

*“Complementi di Fisica”*  
*Lectures 16, 17*



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# Course Outline - Reminder

- The physics of semiconductor devices: an introduction
- Quantum Mechanics: an introduction
  - Reminder on waves
  - Waves as particles and particles as waves (the crisis of classical physics); atoms and the Bohr model
  - The Schrödinger equation and its interpretation
  - (1-d) free and confined (infinite well) electron; wave packets, uncertainty relations; **barriers and wells; periodic potential**
  - (3-d) Hydrogen atom, angular momentum, spin
  - Systems with many particles
- **Advanced semiconductor fundamentals** (bands, etc...)



# Lectures 16, 17 - outline

- 1-d applications of Wave Mechanics:
  - Reminder of the analysis method:
    - Solutions of the S. time-independent equation;
    - Continuity conditions (wave function and its derivative)
    - Wave functions, energy eigenvalues
  - Finite potential well:
    - “bound” states
    - (“free” states: transmission and reflection coefficients)
  - Finite potential barrier:
    - “bound”, “free” states: reflection, transmission coefficients
    - “Tunnel” effect
  - Periodic potential:
    - Bloch theorem
    - Kronig-Penney model
    - Energy bands, effective mass



# Analysis method

- Solutions of the time-independent Schrödinger equation
  - The energy eigenvalue must be the same everywhere; it may correspond to
    - A “bound” particle state
    - A “free” particle state
  - the energy value  $E$  determines the type of solution in each region (interval)
  - Continuity of the wave function and its derivative, at the boundaries between different intervals, determine the coefficients of the different terms
- transmission and reflection coefficients for a given finite barrier or well can be defined for “free” particle states



# Solution types

- If in some region the potential  $V(x)=V$  is constant, there are three possible stationary solution types:

- If  $E > V$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} + k^2\psi = 0, \quad k^2 = \frac{2m(E-V)}{\hbar^2} > 0$$

$$\Rightarrow \quad \psi(x) = Ae^{ikx} + Be^{-ikx}, \quad A \text{ and } B \text{ arbitrary complex constants, or}$$
$$\psi(x) = C \sin kx + D \cos kx \quad (\text{equivalent})$$

- If  $E < V$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} - \alpha^2\psi = 0, \quad \alpha^2 = \frac{2m(V-E)}{\hbar^2} > 0$$

$$\Rightarrow \quad \psi(x) = Ae^{\alpha x} + Be^{-\alpha x}, \quad A \text{ and } B \text{ arbitrary complex constants}$$

- If  $E = V$ :

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} = 0$$

$$\Rightarrow \quad \psi(x) = Ax + B, \quad A \text{ and } B \text{ arbitrary complex constants}$$



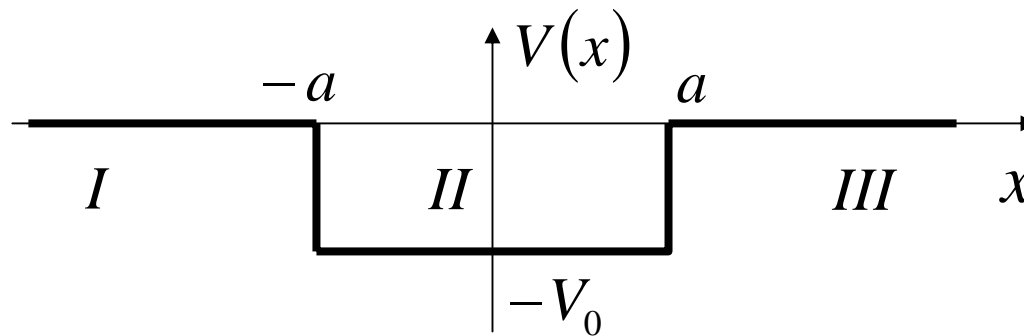
# Finite potential well

“bound” particle

“free” particle

transmission coefficient

# Finite potential well: (a) bound solutions



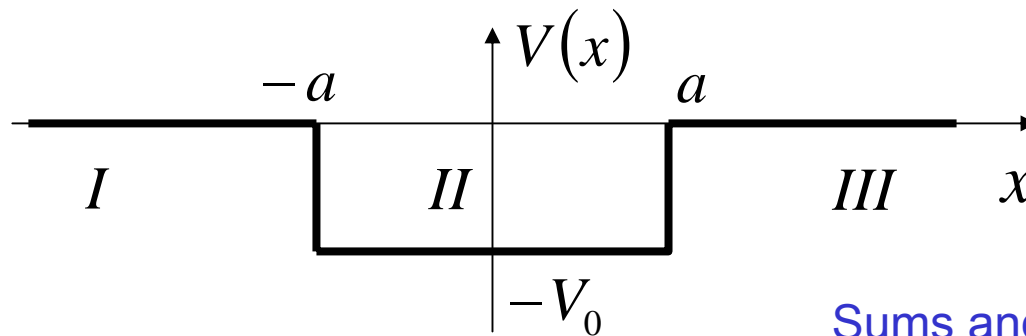
Bound stationary solutions ( $-V_0 < E < 0$ )

$$I: \quad \psi_I = Ae^{\alpha x} \xrightarrow{x \rightarrow -\infty} 0 \quad \alpha = \sqrt{(-E)2m/\hbar^2}$$

$$II: \quad \psi_{II} = B \sin kx + C \cos kx \quad k = \sqrt{(E - V_0)2m/\hbar^2}$$

$$III: \quad \psi_{III} = De^{-\alpha x} \xrightarrow{x \rightarrow +\infty} 0 \quad \alpha = \sqrt{(-E)2m/\hbar^2}$$

# “Bound” solutions: (b) continuity



Sums and differences:

$$x = -a: Ae^{-\alpha a} = -B \sin(ka) + C \cos(ka) \quad \Rightarrow \quad (A - D)e^{-\alpha a} = -2B \sin(ka)$$

$$x = a: De^{-\alpha a} = B \sin(ka) + C \cos(ka) \quad \Rightarrow \quad (A + D)e^{-\alpha a} = 2C \cos(ka)$$

$$x = -a: \alpha Ae^{-\alpha a} = kB \cos(ka) + kC \sin(ka) \quad \Rightarrow \quad \alpha(A + D)e^{-\alpha a} = 2kC \sin(ka)$$

$$x = a: -\alpha De^{-\alpha a} = kB \cos(ka) - kC \sin(ka) \quad \Rightarrow \quad \alpha(A - D)e^{-\alpha a} = 2kB \cos(ka)$$

Compatible only if:

Ratios:

$$\text{odd solutions: } A = -D, \quad C = 0 \quad \Leftrightarrow \quad \alpha = -k \cot(ka)$$

$$\text{even solutions: } A = D, \quad B = 0 \quad \Leftrightarrow \quad \alpha = k \tan(ka)$$





# “bound” solutions: (c) eigenvalues - 1

Equations:

$$\alpha = -k \cot(ka)$$

$$\alpha = k \tan(ka)$$

Incompatible unless:

$$\text{odd solutions: } A = -D, \quad C = 0$$

$$\text{even solutions: } A = D, \quad B = 0$$

These equations express conditions on the energy eigenvalues  $E_i$ :  
Recall the definitions of  $\alpha$  and  $k$  in terms of  $E$ :

$$k = \sqrt{\frac{(E_i - V_0)2m}{\hbar^2}} \quad \alpha = \sqrt{\frac{(-E_i)2m}{\hbar^2}} \quad \alpha^2 + k^2 = (-V_0) \frac{2m}{\hbar^2}$$

To find the solutions for  $E_i$ , it is convenient to consider the normalized a-dimensional variables:

$$\xi = ka \quad \eta = \alpha a \quad \xi^2 + \eta^2 = (-V_0) \frac{2m}{\hbar^2} a^2$$



# “bound” solutions: (c) eigenvalues - 2

The equations to be solved take the reduced form:

$$\alpha^2 + k^2 = (-V_0) \frac{2m}{\hbar^2}$$

$$\alpha = -k \cot(ka)$$

$$\alpha = k \tan(ka)$$



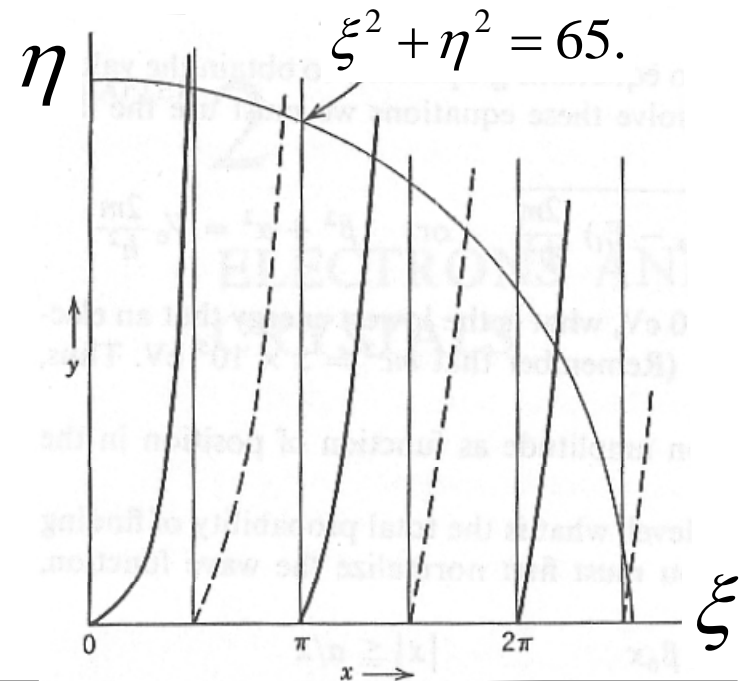
$$\xi^2 + \eta^2 = (-V_0) \frac{2m}{\hbar^2} a^2$$

$$\eta = -\xi \cot(\xi)$$

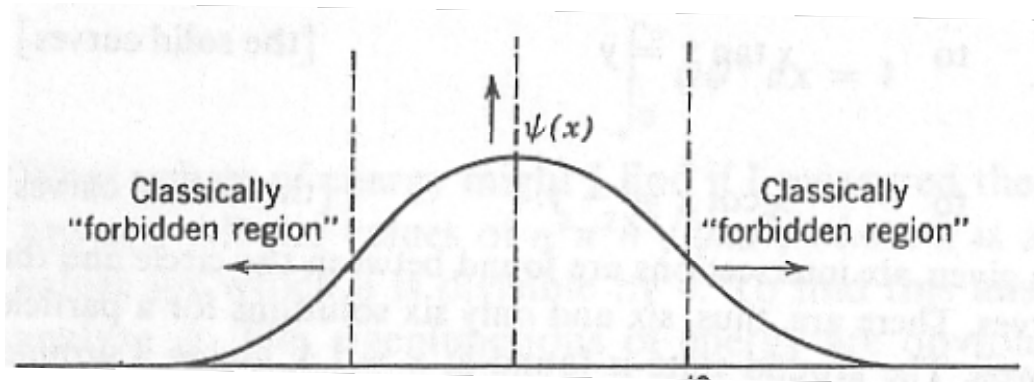
$$\eta = \xi \tan(\xi)$$

Example of graphical (numerical) solution, for  $a = 500\text{\AA}$  and  $V_0 = 10\text{eV}$ :  
6 bound state solutions;  
ground state at  $x = 1.4$ ,  
corresponding to:  
 $E - V_0 = 0.61\text{ eV}$

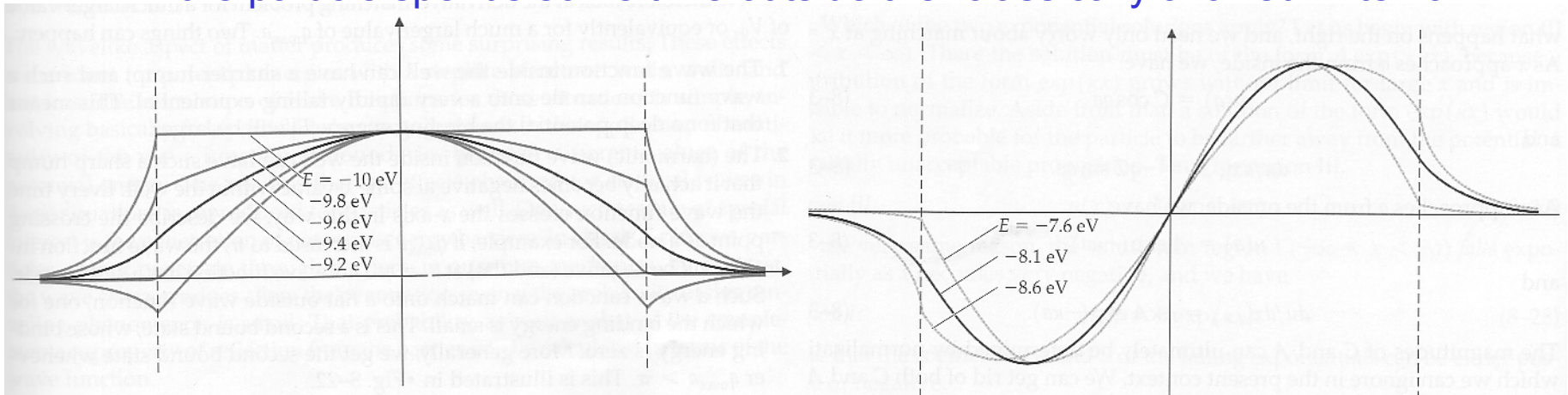
The number of solutions depends on  $a$  and  $V_0$  !



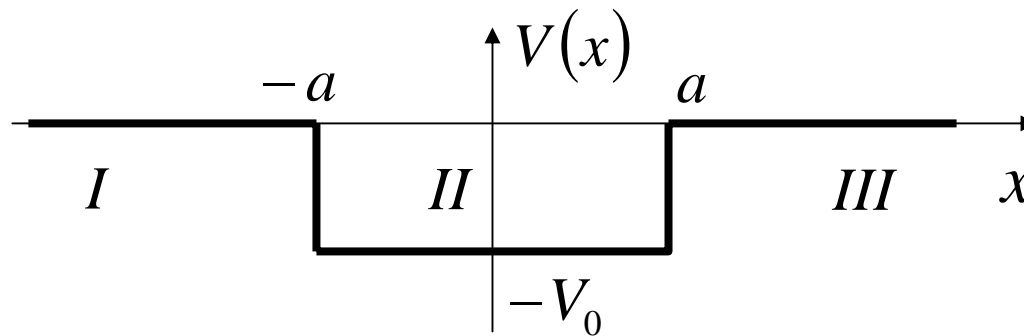
# “bound” solutions: (d) eigenfunctions



Examples of the lowest even and odd solutions, showing the effect of the request that the derivative should be continuous: the particle spends some time *outside* the “classically allowed” interval !



# Finite potential well: (a) “free” solutions



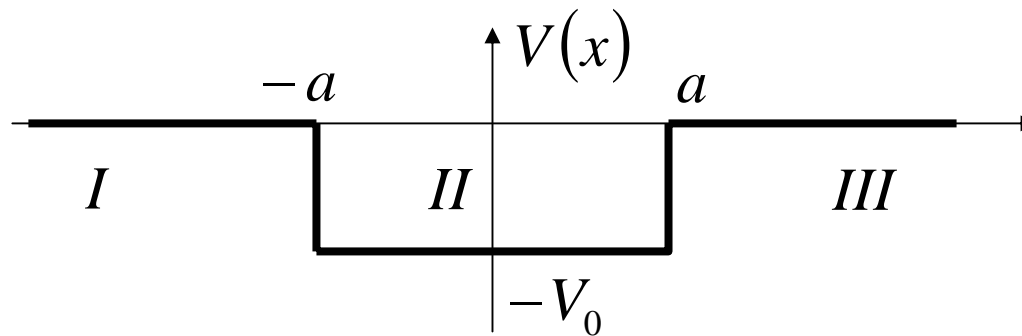
free stationary solutions ( $E > 0$ ); particles coming from the left, towards positive  $x$

$$I: \quad \psi_I = Ae^{ikx} + Be^{-ikx} \quad k = \sqrt{2mE/\hbar^2}$$

$$II: \quad \psi_{II} = C \sin lx + D \cos lx \quad l = \sqrt{(E + V_0)2m/\hbar^2}$$

$$III: \quad \psi_{III} = Fe^{ikx} \quad k = \sqrt{2mE/\hbar^2}$$

# “free” solutions: transmission coefficient

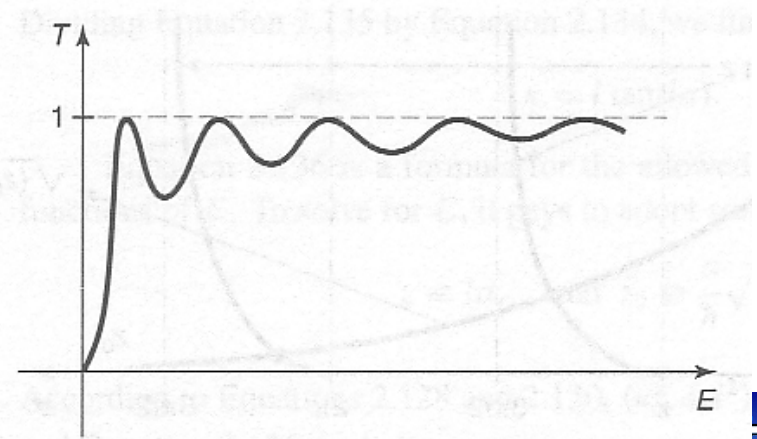


As before, from continuity relations one can extract the coefficients (in particular A and F) and then define the “transmission coefficient”:

$$T = \frac{|F|^2}{|A|^2} = \dots = \frac{1}{1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar} \sqrt{2m(E+V_0)}\right)}$$

The following energies correspond to “perfect transmission”  $T=1$  over the well:

$$E_n + V_0 = \frac{n^2 \pi^2 \hbar^2}{2m(2a)^2}$$



# Finite potential barrier

“bound” particle

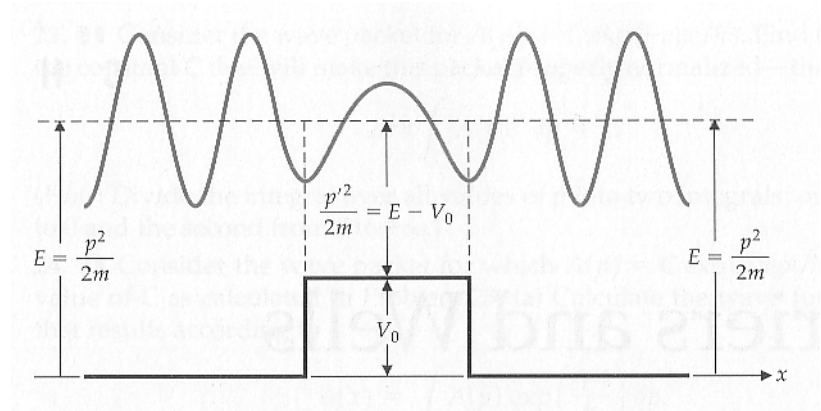
“free” particle

Reflection and transmission  
coefficients

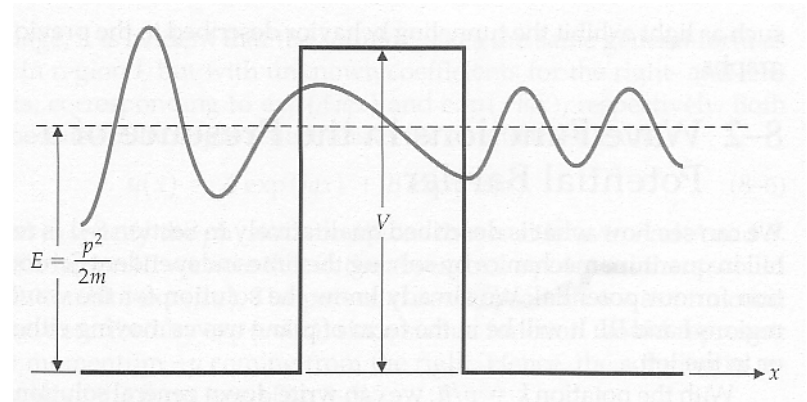
Tunnel effect

# Finite potential barrier - introduction

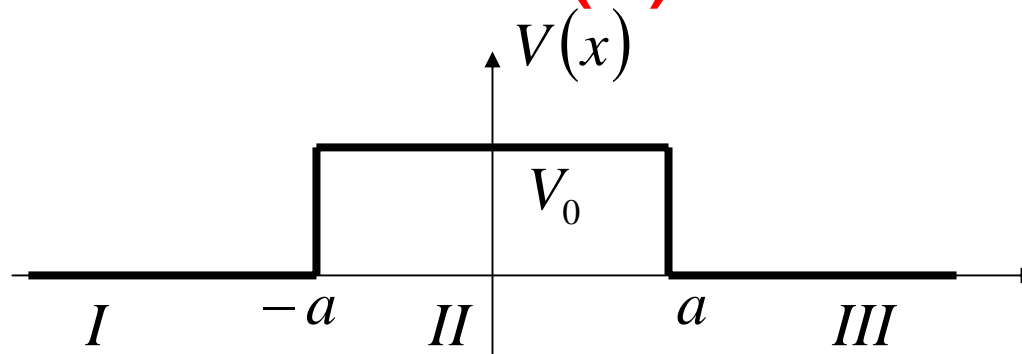
- $E > V_0$ : wavelength always real;
  - But: there is usually reflection in addition to transmission!



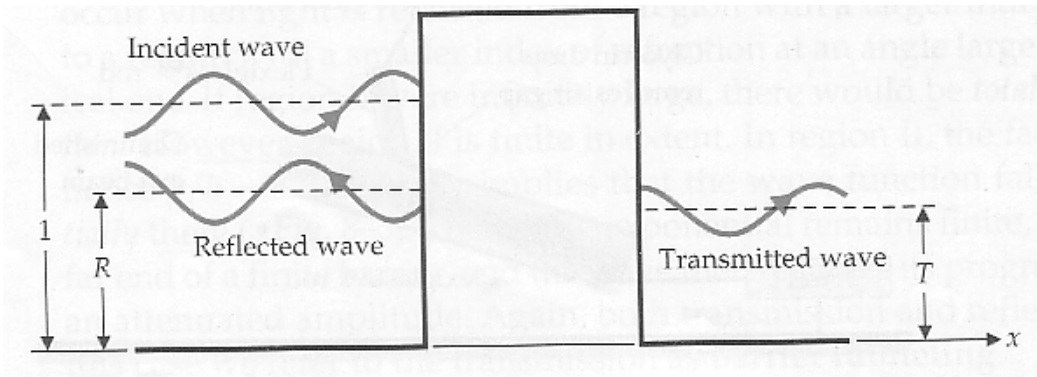
- $E < V_0$ : wavelength becomes imaginary (analog to classical: “evanescent waves”);
  - the wave function falls off exponentially in the barrier
  - There is a “transmitted” wave with reduced amplitude



# Finite barrier: (a) solutions



Similar to finite well, but we use slightly different notations: to describe both “bound” and “free” solutions with the same equations, here  $q$  may be real or imaginary depending on the sign of  $E - V_0$



$$I: \psi_I = e^{ikx} + R e^{-ikx}$$

$$k = \sqrt{2mE/\hbar^2}$$

$$II: \psi_{II} = A e^{iqx} + B e^{-iqx}$$

$$q = \sqrt{(E - V_0)2m/\hbar^2}$$

$$III: \psi_{III} = T e^{ikx}$$

$$k = \sqrt{2mE/\hbar^2}$$



# Reflection and transmission

Continuity conditions:

$$x = -a: \quad e^{-ika} + R e^{ika} = A e^{-iqa} + B e^{iqa}$$

$$i k e^{-ika} + -i k R e^{ika} = i q A e^{-iqa} - i q B e^{iqa}$$

$$x = a: \quad A e^{iqa} + B e^{-iqa} = T e^{ika}$$

$$i q A e^{iqa} - i q B e^{-iqa} = i k T e^{ika}$$

4 equations for 4 unknowns: A, B, R, T; we are interested mainly in reflection and transmission probabilities, represented by  $|R|^2$  and  $|T|^2$ , where R and T are given by (see details in back-up slides):

$$R = \frac{i(q^2 - k^2) \sin(2qa)}{2kq \cos(2qa) - i(k^2 + q^2) \sin(2qa)} e^{-2ika}$$

$$T = \frac{2kq}{2kq \cos(2qa) - i(k^2 + q^2) \sin(2qa)} e^{-2ika}$$



# “free” solution for $E > V_0$

- By inspection of the equations for  $R$  and  $T$ , their features for  $E > V_0$ :
  - $R$  and  $T$  are complex numbers (“probability amplitudes”)
  - $R$  is not zero, even for  $E > V_0$
  - $R \rightarrow 0$  for  $V_0 \rightarrow 0$
  - $|R| \leq 1$
  - $|R|^2 + |T|^2 = 1$
  - $|R|^2$  and  $|T|^2$  can be interpreted respectively as *probabilities for reflection and transmission of the particle* by the potential barrier
- A similar method is used in more complicated 3-d problems found in the physics of semiconductors !
  - For instance, scattering of an electron by an impurity or defect in a crystal lattice...
  - computation of “scattering amplitudes” and “probabilities” !



# “tunneling” solution for $E < V_0$

- When  $E < V_0$ :
  - Classically, the particle can only bounce back (perfect reflection)
  - Here: non-zero transmission probability
  - Convenient to show explicitly that  $q$  becomes purely imaginary

$$q^2 = \frac{2m}{\hbar^2}(E - V_0) < 0 \Rightarrow \text{express it as } q = i\eta \text{ purely imaginary}$$

$$\eta^2 = \frac{2m}{\hbar^2}(V_0 - E) > 0$$

$$\cos(2qa) \rightarrow \frac{e^{-2\eta a} + e^{2\eta a}}{2}$$

$$\sin(2qa) \rightarrow \frac{i(e^{2\eta a} - e^{-2\eta a})}{2}$$

$$T = \frac{4ik\eta e^{-2\eta a}}{2ik\eta(1 + e^{-4\eta a}) + (k^2 - \eta^2)(1 - e^{-4\eta a})} e^{-2ika}$$
$$e^{-4\eta a} \ll 1 \Rightarrow |T|^2 \approx \frac{16k^2\eta^2}{(k^2 + \eta^2)^2} e^{-4\eta a}$$

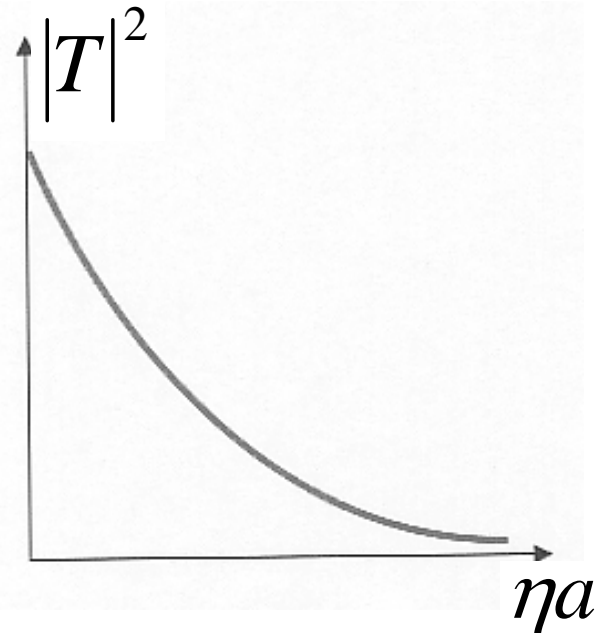
# “tunneling” solution for $E < V_0$

Exponentially decreasing “tunneling” (transmission) probability, depending both on  $\eta$  (barrier “height”) and on  $a$  (barrier “width”):

$$e^{-4\eta a} \ll 1 \Rightarrow |T|^2 \approx \frac{16k^2\eta^2}{(k^2 + \eta^2)^2} e^{-4\eta a}$$

$\eta$  = barrier “height”  
 $a$  = barrier “width”

Qualitatively similar behavior for arbitrary barrier shape, with more complicated coefficients in the exponential, obtained by integrating over many “thin square barriers”



# Electrons in a “perfect crystal”: “Periodic potential”

Bloch Theorem

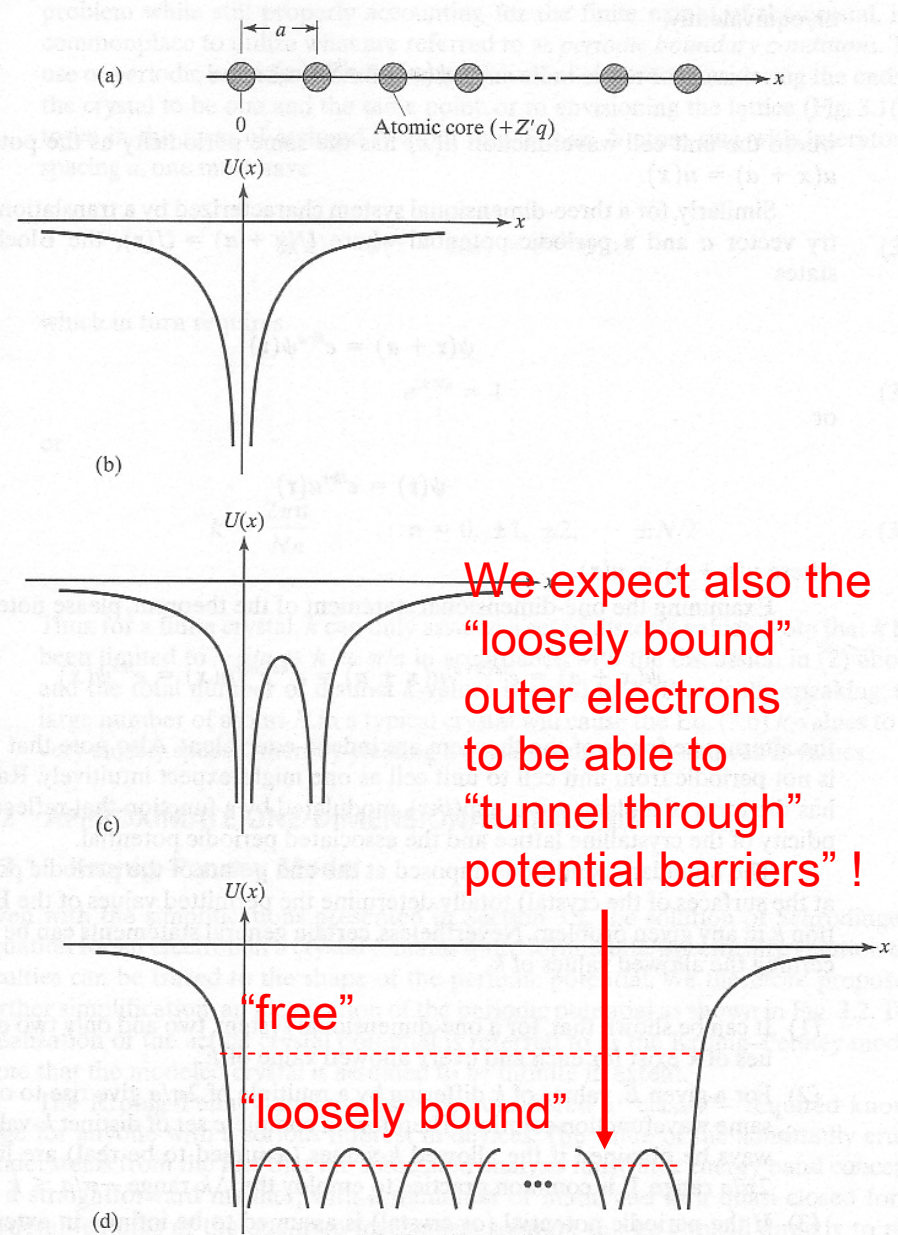
Kronig-Penney model

Energy bands and Brillouin zones

Particle motion and effective mass

# Assumptions

- Approximate the forces felt by each “loosely bound”, “external” electron as the sum of Coulomb potentials:
  - Individual charges  $Z'q$  (nuclei + tightly bound electrons)
  - Separated (in 1-d) by the lattice constant  $a$
- For a first-order approximation, neglect interactions between “external” electrons
  - They become important at very low temperatures (“Cooper pairs”, superconductivity)
- Find the available stationary states and energy eigenvalues
  - To understand how they are occupied we need to come back to multi-particle system and the “Pauli principle”



We expect also the “loosely bound” outer electrons to be able to “tunnel through” potential barriers” !

Figure 3.1 (a) One-dimensional crystalline lattice. (b–d) Potential energy of an electron inside the lattice considering (b) only the atomic core at  $x = 0$ , (c) the atomic cores at both  $x = 0$  and  $x = a$ , and (d) the entire lattice chain.



# The Bloch Theorem

IF  $V(x)$  periodic:  $V(x+a) = V(x)$

THEN the solutions of S. equation can be taken to satisfy the condition, for some constant  $k$ :

$$\psi(x+a) = e^{ika} \psi(x) \quad \text{or, equivalently:}$$

$$\psi(x) = e^{ikx} u(x), \quad u(x+a) = u(x)$$

(Proof: not too complicated, based on the fact that the “translation” operator  $x \rightarrow x+a$  commutes with the hamiltonian...)

**NB:** The solution  $\psi(x)$  is not periodic itself: it has the form of a plane wave  $\exp(ikx)$  modulated by a function  $u(x)$  that reflects the periodicity of the crystal. One can show that  $k$  is real, so that the probability density  $|\psi(x)|^2$  is periodic, as one would expect



# Allowed values of $k$ ?

- Independently of the specific shape of  $V(x)$ , some general properties of  $k$ :
  - For a 1-d system: 2 distinct values of  $k$  exist for each allowed value of  $E$
  - For a given  $E$ : values of  $k$  differing by  $2\pi/a$  give the same wavefunction solution ( $\Rightarrow$  range restricted to  $-\pi/a < k < \pi/a$ )
  - For “infinite” crystals, one can show that  $k$  must be real and that it can assume a continuum of values
  - To describe electrons inside crystals of finite extent, it is customary to assume “periodic boundary conditions” (equivalent to a “closed N-atom ring”): this implies that  $k$  can only assume a set of discrete values; since N is large, this is a “quasi-continuum”.

$$\psi(x) = \psi(x + Na) = e^{ikNa} \psi(x) \quad \Rightarrow \quad e^{ikNa} = 1 \quad \Rightarrow \quad k = \frac{2\pi n}{Na} \quad n = 0, \pm 1, \pm 2, \dots \pm N/2$$

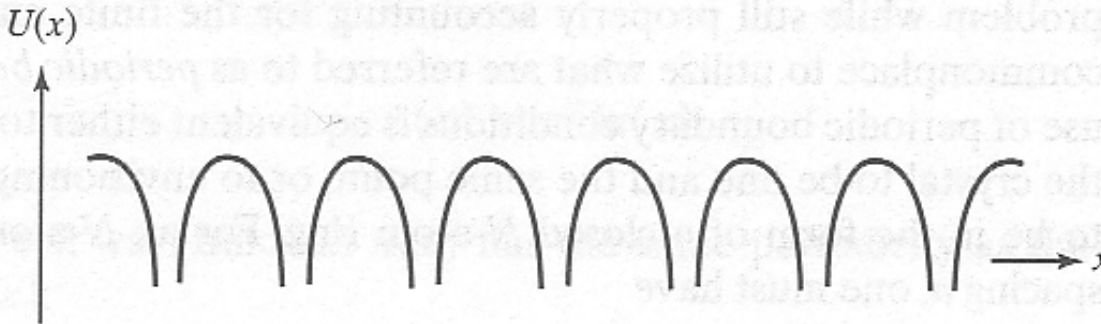
- Bloch's theorem allows us to solve the Schrödinger equation on a single cell and generate recursively the wavefunction everywhere else



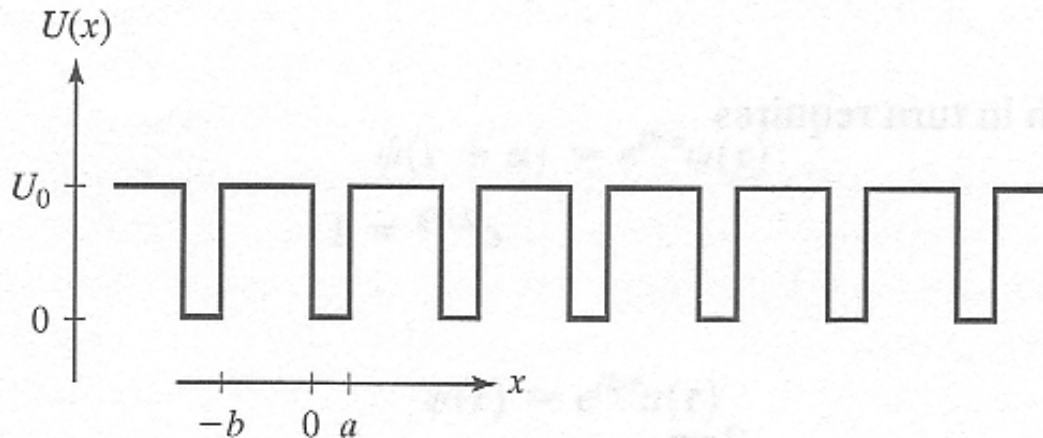


# The Kronig-Penney model

- Approximation:



(a)



(b)

# Kronig-Penney (1): S.equation in one cell

- Schrödinger equation and solutions: similar to what we saw for wells and barriers

$$\frac{d^2\psi_a}{dx^2} + \alpha^2\psi_a = 0 \quad 0 < x < a$$

$$\alpha = \sqrt{2mE/\hbar^2}$$

$$\frac{d^2\psi_b}{dx^2} + \beta^2\psi_b = 0 \quad -b < x < 0$$

$$\beta = \begin{cases} i\beta_-; & \beta_- = \sqrt{2m(U_0 - E)/\hbar^2} & 0 < E < U_0 \\ \beta_+; & \beta_+ = \sqrt{2m(E - U_0)/\hbar^2} & E > U_0 \end{cases}$$



$$\psi_a(x) = A_a \sin \alpha x + B_a \cos \alpha x$$

$$\psi_b(x) = A_b \sin \beta x + B_b \cos \beta x$$

# Kronig-Penney (2): boundary conditions

- No surprise... they produce constraints on  $\alpha$ ,  $\beta_-$ ,  $\beta_+ \Rightarrow$  on  $k$ ,  $E$

$\psi_a(0) = \psi_b(0)$	$\left. \vphantom{\begin{matrix} \psi_a(0) = \psi_b(0) \\ \frac{d\psi_a}{dx}\big _0 = \frac{d\psi_b}{dx}\big _0 \end{matrix}} \right\} \text{Continuity requirements}$	$\longrightarrow$	$B_a = B_b$
$\frac{d\psi_a}{dx}\bigg _0 = \frac{d\psi_b}{dx}\bigg _0$			
$\psi_a(a) = e^{ik(a+b)}\psi_b(-b)$	$\left. \vphantom{\begin{matrix} \psi_a(a) = e^{ik(a+b)}\psi_b(-b) \\ \frac{d\psi_a}{dx}\big _a = e^{ik(a+b)}\frac{d\psi_b}{dx}\big _{-b} \end{matrix}} \right\} \text{Periodicity requirements}$	$\longrightarrow$	$\alpha A_a = \beta A_b$
$\frac{d\psi_a}{dx}\bigg _a = e^{ik(a+b)}\frac{d\psi_b}{dx}\bigg _{-b}$			

$$A_a \sin \alpha a + B_a \cos \alpha a = e^{ik(a+b)}[-A_b \sin \beta b + B_b \cos \beta b]$$

$$\alpha A_a \cos \alpha a - \alpha B_a \sin \alpha a = e^{ik(a+b)}[\beta A_b \cos \beta b + \beta B_b \sin \beta b]$$

$$A_a[\sin \alpha a + (\alpha/\beta)e^{ik(a+b)}\sin \beta b] + B_a[\cos \alpha a - e^{ik(a+b)}\cos \beta b] = 0$$

$$A_a[\alpha \cos \alpha a - \alpha e^{ik(a+b)}\cos \beta b] + B_a[-\alpha \sin \alpha a - \beta e^{ik(a+b)}\sin \beta b] = 0$$

# Kronig-Penney (3): equations for $\alpha, \beta$ ( $k, E$ )

System of 2 linear equations:  
determinant must be zero  
to give non-trivial solution

$$-\frac{\alpha^2 + \beta^2}{2\alpha\beta} \sin\alpha a \sin\beta b + \cos\alpha a \cos\beta b = \cos k(a + b) \quad (3.15)$$

Finally, reintroducing  $\beta = i\beta_-$  for  $0 < E < U_0$  and  $\beta = \beta_+$  for  $E > U_0$ , noting  $\sin(ix) = i\sinh x$  and  $\cos(ix) = \cosh x$ , and defining

Another old trick:  
change of variables:

$$\alpha_0 \equiv \sqrt{2mU_0/\hbar^2} \quad (3.16)$$

Express  $\alpha, \beta$  in terms of  
an a-dimensional variable

$$\xi \equiv E/U_0 \quad (3.17)$$

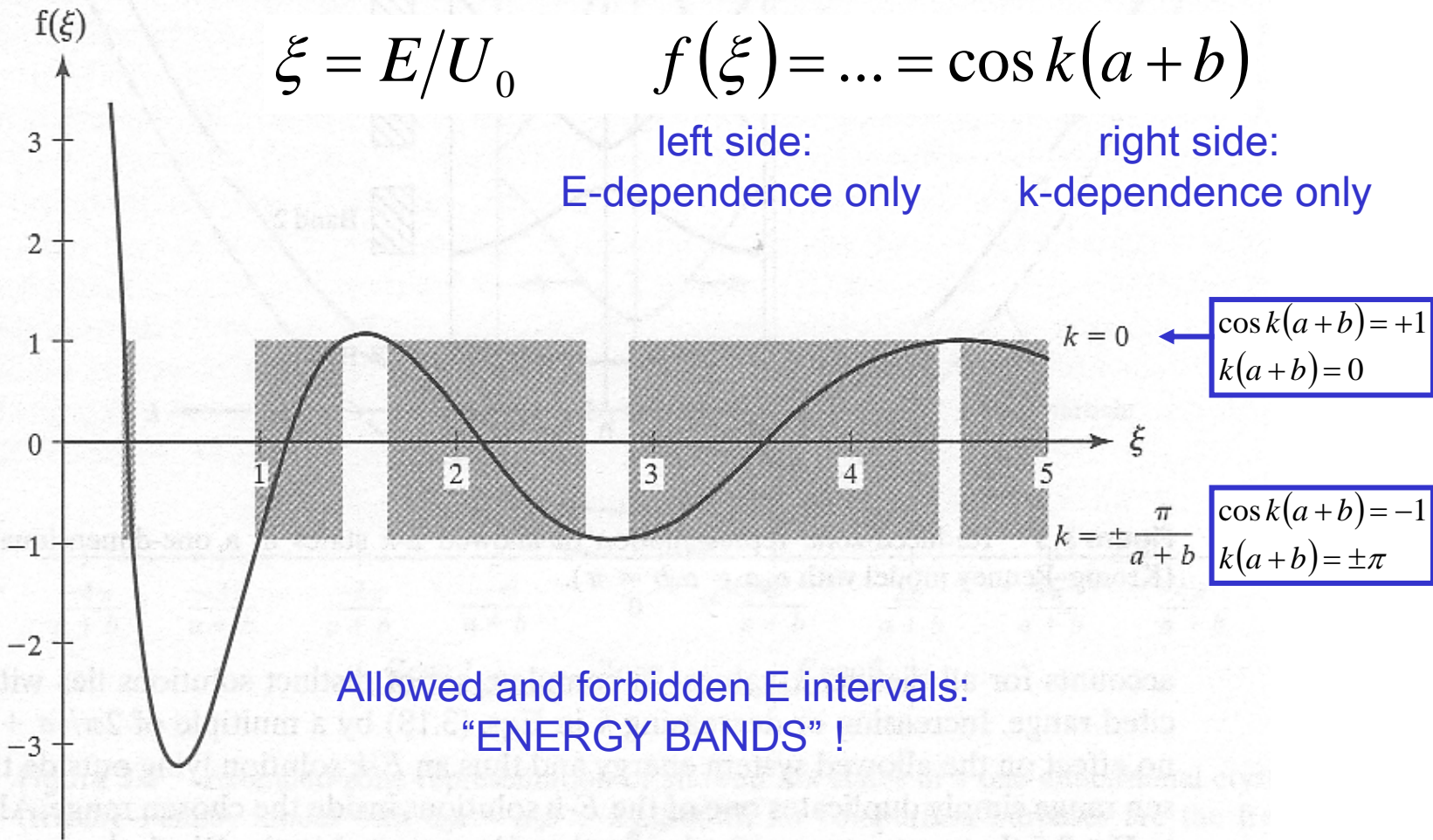
such that  $\alpha = \alpha_0\sqrt{\xi}$ ,  $\beta_- = \alpha_0\sqrt{1 - \xi}$  and  $\beta_+ = \alpha_0\sqrt{\xi - 1}$ , we arrive at the result

$$f(\xi) = \frac{1 - 2\xi}{2\sqrt{\xi(1 - \xi)}} \sin\alpha_0 a \sqrt{\xi} \sinh\alpha_0 b \sqrt{1 - \xi} + \cos\alpha_0 a \sqrt{\xi} \cosh\alpha_0 b \sqrt{1 - \xi} = \cos k(a + b) \quad \dots 0 < E < U_0 \quad (3.18a)$$

$$\frac{1 - 2\xi}{2\sqrt{\xi(\xi - 1)}} \sin\alpha_0 a \sqrt{\xi} \sin\alpha_0 b \sqrt{\xi - 1} + \cos\alpha_0 a \sqrt{\xi} \cos\alpha_0 b \sqrt{\xi - 1} = \cos k(a + b) \quad \dots E > U_0 \quad (3.18b)$$



# Kronig-Penney: allowed k, E

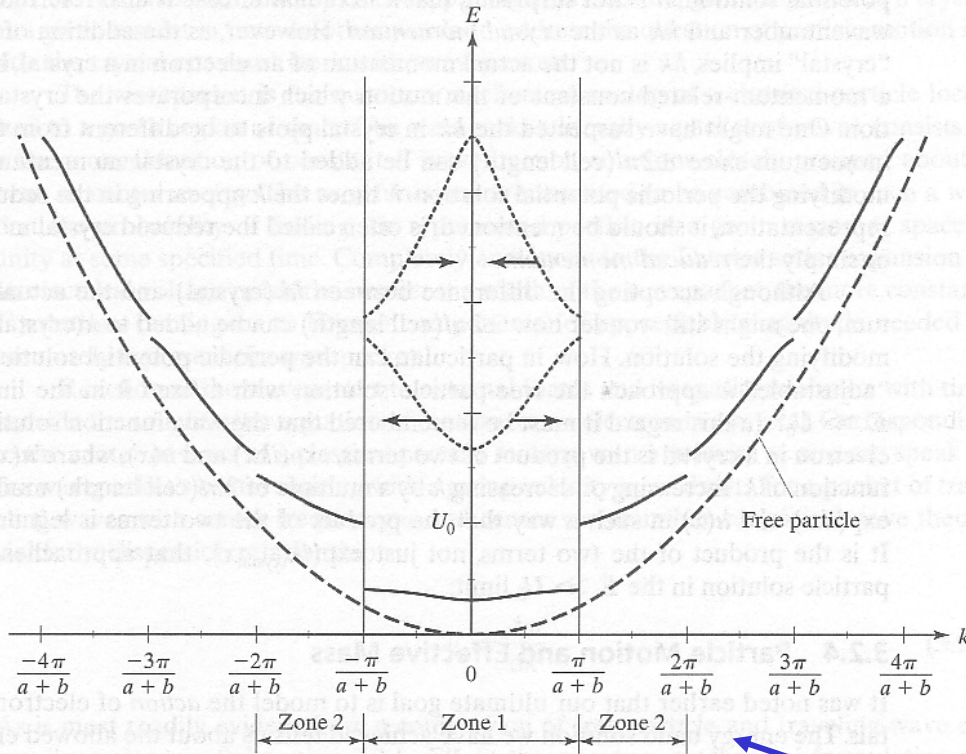


**Figure 3.3** Graphical determination of allowed electron energies. The left-hand side of the Eqs. (3.18) Kronig-Penney model solution is plotted as a function of  $\xi = E/U_0$ . The shaded regions where  $-1 \leq f(\xi) \leq 1$  identify the allowed energy states  $(\alpha_0 a = \alpha_0 b = \pi)$ . **Specific example**



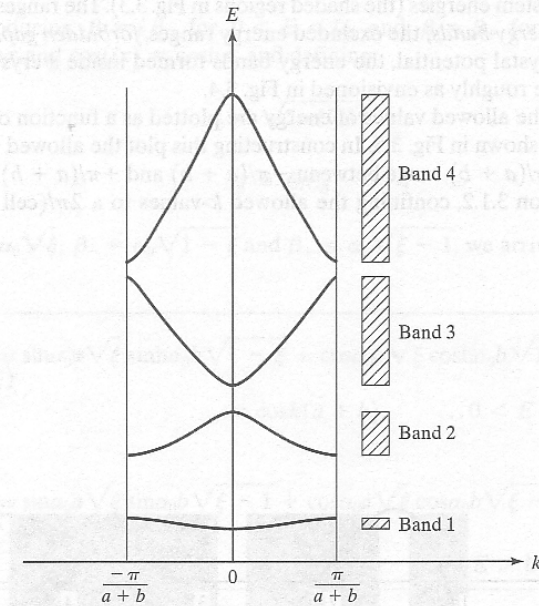
# Kronig-Penney: E-k relation

“extended zone representation”  
of allowed E-k states



**Figure 3.6** Extended-zone representation of allowed  $E-k$  states in a one-dimensional crystal (Kronig-Penney model with  $\alpha_0 a = \alpha_0 b = \pi$ ). Shown for comparison purposes are the free-particle  $E-k$  solution (dashed line) and selected bands from the reduced-zone representation (dotted lines). Arrows on the reduced-zone band segments indicate the directions in which these band segments are to be translated to achieve coincidence with the extended-zone representation. Brillouin zones 1 and 2 are also labeled on the diagram.

“reduced zone representation”  
of allowed E-k states



**Figure 3.5** Reduced-zone representation of allowed  $E-k$  states in a one-dimensional crystal (Kronig-Penney model with  $\alpha_0 a = \alpha_0 b = \pi$ ).

“Brillouin zones”

# Lectures 16, 17 - summary

- Potential wells + barriers and the Bloch theorem for periodic potentials led us to understand the allowed energy band structure for electrons in a simplified 1-d crystal model
- In particular we understood how the E-k relation is obtained
- Two k values correspond to each allowed E value; multiples of  $\pm 2\pi/(\text{cell length})$  can be added to k without modifying the periodic potential solution.
- For a free particle, k is the wave-number and  $hk/2\pi = \langle p \rangle$  is the particle momentum. In a crystal,  $hk/2\pi$  is the “crystal” momentum: it is not the actual momentum of the electron, but rather a constant of the motion that incorporates the interaction with the periodic crystal!
- Next: let us revisit electron effective mass, etc...



# Lecture 16, 17 - exercises

- **Exercise 16.1:** Consider the derivation of “bound” solutions for the finite well; following the track given in this lecture, fill in the calculations leading to the equation for the energy eigenvalues for the “even” solutions. Find the numerical energy eigenvalue for the lowest energy “even” state, assuming  $a = 500\text{\AA}$  and  $V_0 = 10\text{eV}$ .
- **Exercise 16.2:** Following the method described in this lecture (see also back-up slides for details), derive the transmission amplitude  $T$  for a “square” potential barrier for  $E < V_0$  and the approximate expression for the tunneling probability  $|T|^2$ . Compute the numerical value of the transmission (tunneling) probability for a particle with energy  $E = 9\text{eV}$ , incident on a “square” potential barrier ( $V_0 = 10\text{ eV}$ ,  $a = 50\text{\AA}$  and  $100\text{\AA}$ )
- **Exercise 17.1:** (a) Check that the two forms given for the Bloch wave functions in the Bloch theorem are indeed equivalent. (b) Explain in words what is meant by “Brillouin zones”





**Back-up slides**

# Reflection and Transmission

We are interested in finding  $R$  and  $T$ , given the four linear equations (8-8) through (8-11) for  $A$ ,  $B$ ,  $R$ , and  $T$ . We start by defining  $X = A \exp(ika)$  and  $Y = B \exp(-ika)$ . Then Eqs. (8-10) and (8-11) become, respectively,

$$X + Y = T \exp(ika) \quad (\text{A-1})$$

and

$$X - Y = \left(\frac{k}{q}\right) T \exp(ika). \quad (\text{A-2})$$

We can solve for  $X$  and  $Y$  by taking the sum and difference, respectively, of these equations. Once we have  $X$  and  $Y$ , we have, in turn,  $A = X \exp(-ika)$  and  $B = Y \exp(+ika)$ . These can be substituted into Eqs. (8-8) and (8-9), respectively giving

$$\begin{aligned} \exp(-ika) + R \exp(ika) &= \frac{q+k}{2q} T \exp[i(k-2q)a] \\ &+ \frac{q-k}{2q} T \exp[i(k+2q)a] \end{aligned} \quad (\text{A-3})$$

and

$$\begin{aligned} \exp(-ika) - R \exp(ika) &= \frac{q+k}{2k} T \exp[i(k-2q)a] \\ &- \frac{q-k}{2k} T \exp[i(k+2q)a]. \end{aligned} \quad (\text{A-4})$$

If we now take the sum of these two equations, we get a linear equation for  $T$  alone, which we can easily solve, giving Eq. (8-13). In turn, we substitute our result for  $T$  into either Eq. (A-3) or Eq. (A-4), which then becomes a linear equation for  $R$ , and this immediately gives Eq. (8-12).

