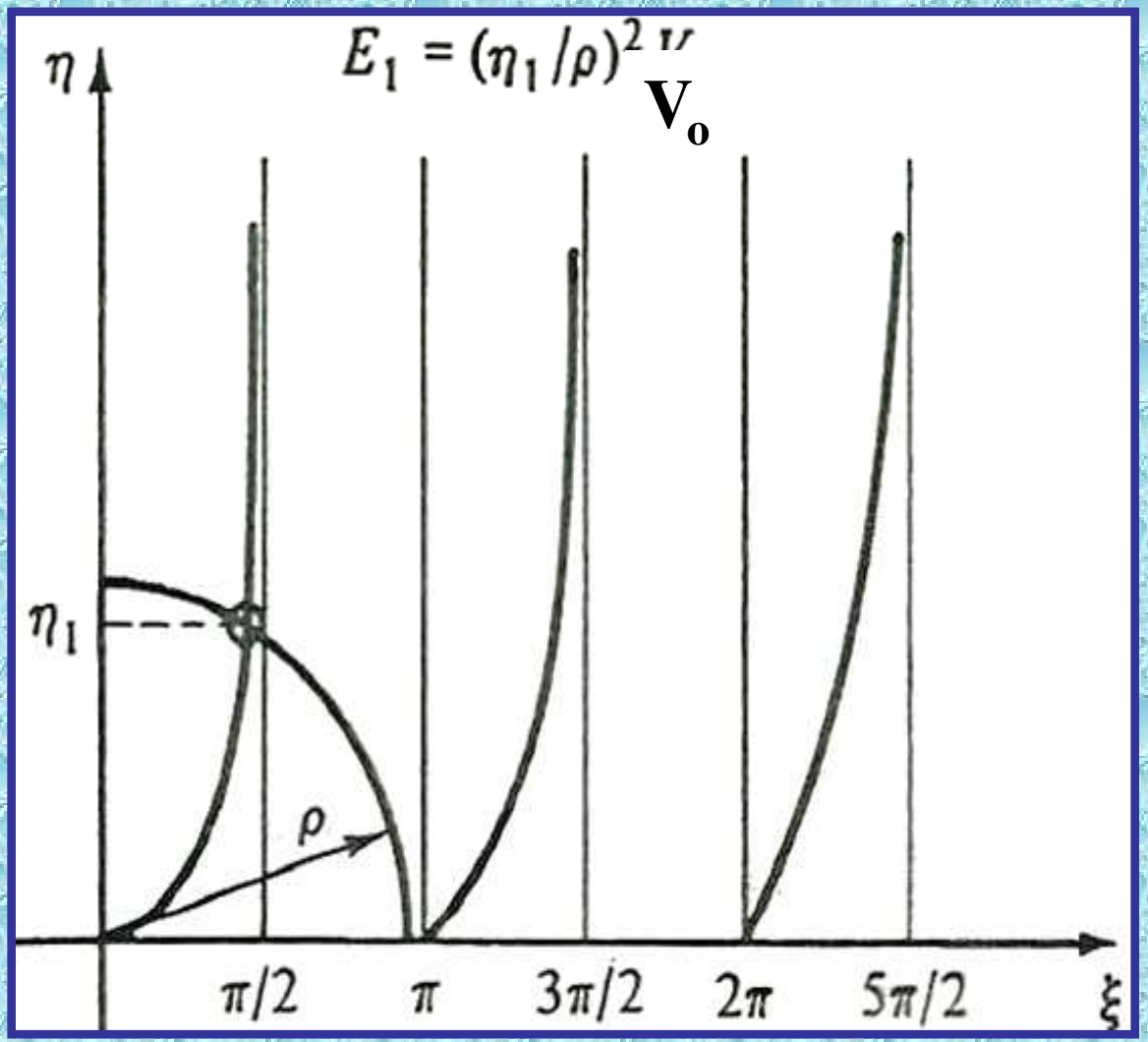
- **ε, α, β** are related to each other by transcendental equations.
- **For Example:**

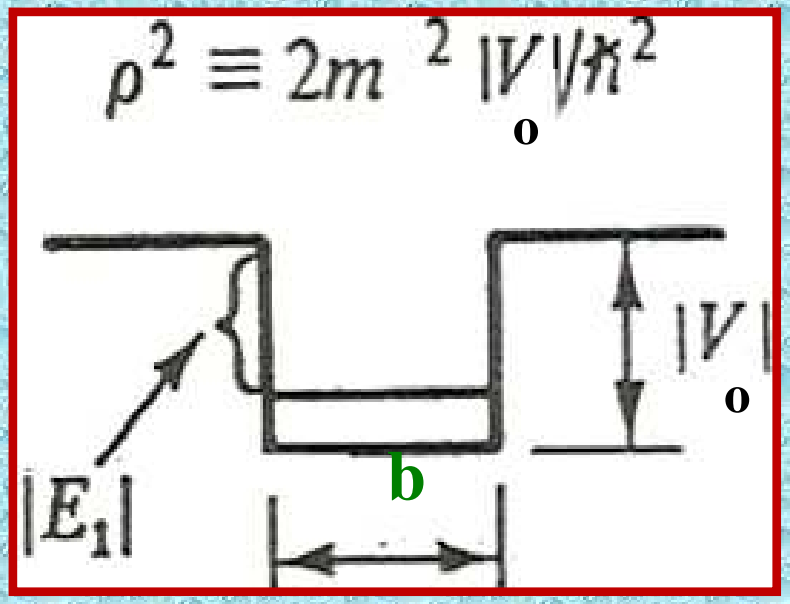
$$\tan(\alpha b) = (2\alpha\beta)/(\alpha^2 - \beta^2)$$

- Solve graphically or numerically.
- **Get:** ***Discrete energy levels*** in the well (a finite number of finite well levels!)

Even Eigenfunction solutions (a finite number):

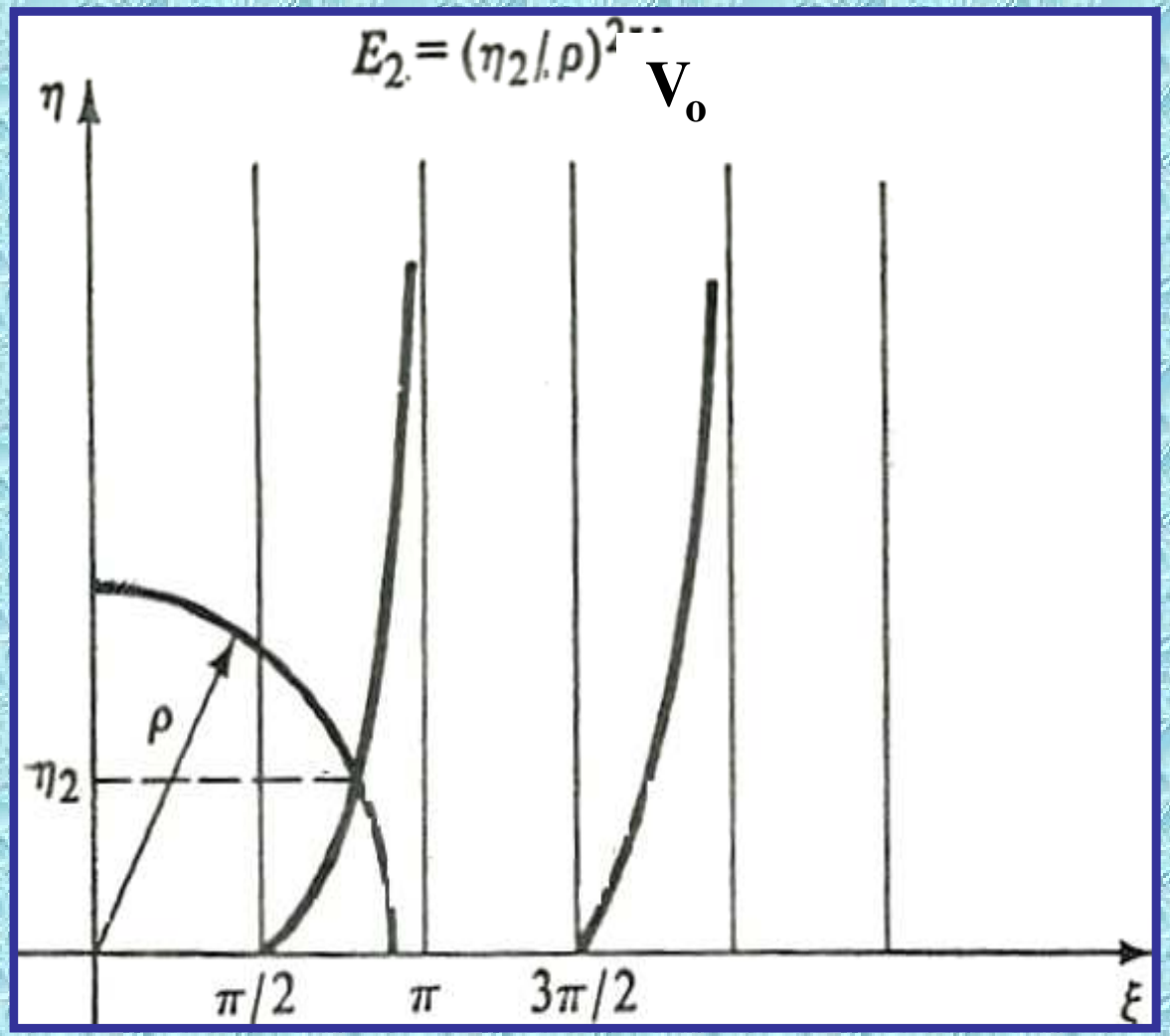
Circle, $\xi^2 + \eta^2 = \rho^2$, Crosses, $\eta = \xi \tan(\xi)$

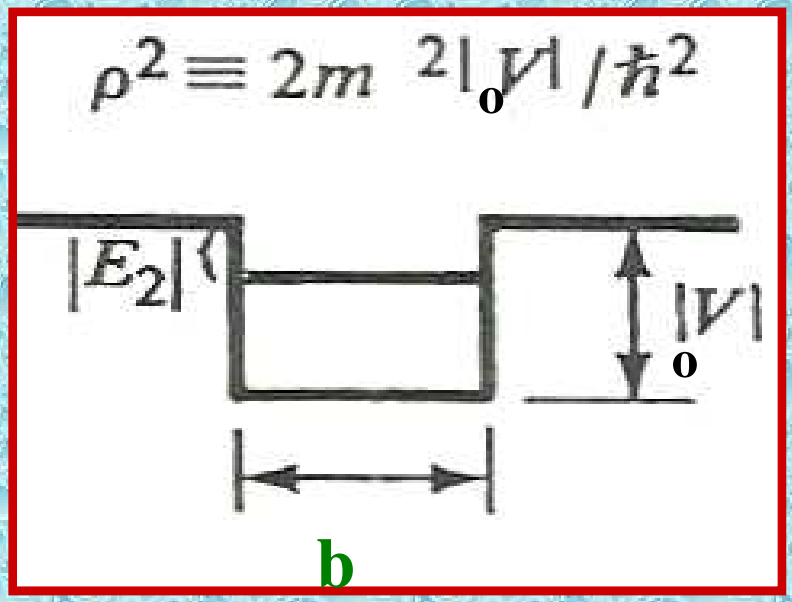




Odd Eigenfunction solutions (a finite number):

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

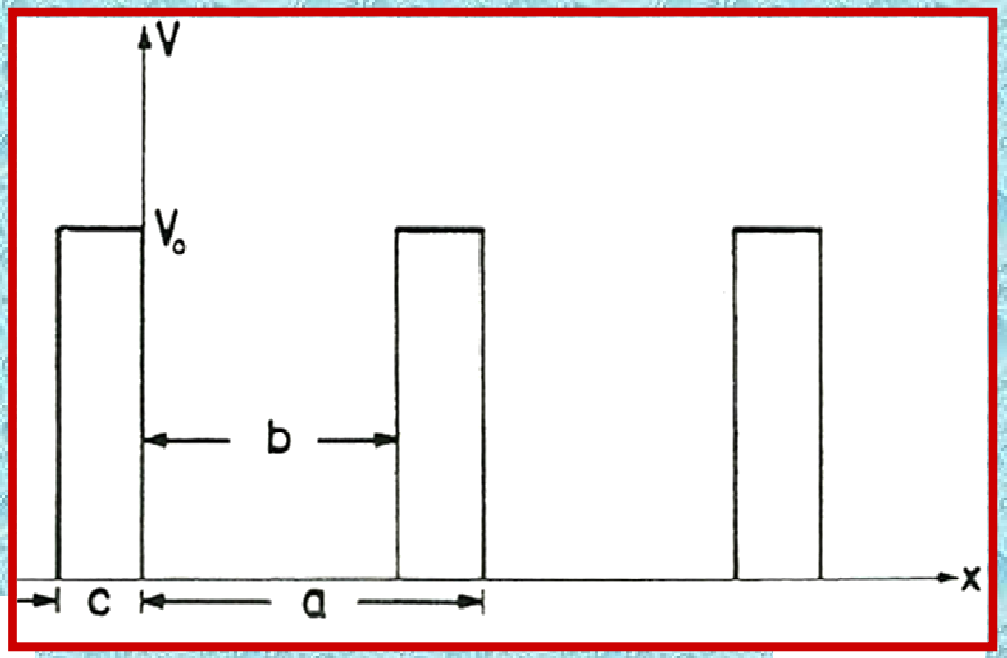




The Krönig-Penney Model

Repeat distance **a = b + c.** Periodic potential **V(x) = V(x + na), n** = integer

Periodically Repeated Wells & Barriers. →



Schrödinger Equation:

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

V(x) = Periodic Potential

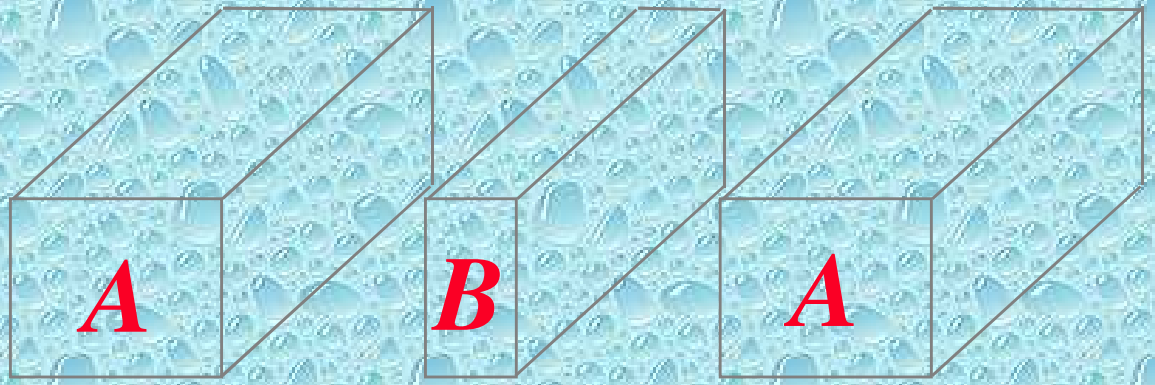
⇒ The **Wavefunctions** must have the **Bloch Form**: $\psi_k(x) = e^{ikx}\, u_k(x);\ u_k(x) = u_k(x+a)$

- Boundary conditions at **x = 0, b:**

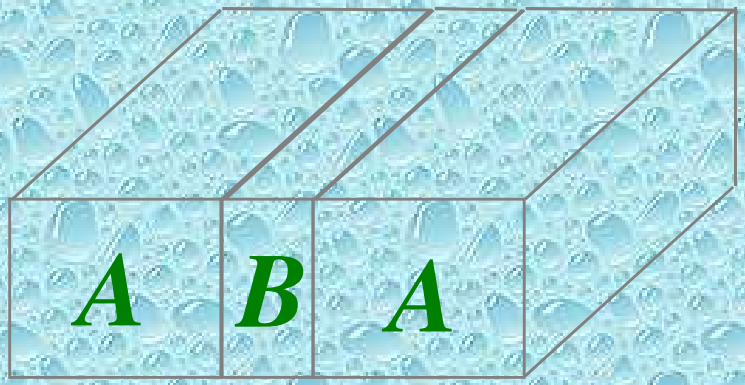
ψ, (dψ/dx) are continuous ⇒

Quantum Wells & Superlattices

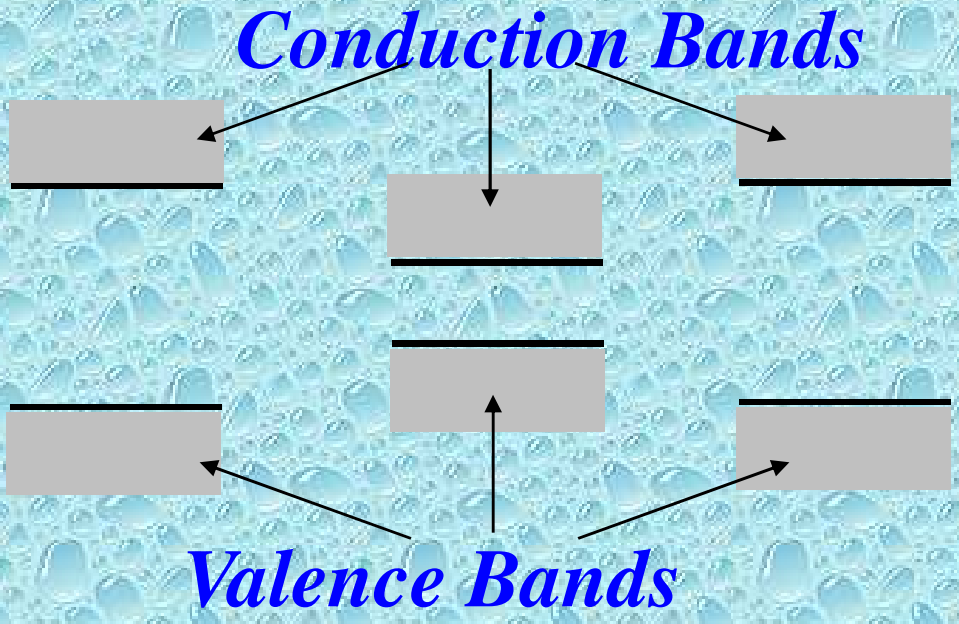
Bulk Semiconductors

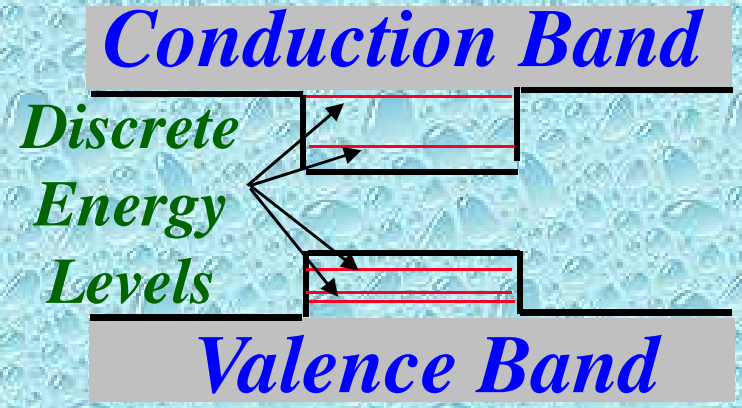


Epitaxial Layers



In Energy Space





"Quantum Well"

- **Algebra &Calculus give: *A MESS!***
- But doable ***EXACTLY!*** Instead of an explicit form for the bandstructure ε_k or $\varepsilon(\mathbf{k})$, we get:

$$\mathbf{k = k(\varepsilon) = (1/a)\cos^{-1}[L(\varepsilon/V_o)]}\ \textbf{\textit{OR}}$$

$$\mathbf{L = L(\varepsilon/V_o) = \cos(ka)}\quad \textbf{\textit{WHERE}}$$

$$\mathbf{L = L(\varepsilon/V_o) =}$$

$$L = \frac{1 - 2\varepsilon/V_0}{2\sqrt{(\varepsilon/V_0) - (\varepsilon/V_0)^2}} \sinh\left[\sqrt{\frac{2m\,V_0}{\hbar^2}\left(1 - \frac{\varepsilon}{V_0}\right)}\,c\right] \sin\left(\sqrt{\frac{2m\,V_0}{\hbar^2}\frac{\varepsilon}{V_0}}\,b\right)$$

$$+ \cosh\left[\sqrt{\frac{2m\,V_0}{\hbar^2}\left(1 - \frac{\varepsilon}{V_0}\right)}\,c\right] \cos\left(\sqrt{\frac{2m\,V_0}{\hbar^2}\frac{\varepsilon}{V_0}}\,b\right)$$

$$L = L(\varepsilon/V_o) = \cos(ka) \Rightarrow -1 < L < 1$$

- The ε in this range are the ***allowed energies***

(The Allowed BANDS!)

- But also, $L(\varepsilon/V_o) =$ a messy function with no limit on L
- The k's in the range where $|L| > 1$ are imaginary.

$\Rightarrow$ **These are regions of *forbidden energy*.**

(The Forbidden GAPS!)

- No solutions exist there for real k; math solutions exist, but with imaginary k!
- The wavefunctions have the Bloch form for all k (& all L):

$$\psi_k(x) = e^{ikx} u_k(x)$$

$\Rightarrow$ For imaginary k, $\psi_k(x)$ decays instead of propagating!

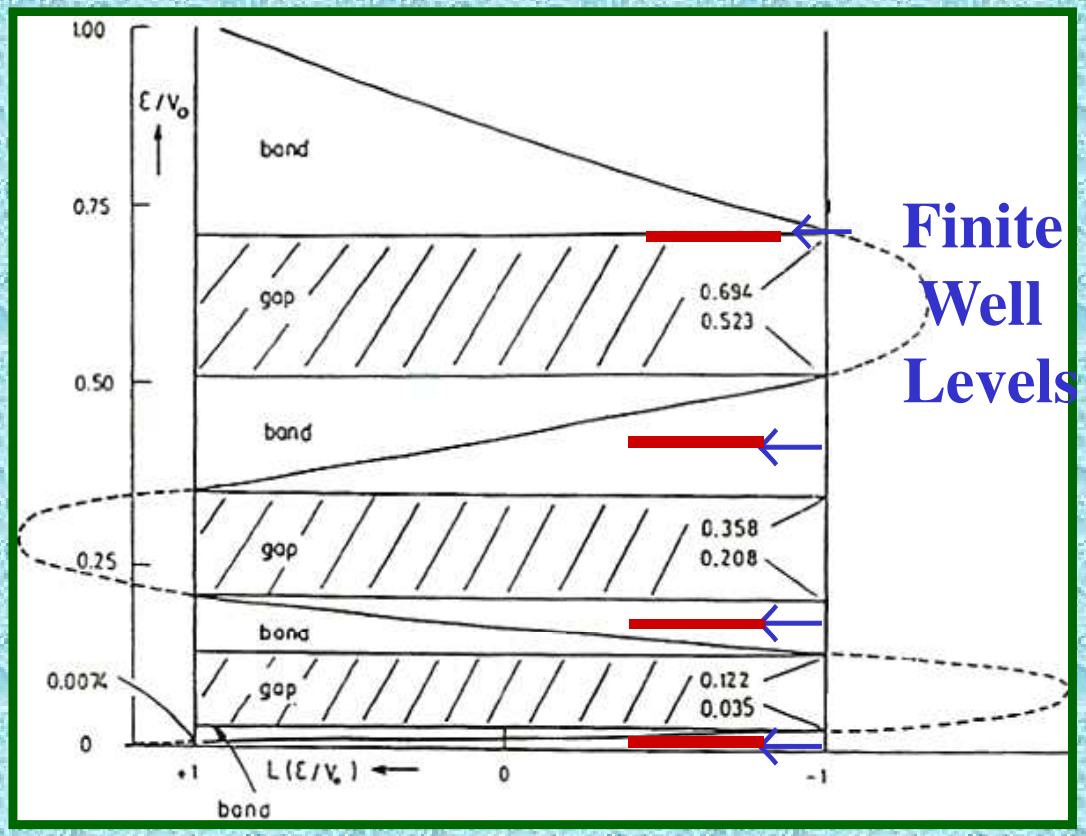
Krönig-Penney Results: For particular a, b, c, V_o

- Each band has a finite well level "parent":

$$L(\varepsilon/V_o) = \cos(ka)$$

$$\Rightarrow -1 < L < 1$$

- But also $L(\varepsilon/V_o)$ = a messy function with no limits. For ε in the range



$$-1 < L < 1 \Rightarrow \text{Gives}$$

Allowed **Energies (*Bands!*)**

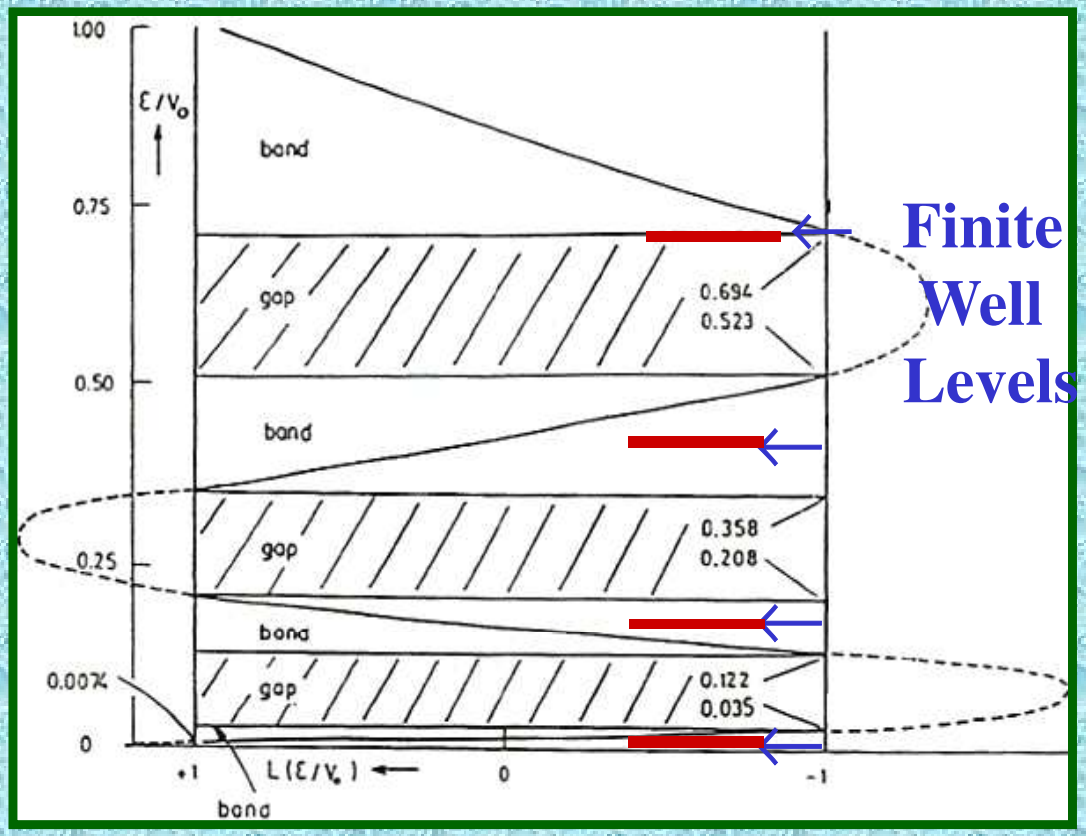
Krönig-Penney Results: For particular a, b, c, V_o

- Each band has a finite well level "parent":

$$L(\varepsilon/V_o) = \cos(ka)$$

$$\Rightarrow -1 < L < 1$$

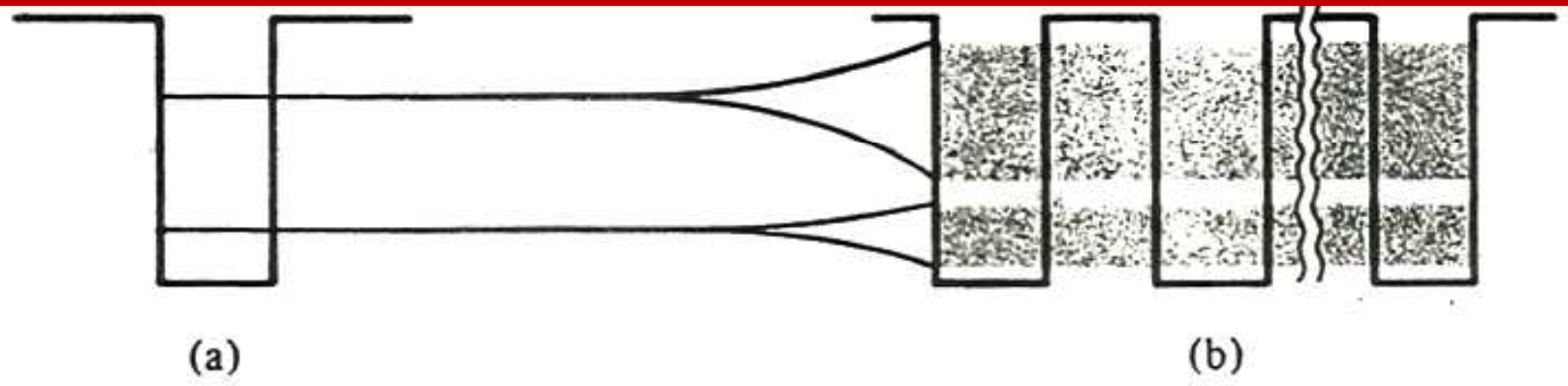
- But also $L(\varepsilon/V_o) =$ a messy function with no limits. For ε in the range



$$|L| > 1 \Rightarrow \text{Gives}$$

***Forbidden* Energies (*Gaps*!)**

- ***Every band*** in **the Krönig-Penney model** has a finite well **discrete level as its "parent"**! ⇒ In its ***implementation,*** the **Krönig-Penney** model is similar to the **"almost free" e⁻ approach**, but ***the results*** are **similar to the tightbinding approach!** (As we'll see). Each band is associated with an "atomic" level from the well.



(a) Single isolated finite potential well with two bound states. (b) Corresponding periodic potential with two energy bands. For N wells each band contains N states.

The figure is ***a schematic representation*** of the **evolution *from*** the finite well ***to*** the periodic potential.

More on the Krönig-Penney Solutions

$L(\varepsilon/V_o) = \cos(ka) \Rightarrow$ *BANDS & GAPS!*

- **The Gap Size** depends on the **c/b** ratio
- Within a band (previous Figure) a good approximation is that **L ~** a linear function of **ε**. Use this to simplify the results:
- For (say) the lowest band, let $\varepsilon \equiv \varepsilon_1$ (L = -1) & $\varepsilon \equiv \varepsilon_2$ (L = 1) use the linear approximation for $L(\varepsilon/V_o)$. Invert this & get:

$$\varepsilon_-(k) = (1/2)(\varepsilon_2 + \varepsilon_1) - (1/2)(\varepsilon_2 - \varepsilon_1)\cos(ka)$$

For the next lowest band,

$$\varepsilon_+(k) = (1/2)(\varepsilon_4 + \varepsilon_3) + (1/2)(\varepsilon_4 - \varepsilon_3)\cos(ka)$$

- ***In this approximation, all bands are cosine functions!!!*** This is identical, as we'll see, to some simple tightbinding results.

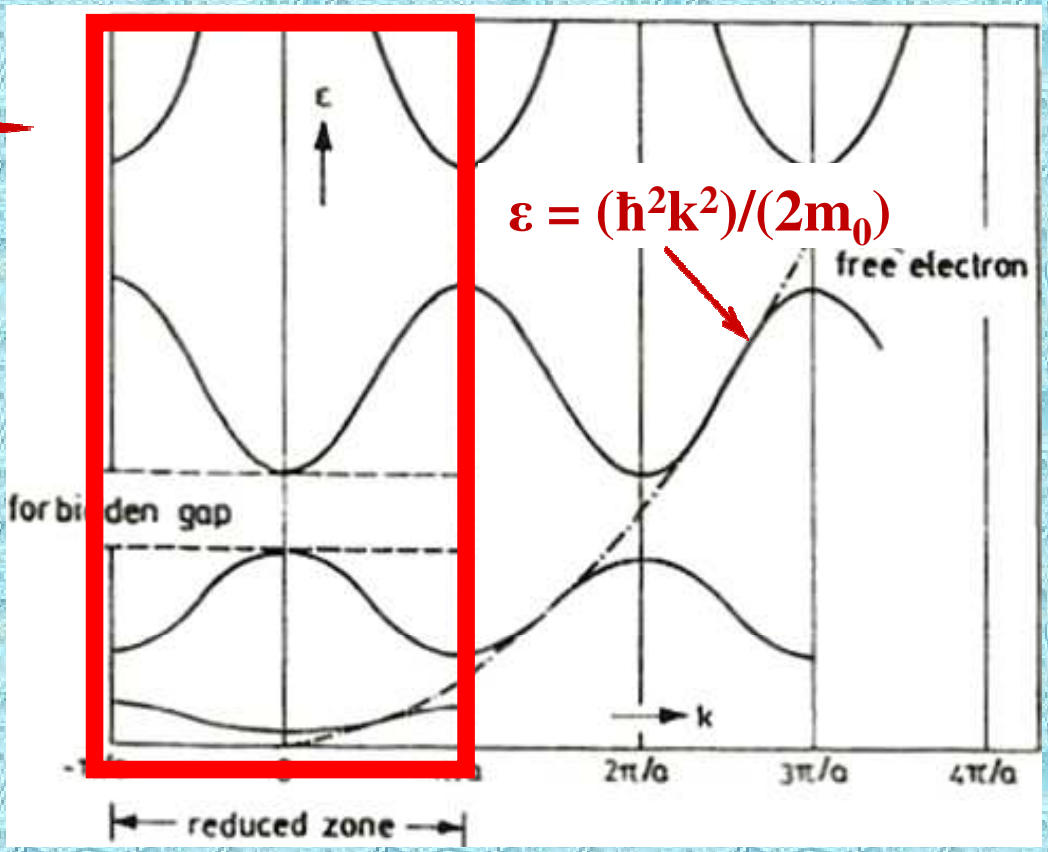
The Lowest Krönig-Penney Bands

- In the linear approximation for $L(\varepsilon/V_o)$:

  All Bands are cos(ka) Functions!

- The figure shows the bands in this approximation, plotted in **the extended zone scheme.** Note the discontinuities in the bands at the BZ edges:

$$k = \pm(n\pi/a)$$



- Because of the periodicity of **ε(k)**, **the reduced zone scheme (red)** gives **the same information as the extended zone scheme** (as is true in general).