

Lecture 33 & 34

10/12/20

T. 26.1: Funzione d'onda e equazione di Schrödinger dipendente dal tempo.

Revanth Reddy Pannala
EBIT, Unibo
రేవంథ రెడ్డి పానలా

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Hamiltonian Operator — I

For systems of microscopic particles q_{i0} and p_{i0} are not available, hence $q_i(t)$ and $p_i(t)$ cannot be calculated. The information about the system must be limited to a statistical description, which is carried out by means of the (complex) wave function $\psi(\mathbf{q}, t)$. Here, only the wave functions such that $|\psi|^2$ is integrable will be considered, whence the normalization condition holds:

$$\int_{\infty} |\psi|^2 dq = 1, \quad dq \doteq dq_1 \dots dq_s$$

The meaning of ψ is that $|\psi(\mathbf{q}', t)|^2 dq$ is the probability that at time t the i th coordinate q_i belongs to the interval dq_i around q'_i , $i = 1, \dots, s$. Since $|\psi(\mathbf{q}', t)|^2 dq$ is a probability, then $|\psi(\mathbf{q}', t)|^2$ is a probability density.

The wave function is a solution of a differential equation. Such equation is the time-dependent Schrödinger equation

$$\mathcal{H}\psi = j\hbar \frac{\partial \psi}{\partial t}$$

where \mathcal{H} is the Hamiltonian operator.

T. 26.2: Operatore hamiltoniano.

Hamiltonian Operator — II

The Hamiltonian operator is derived from the Hamiltonian function by replacing each pair q_i, p_i of conjugate coordinates with a pair of operators:

$$q_i \leftarrow \hat{q}_i = q_i, \quad p_i \leftarrow \hat{p}_i = -j\hbar \frac{\partial}{\partial q_i}$$

where $\hbar \simeq 1.055 \cdot 10^{-34} \text{ Js}$ is the reduced Planck constant.

Example: if the system is described by Cartesian orthogonal coordinates \mathbf{r}_j , $j = 1, \dots, N$, and $H = T + V = E = \text{const}$, it is

$$\begin{aligned} H &= \sum_{j=1}^N \frac{1}{2m_j} (p_{1j}^2 + p_{2j}^2 + p_{3j}^2) + V(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ \mathcal{H} &= \sum_{j=1}^N \frac{-\hbar^2}{2m_j} \nabla_j^2 + V(\mathbf{r}_1, \dots, \mathbf{r}_N) \end{aligned}$$

For $N = 1$ it is $\mathcal{H} = -\hbar^2/(2m) \nabla^2 + V(\mathbf{r})$. In this case:

$$\psi = \sum_{k_1 k_2 k_3} c(\mathbf{k}) w(\mathbf{r}, \mathbf{k}) \exp[-jE(\mathbf{k})t/\hbar]$$

where the components of vector $\mathbf{k} \equiv (k_1, k_2, k_3)$, (wave vector, $[k_i] = \text{cm}^{-1}$), are proportional to integers.

T. 26.3: Il vettore d'onda nel caso dell'energia potenziale periodica.

Hamiltonian Operator — III

Replacing ψ in the Schrödinger equation shows that $w(\mathbf{r}, \mathbf{k})$ and $E(\mathbf{k})$ are the eigenfunctions and eigenvalues of the equation $\mathcal{H}w = Ew$. The meaning of $E(\mathbf{k})$ is that it provides the possible values of the particle's energy in the potential $V(\mathbf{r})$. The orthonormality condition holds:

$$\int w^*(\mathbf{r}, \mathbf{k}) w(\mathbf{r}, \mathbf{k}') d^3r = \delta[\mathbf{k} - \mathbf{k}']$$

while $|c(\mathbf{k})|^2$ is the probability that the particle's state is \mathbf{k} .

In crystals, V has the periodicity of the direct lattice:

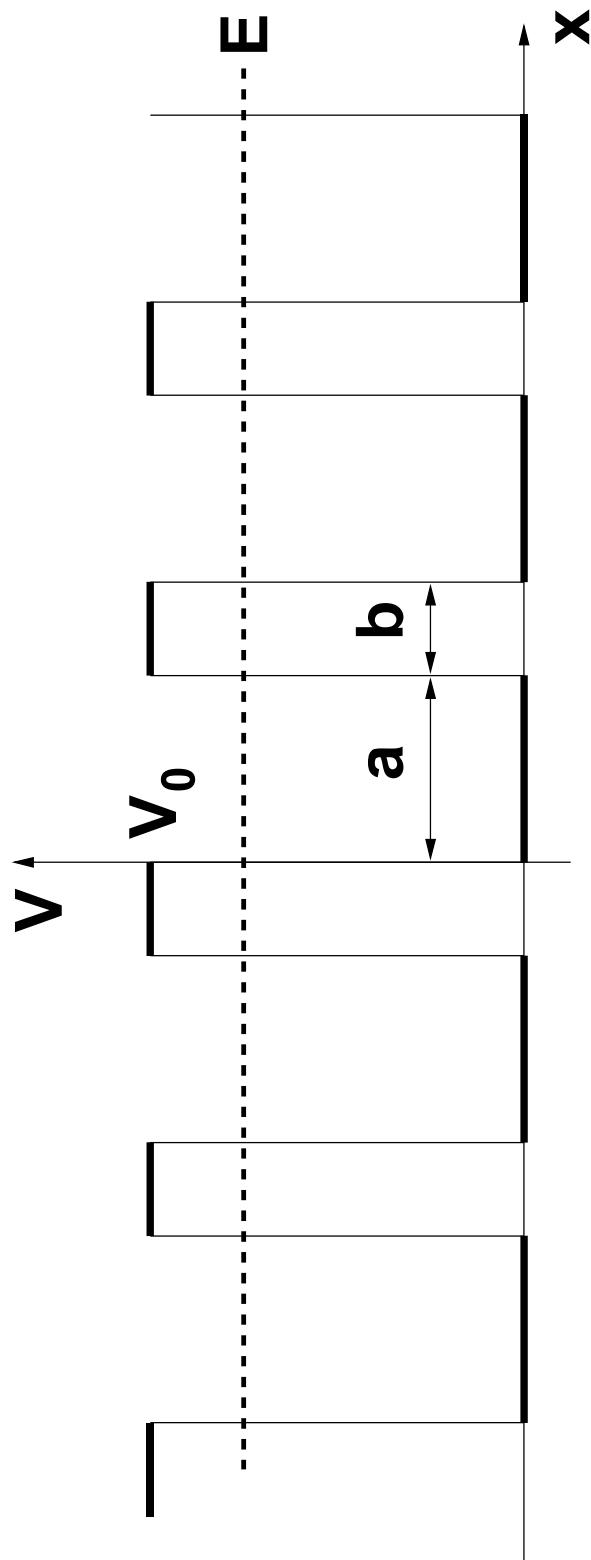
$$V(\mathbf{r} + \mathbf{l}) = V(\mathbf{r}), \quad \mathbf{l} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$$

If the crystal is limited, and has N_i cells along the i th side, the following holds:

$$\mathbf{k} = \frac{n_1}{N_1} 2\pi \mathbf{b}_1 + \frac{n_2}{N_2} 2\pi \mathbf{b}_2 + \frac{n_3}{N_3} 2\pi \mathbf{b}_3$$

where $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the characteristic vectors of the reciprocal lattice and $n_1 = 0, 1, \dots, N_1 - 1$ etc. As a consequence, \mathbf{k} belongs to the Brillouin zone and has $N_c = N_1 N_2 N_3$ possible values.

T. 26.4: Schematizzazione del potenziale periodico in una dimensione.



T. 26.5: Il caso del potenziale periodico in una dimensione.

Periodic Potential — I

Taking a one-dimensional case, let $V = 0$ for $n(a+b) < x < n(a+b)+a$ and $V = V_0 > 0$ for $n(a+b)-b < x < n(a+b)$, with $n = 0, \pm 1, \pm 2, \dots$. The first characteristic vector is $\mathbf{a}_1 = (a+b)\mathbf{i}_1$, whereas the remaining two can be chosen arbitrarily, e.g., $\mathbf{a}_2 = a_2\mathbf{i}_2$, $\mathbf{a}_3 = a_3\mathbf{i}_3$. It follows

$$\mathbf{b}_1 = \frac{a_2\mathbf{i}_2 \wedge a_3\mathbf{i}_3}{(a+b)\mathbf{i}_1 \bullet a_2\mathbf{i}_2 \wedge a_3\mathbf{i}_3} = \frac{\mathbf{i}_1}{a+b}, \quad \mathbf{b}_2 = \frac{\mathbf{i}_2}{a_2}, \quad \mathbf{b}_3 = \frac{\mathbf{i}_3}{a_3}.$$

The first Brillouin zone extends from $-\pi/(a+b)$ to $+\pi/(a+b)$ in the \mathbf{i}_1 direction, whereas it can be made arbitrarily small in the other two directions by taking a_2, a_3 large.

From the general properties of the time-independent Schrödinger equation it follows $E \geq 0$. A non-localized wavefunction w should be expected even in the $E < V_0$ case due to the tunnel effect. In fact, the case $E < V_0$ will be considered here, whence

$$\begin{cases} \text{if } V = 0 : & -w'' = \alpha^2 w, \quad \alpha \doteq \sqrt{2mE}/\hbar \\ \text{if } V = V_0 : & w'' = \beta^2 w, \quad \beta \doteq \sqrt{2m(V_0 - E)}/\hbar \end{cases}$$

T. 26.6: Condizioni di saldatura della funzione d'onda (I).

Periodic Potential — II

Due to the Bloch theorem, the wavefunction has the form

$$w_k = u_k \exp(jkx), \quad u_k(x + a + b) = u_k(x),$$

where k belongs to the first Brillouin zone. It follows:

$$\begin{cases} \text{if } V = 0 : & u_k'' + 2jk u_k' - (k^2 - \alpha^2) u_k = 0 \\ \text{if } V = V_0 : & u_k'' + 2jk u_k' - (k^2 + \beta^2) u_k = 0 \end{cases}$$

The associated algebraic equations have the roots

$$\begin{cases} \text{if } V = 0 : & s = -jk \pm \sqrt{-k^2 + (k^2 - \alpha^2)} = -jk \pm j\alpha \\ \text{if } V = V_0 : & s = -jk \pm \sqrt{-k^2 + (k^2 + \beta^2)} = -jk \pm \beta \end{cases}$$

whence

$$\begin{cases} \text{if } V = 0 : & u_k^+ = c_1 \exp[j(\alpha - k)x] + c_2 \exp[-j(\alpha + k)x] \\ \text{if } V = V_0 : & u_k^- = c_3 \exp[(\beta - jk)x] + c_4 \exp[-(\beta + jk)x] \end{cases}$$

The continuity conditions at $x = 0$ yield

$$\begin{aligned} \begin{cases} u_k^+(0) = u_k^-(0) \\ (u_k^+)'(0) = (u_k^-)'(0) \end{cases} &\Rightarrow c_1 + c_2 = c_3 + c_4 \\ &\Rightarrow j\alpha(c_1 - c_2) = \beta(c_3 - c_4) \\ \Rightarrow c_1 = \sigma c_3 + \sigma^* c_4, \quad c_2 = \sigma^* c_3 + \sigma c_4, \quad 2\sigma &\doteq 1 - j\beta/\alpha. \end{aligned}$$

T. 26.7: Condizioni di saldatura della funzione d'onda (II).

Periodic Potential — III

The periodicity of u (namely, $u_k^+(a) = u_k^-(-b)$) yields

$$c_1 A + c_2 / A = K L (c_3 / B + c_4 B),$$

with $A = \exp(j\alpha a)$, $B = \exp(\beta b)$ and, similarly, $K = \exp(jka)$, $L = \exp(jkb)$. Finally, from the periodicity of u' (namely, $(u_k^+)'(a) = (u_k^-)'(-b)$) one finds

$$c_1 A - c_2 / A = -K L (c_3 / B - c_4 B) j\beta / \alpha.$$

Coupling the last two equations provides two more expressions for c_1 and c_2 :

$$c_1 = \frac{KL}{A} \left(\frac{\sigma}{B} c_3 + \sigma^* B c_4 \right), \quad c_2 = A K L \left(\frac{\sigma^*}{B} c_3 + \sigma B c_4 \right).$$

Using $c_1 = \sigma c_3 + \sigma^* c_4$, $c_2 = \sigma^* c_3 + \sigma c_4$ yields the system

$$\sigma \left(1 - \frac{KL}{AB} \right) c_3 + \sigma^* \left(1 - \frac{BKL}{A} \right) c_4 = 0$$

$$\sigma^* \left(1 - \frac{AKL}{B} \right) c_3 + \sigma (1 - ABKL) c_4 = 0$$

A solution is possible only if the determinant vanishes. This in turn determines a relation between $\alpha(E)$, $\beta(E)$, and k .

T. 26.8: Calcolo della relazione $E(k)$.

Periodic Potential — IV

The determinant vanishes if

$$(\sigma^{*2} - \sigma^2) \left(KL + \frac{1}{KL} \right) = \sigma^{*2} \left(\frac{A}{B} + \frac{B}{A} \right) - \sigma^2 \left(AB + \frac{1}{AB} \right).$$

Introducing the expression of σ and those of A, B, K, L transforms the above into

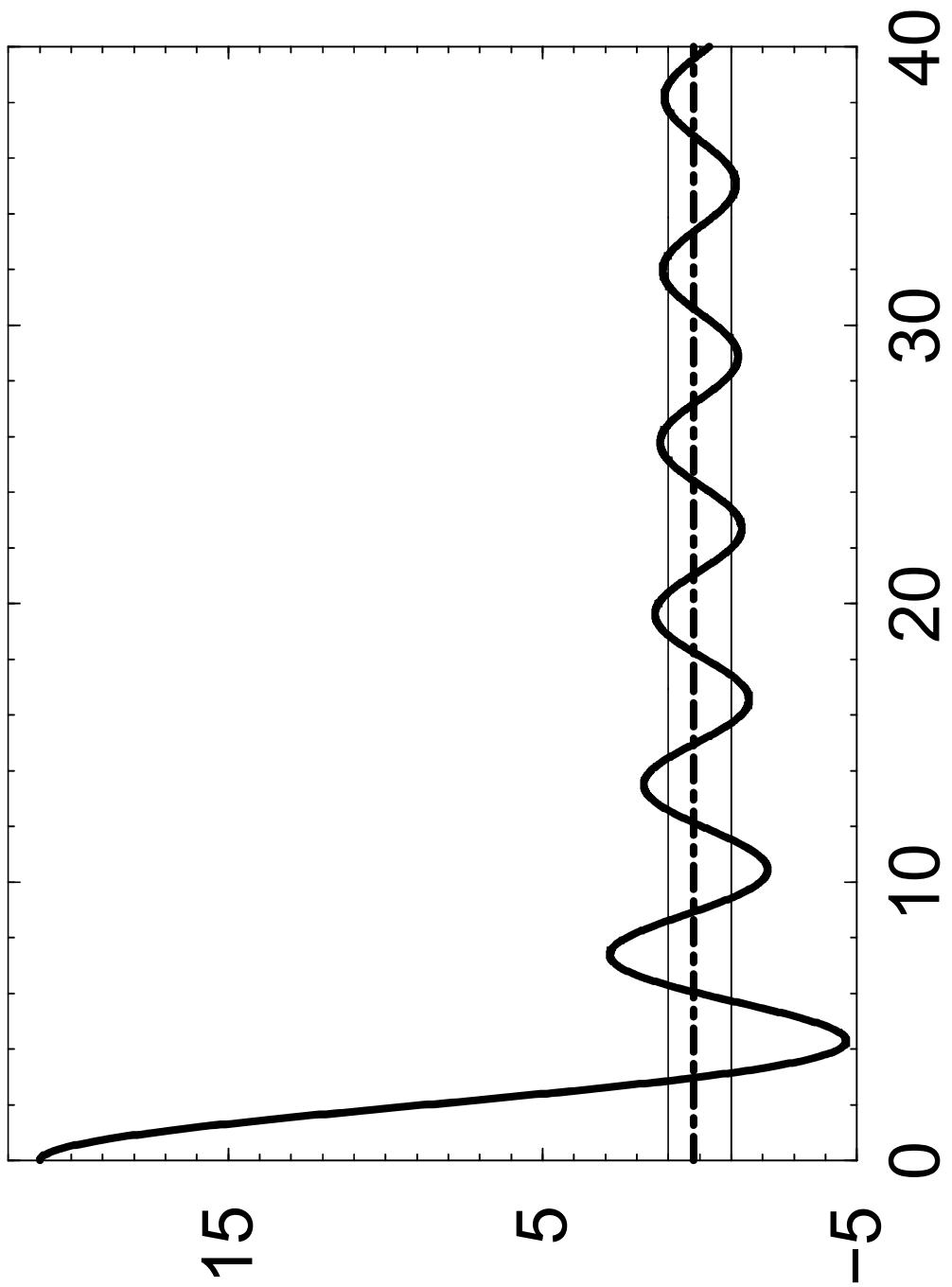
$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin(\alpha a) \sinh(\beta b) + \cos(\alpha a) \cosh(\beta b) = \cos[k(a+b)]$$

which has the form $F(E) = G(k)$. From this, the relation $E = E(k)$ can be determined. It is worth noting that $G(-k) = G(k)$ and $G[k+2\pi/(a+b)] = G(k)$. As a consequence the function $E(k)$ is even, and has the periodicity of the reciprocal scaled lattice.

A simplified expression is found by taking $V_0 \gg E$, so that $\beta^2 \gg \alpha^2$. This, however, would eliminate the tunnel effect, unless $b \rightarrow 0$ as $V_0 \rightarrow \infty$. In this case $\beta^2 b \rightarrow \text{const} \neq 0$, $\beta b \rightarrow 0$, $\sinh(\beta b) \rightarrow \beta b$, $\cosh(\beta b) \rightarrow 1$, and

$$\frac{\beta^2}{2\alpha\beta} \sin(\alpha a) \beta b + \cos(\alpha a) = \cos(ka).$$

T. 26.9: Determinazione grafica della relazione $E(k)$.



T. 26.10: Modello di Krönig e Penney.

Periodic Potential — V

Krönig-Penney Model

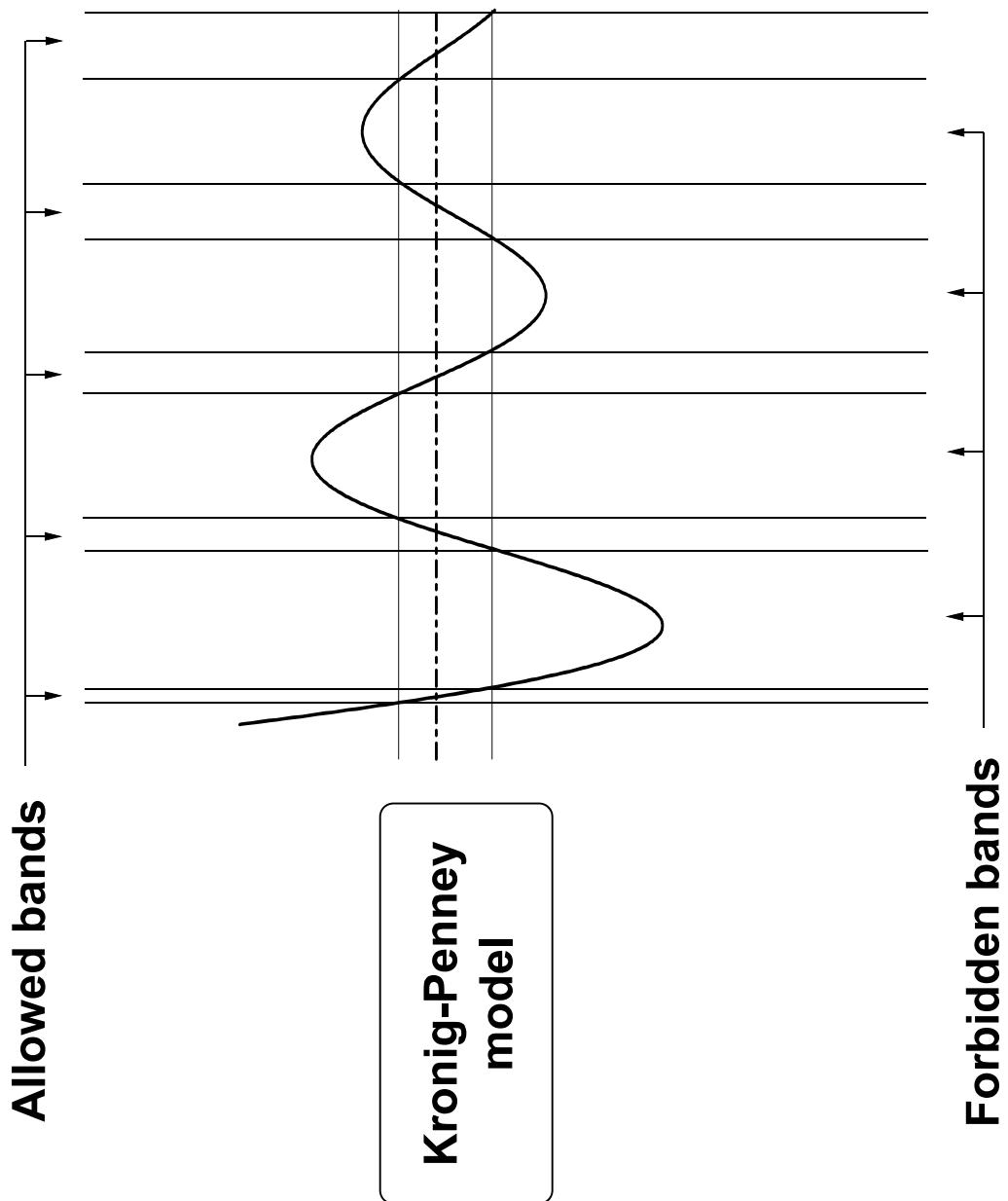
Letting $\theta \doteq \lim(ab\beta^2/2)$, the relation $F(E) = G(k)$ becomes

$$\theta \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka), \quad \theta > 0, \quad \alpha = \frac{\sqrt{2mE}}{\hbar}.$$

The function $E = E(k)$ can be determined from the above by numerical calculation: given k , the right hand side is fixed at some value $-1 \leq \cos(ka) \leq 1$. The energy E can then be found by seeking αa such that the two sides become equal. The following are worth noting:

- As the left hand side oscillates, there is more than one solution for a given k , namely, $E(k)$ is a multi-valued function.
- There is no solution for $\alpha a \rightarrow 0$ as the left hand side tends to $\theta + 1 > 0$. Actually, there are intervals of energy such that no solution exists, called *forbidden energy bands*.
- At large energies the relation tends to $\cos(\alpha a) = \cos(ka)$, namely, to the free-particle one: $k = \alpha = \sqrt{2mE}/\hbar$.
- For a finite structure the above treatment still holds, with k a discrete variable.

T. 26.11: Bande permesse e bande proibite.



Hamiltonian Operator — III

Replacing ψ in the Schrödinger equation shows that $w(\mathbf{r}, \mathbf{k})$ and $E(\mathbf{k})$ are the eigenfunctions and eigenvalues of the equation $\mathcal{H}w = Ew$. The meaning of $E(\mathbf{k})$ is that it provides the possible values of the particle's energy in the potential $V(\mathbf{r})$. The orthonormality condition holds:

$$\int w^*(\mathbf{r}, \mathbf{k}) w(\mathbf{r}, \mathbf{k}') d^3r = \delta[\mathbf{k} - \mathbf{k}']$$

while $|c(\mathbf{k})|^2$ is the probability that the particle's state is \mathbf{k} .

In crystals, V has the periodicity of the direct lattice:

- $V(\mathbf{r} + \mathbf{l}) = V(\mathbf{r})$, $\mathbf{l} = m_1 \mathbf{a}_1 + m_2 \mathbf{a}_2 + m_3 \mathbf{a}_3$ Translational vectors in direct lattice

If the crystal is limited, and has N_i cells along the i th side, the lattice following holds:

$$\mathbf{k} = \frac{n_1}{N_1} 2\pi \mathbf{b}_1 + \frac{n_2}{N_2} 2\pi \mathbf{b}_2 + \frac{n_3}{N_3} 2\pi \mathbf{b}_3$$

where $\mathbf{b}_1, \mathbf{b}_2, \mathbf{b}_3$ are the characteristic vectors of the reciprocal lattice and $n_1 = 0, 1, \dots, N_1 - 1$ etc. As a consequence, \mathbf{k} belongs to the Brillouin zone and has $N_c = N_1 N_2 N_3$ possible values.

The exercise of this lecture is the solution of the Schrödinger eqⁿ independent of time in a Periodic Potential energy. Because it is a typical case that occurs in the Crystals as they are periodic structures.

→ If we assume atoms are fixed in equilibrium positions then the force felt by the e^- that moves inside the crystal is due to a Potential Period Energy. Otherwise the form of the PPE is complicated

* But we shall take a simplified model for our Analytic purposes. However many important features of the actual solution are kept by the simplified Model.

→ Any vector \mathbf{k}' in the reciprocal scaled lattice

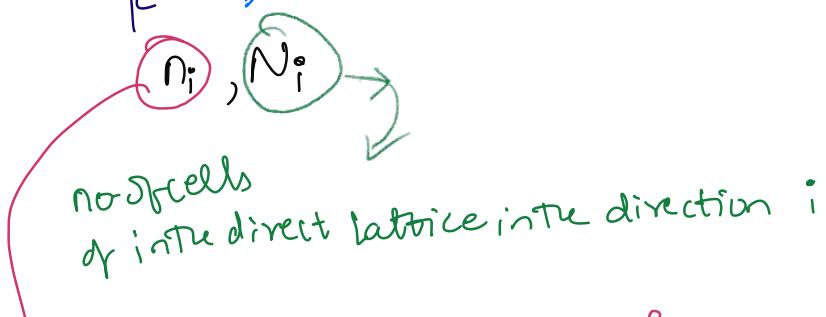
$$\mathbf{k}' = \frac{n_1}{N_1} 2\pi \mathbf{b}_1 + \frac{n_2}{N_2} 2\pi \mathbf{b}_2 + \frac{n_3}{N_3} 2\pi \mathbf{b}_3$$

- In principle the coefficients of the linear combination should be real numbers, at

Some point we introduced the Periodic Boundary Conditions and they have the effect ~~to~~ one to restore periodicity in a finite volume of the material.

That in principle is not periodic

- Two the second effect is that if we impose the periodic Boundary conditions, the coefficients of ' k ' become discrete. They become rational



nodes in the direct lattice or in the reciprocal lattice

are integers that go from 0 to $N_i - 1$

→ That means we can limit the consideration of the k -vector only to one period of reciprocal scaled lattice and this period is the Elementary cell i.e. the Brillouin Zone.

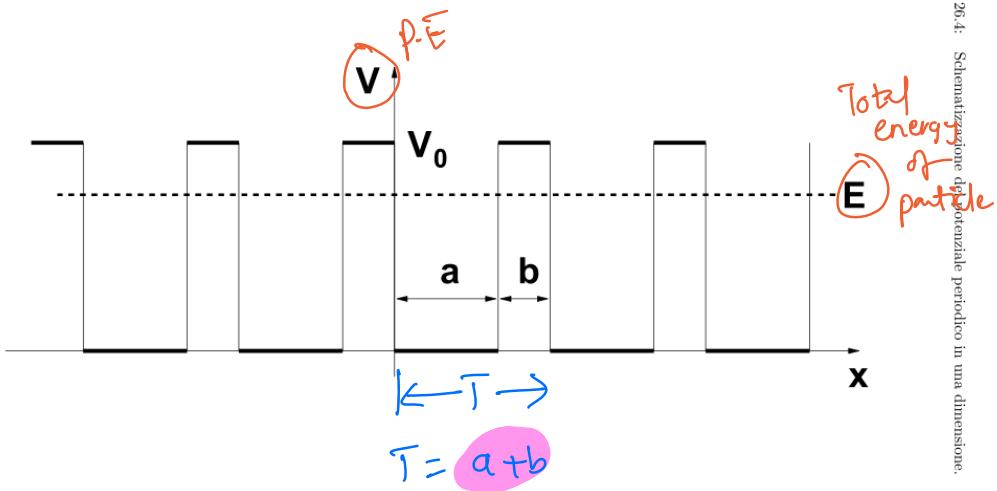
- The 2nd consequence is that the total no. of distinct k -vectors in the BZ is the product of N_1, N_2, N_3 i.e. the k -vectors although discrete are many. They are very dense and when we take derivatives we can do it safely.

→ we can exploit a result which is full General before solving for the Schrödinger eq with approximation.

This result is for P.E which is Periodic we find that the solutions have a special form. This applies to operators that are periodic

* Hamiltonian is periodic if P.E is periodic.
because kinetic part is invariant upon Translation

The simplest form of periodic P.E is piecewise constant 1D we see below.



T. 26.4: Schematizzazione del potenziale periodico in una dimensione.



Revanth Reddy Pannala
EBIT, Unibo
ఫ్లోట్ బెన్జి

Periodic Potential — I

- Taking a one-dimensional case, let $V = 0$ for $n(a+b) < x < n(a+b)+a$ and $V = V_0 > 0$ for $n(a+b)-b < x < n(a+b)$, with $n = 0, \pm 1, \pm 2 \dots$. The first characteristic vector is $\mathbf{a}_1 = (a+b)\mathbf{i}_1$, whereas the remaining two can be chosen arbitrarily, e.g., $\mathbf{a}_2 = a_2\mathbf{i}_2$, $\mathbf{a}_3 = a_3\mathbf{i}_3$. It follows *assuming $\mathbf{i}_1, \mathbf{i}_2, \mathbf{i}_3$ are mutually orthogonal.*

$$\mathbf{b}_1 = \frac{a_2\mathbf{i}_2 \wedge a_3\mathbf{i}_3}{(a+b)\mathbf{i}_1 \bullet a_2\mathbf{i}_2 \wedge a_3\mathbf{i}_3} = \frac{\mathbf{i}_1}{a+b}, \quad \mathbf{b}_2 = \frac{\mathbf{i}_2}{a_2}, \quad \mathbf{b}_3 = \frac{\mathbf{i}_3}{a_3}.$$

- The first Brillouin zone extends from $-\pi/(a+b)$ to $+\pi/(a+b)$ in the \mathbf{i}_1 direction, whereas it can be made arbitrarily small in the other two directions by taking a_2, a_3 large.
- From the general properties of the time-independent Schrödinger equation it follows $E \geq 0$. A non-localized wavefunction w should be expected even in the $E < V_0$ case due to the tunnel effect. In fact, the case $E < V_0$ will be considered here, whence

$$\begin{cases} \text{if } V = 0 : & -w'' = \alpha^2 w, \\ \text{if } V = V_0 : & w'' = \beta^2 w, \end{cases} \quad \begin{array}{l} \alpha \doteq \sqrt{2mE/\hbar} \\ \beta \doteq \sqrt{2m(V_0 - E)/\hbar} \end{array}$$

The sol'n of S-E is expected to be oscillatory for $V=0$

- We remember that the Brillouin zone is symmetric w.r.t. Origin.



Due to the Bloch theorem, the wavefunction has the form

$$w_k = u_k \exp(jkx), \quad u_k(x + a + b) = u_k(x),$$

where k belongs to the first Brillouin zone. It follows:

$$\begin{cases} \text{if } V = 0 : & u_k'' + 2jk u_k' - (k^2 - \alpha^2) u_k = 0 \\ \text{if } V = V_0 : & u_k'' + 2jk u_k' - (k^2 + \beta^2) u_k = 0 \end{cases}$$

This is similar
to potential
STEP, Barrier
+ well calculations
we did earlier.

Since there
are infinite
periods, it is
possible to do
calculations only
in one period
because of a
Theorem
"Bloch
Theorem"

↳

* 'K' is a wave vector in 1D
 & it is related to expectation value of the Momentum.

Periodic Potential — II

- Due to the Bloch theorem, the wavefunction has the form

$$w_k = u_k \exp(jkx), \quad u_k(x + a + b) = u_k(x), \quad \text{Time period}$$

where k belongs to the first Brillouin zone. It follows:

$$\begin{cases} \text{if } V = 0 : & u_k'' + 2jk u_k' - (k^2 - \alpha^2) u_k = 0 \\ \text{if } V = V_0 : & u_k'' + 2jk u_k' - (k^2 + \beta^2) u_k = 0 \end{cases}$$

We have to solve for 'u'
 The associated algebraic equations have the roots

$$\begin{cases} \text{if } V = 0 : & s = -jk \pm \sqrt{-k^2 + (k^2 - \alpha^2)} = -jk \pm j\alpha \\ \text{if } V = V_0 : & s = -jk \pm \sqrt{-k^2 + (k^2 + \beta^2)} = -jk \pm \beta \end{cases}$$

whence

$$\begin{cases} \text{if } V = 0 : & u_k^+ = c_1 \exp[j(\alpha - k)x] + c_2 \exp[-j(\alpha + k)x] \\ \text{if } V = V_0 : & u_k^- = c_3 \exp[(\beta - jk)x] + c_4 \exp[-(\beta + jk)x] \end{cases}$$

The continuity conditions at $x = 0$ yield

$$\begin{cases} u_k^+(0) = u_k^-(0) \Rightarrow c_1 + c_2 = c_3 + c_4 \\ (u_k^+)'(0) = (u_k^-)'(0) \Rightarrow j\alpha(c_1 - c_2) = \beta(c_3 - c_4) \end{cases}$$

$$\Rightarrow c_1 = \sigma c_3 + \sigma^* c_4, \quad c_2 = \sigma^* c_3 + \sigma c_4, \quad 2\sigma \doteq 1 - j\beta/\alpha.$$

K is also related to Energy

c_1, c_2, c_3, c_4
 are 4 unknown coefficients.
 But we are not able to find the solns because the Algebraic

s/s is homogeneous.

Periodic Potential — III

- The periodicity of u (namely, $u_k^+(a) = u_k^-(b)$) yields

$$c_1 A + c_2 / A = K L (c_3 / B + c_4 B),$$

with $A = \exp(j\alpha a)$, $B = \exp(\beta b)$ and, similarly, $K = \exp(jka)$, $L = \exp(jkb)$. Finally, from the periodicity of u' (namely, $(u_k^+)'(a) = (u_k^-)'(-b)$) one finds

$$c_1 A - c_2 / A = -K L (c_3 / B - c_4 B) j\beta / \alpha.$$

- Coupling the last two equations provides two more expressions for c_1 and c_2 :

$$c_1 = \frac{KL}{A} \left(\frac{\sigma}{B} c_3 + \sigma^* B c_4 \right), \quad c_2 = AKL \left(\frac{\sigma^*}{B} c_3 + \sigma B c_4 \right).$$

Using $c_1 = \sigma c_3 + \sigma^* c_4$, $c_2 = \sigma^* c_3 + \sigma c_4$ yields the system

$$\begin{aligned} \sigma \left(1 - \frac{KL}{AB} \right) c_3 + \sigma^* \left(1 - \frac{BKL}{A} \right) c_4 &= 0 \\ \sigma^* \left(1 - \frac{AKL}{B} \right) c_3 + \sigma \left(1 - ABKL \right) c_4 &= 0 \end{aligned}$$

a, b are given because they belong to the structures.

In order to solve the Homogeneous S_S we must impose the Determinant of coefficients to ZERO.

A solution is possible only if the determinant vanishes. This in turn determines a relation between $\alpha(E)$, $\beta(E)$, and k .

Periodic Potential — IV

- The determinant vanishes if

$$(\sigma^{*2} - \sigma^2) \left(KL + \frac{1}{KL} \right) = \sigma^{*2} \left(\frac{A}{B} + \frac{B}{A} \right) - \sigma^2 \left(AB + \frac{1}{AB} \right).$$

- Introducing the expression of σ and those of A, B, K, L transforms the above into

$$\frac{\beta^2 - \alpha^2}{2\alpha\beta} \sin(\alpha a) \sinh(\beta b) + \cos(\alpha a) \cosh(\beta b) = \cos[k(a+b)]$$

which has the form $F(E) = G(k)$. From this, the relation $E = E(k)$ can be determined. It is worth noting that $G(-k) = G(k)$ and $G[k+2\pi/(a+b)] = G(k)$. As a consequence the function $E(k)$ is even, and has the periodicity of the reciprocal scaled lattice.

- A simplified expression is found by taking $V_0 \gg E$, so that $\beta^2 \gg \alpha^2$. This, however, would eliminate the tunnel effect, unless $b \rightarrow 0$ as $V_0 \rightarrow \infty$. In this case $\beta^2 b \rightarrow \text{const} \neq 0$, $\beta b \rightarrow 0$, $\sinh(\beta b) \rightarrow \beta b$, $\cosh(\beta b) \rightarrow 1$, and

$$\frac{\beta^2}{2\alpha\beta} \sin(\alpha a) \beta b + \cos(\alpha a) = \cos(ka).$$

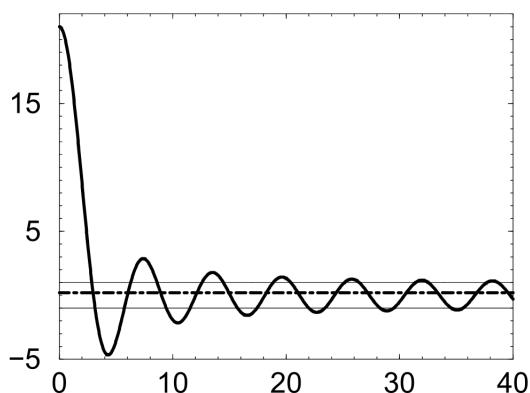
is an even function.
energy momentum

which proves that Energy is even w.r.t Momentum!

Conclusion: Due to the Periodicity of the Direct lattice
The Eigen value of the Problem i.e Energy
is periodic in the reciprocal scaled lattice

• Ultimately we aim to find the relation
between Energy & Momentum after end of this calculation

$F(E) = G(k)$
Function of Energy Function of Momentum



* When we discussed about Semiconductor Bands we studied about relationship between E & k in a crystal.

- We noticed that this Energy Relation is made up of several branches of the functions that are called Bands.

~~* We can clearly remember that Bands are symmetric from left to right also they are shown with the First Brillouin Zone.~~

Periodic Potential — V

Krönig-Penney Model

- Letting $\theta \doteq \lim(ab\beta^2/2)$, the relation $F(E) = G(k)$ becomes

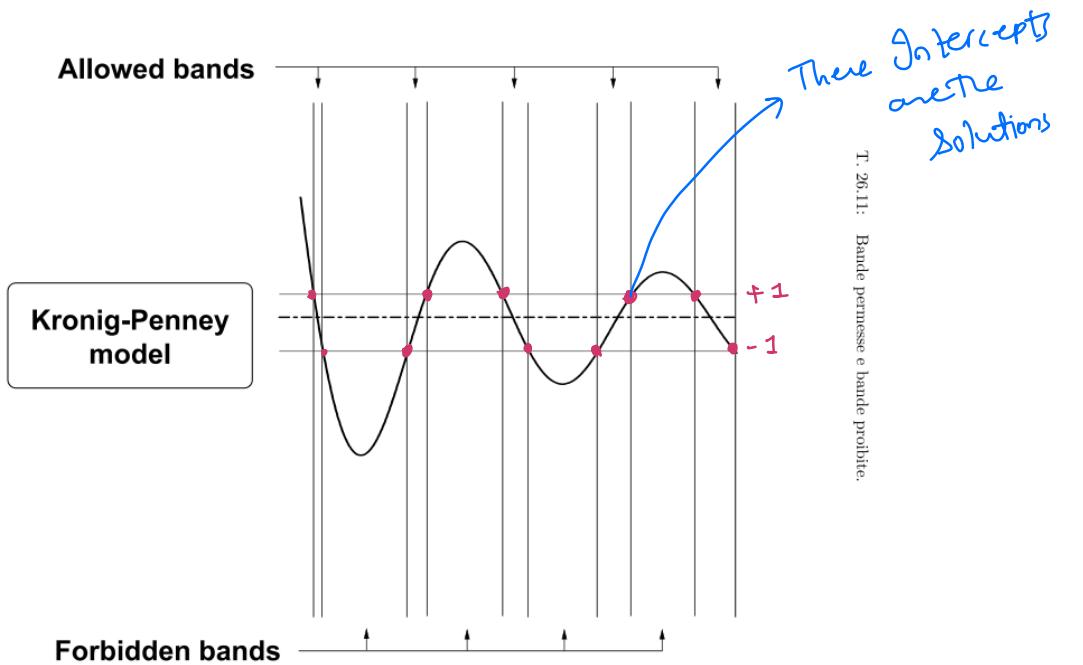
$$\theta \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka), \quad \theta > 0, \quad \alpha = \frac{\sqrt{2mE}}{\hbar}.$$

The function $E = E(k)$ can be determined from the above by numerical calculation: given k , the right hand side is fixed at some value $-1 \leq \cos(ka) \leq 1$. The energy E can then be found by seeking αa such that the two sides become equal. The following are worth noting:

- As the left hand side oscillates, there is more than one solution for a given k , namely, $E(k)$ is a multi-valued function.
- There is no solution for $\alpha a \rightarrow 0$ as the left hand side tends to $\theta + 1 > 0$. Actually, there are intervals of energy such that no solution exists, called *forbidden energy bands*.
- At large energies the relation tends to $\cos(\alpha a) = \cos(ka)$, namely, to the free-particle one: $k = \alpha = \sqrt{2mE}/\hbar$.
- For a finite structure the above treatment still holds, with k a discrete variable.

Simplified form of the relation b/w E & k

$E \propto \alpha'$



Revanth Reddy Pannala
EBIT, Unibo
ఫ్లోట్ ఎస్టేషన్

Chapter 13

Comments on the Kronig-Penney Model

The Kronig-Penney model is simple enough to lend itself to a number of considerations based on an analytical approach. Some of them are shown below.

13.1 Band Calculation

The starting point is the dispersion relation (D.10),

$$\vartheta \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka), \quad \alpha = \frac{\sqrt{2mE}}{\hbar}, \quad (13.1)$$

with $\vartheta > 0$ and $-\pi/a \leq k \leq +\pi/a$. Considering that $\cos(ka)$ is even with respect to k , one can limit the analysis to the interval $-\pi/a \leq k \leq 0$, in which $\cos(ka)$ ranges between -1 and $+1$. The left hand side of (13.1) is shown in Fig. D.8 along with the limiting values $+1$ and -1 of the right hand side. The real solutions of (13.1) lie in the intervals of αa such that the corresponding values of the left hand side belong to the strip limited by the two horizontal lines.

Letting $2u = \alpha a > 0$, the real solutions of the first relation in (13.1) correspond to the inequalities

$$-1 \leq \frac{\vartheta}{2} \frac{2 \sin(u) \cos(u)}{u} + \cos^2(u) - \sin^2(u) \leq +1. \quad (13.2)$$

Excluding for the moment the cases where the equality holds, (13.2) is recast as

$$-\cos^2(u) < \frac{\vartheta}{2u} \sin(u) \cos(u) < \sin^2(u), \quad -1 < \frac{\vartheta}{2u} \tan(u) < \tan^2(u). \quad (13.3)$$

Observing that ϑ and u are positive, the latter splits as

$$\frac{2}{\vartheta} u > -\tan(u), \quad \frac{2}{\vartheta} u > \cot(u). \quad (13.4)$$

which must be fulfilled simultaneously. With reference to Fig. 13.1, the green ver-

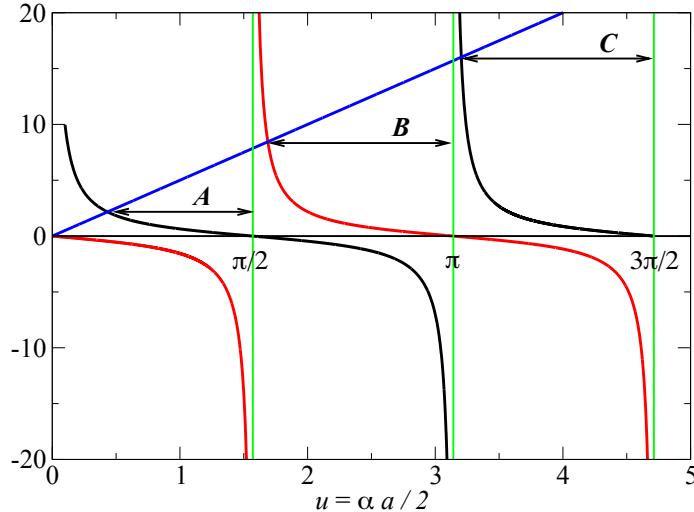


Fig. 13.1 Graphic solution of (13.4), with $\vartheta = 0.4$. The red curves represent $-\tan(u)$, the black curves represent $\cot(u)$, and the blue line represents $(2/\vartheta)u = 5u$.

tical lines mark the position of $u = \pi/2$, $u = \pi$, and $u = 3\pi/2$. In the interval $0 \leq u \leq \pi/2$, inequalities (13.4) are fulfilled for the values of u whose range is indicated with A ; in the subsequent intervals, the ranges are B and C , respectively. The extension of the ranges increases with u and has $\pi/2$ as limiting value.

If u equals an odd multiple of $\pi/2$, namely, $u = \pi/2, u = 3\pi/2, \dots$, the equality on the left of (13.1) is fulfilled; these values of u provide the upper edge of ranges like A and C ; in turn, if u equals an even multiple of $\pi/2$, namely, $u = \pi, u = 2\pi, \dots$, the equality on the right is fulfilled, and these values of u provide the upper edge of ranges like B . The $u \rightarrow 0$ limit, instead, yields $-1 \leq \vartheta + 1 \leq 1$, where the inequality on the right is impossible; this shows that the lowest value u_L of the A range is strictly positive, $0 < u_L \leq u \leq \pi/2$. From the second relation in (13.1) it follows that E is strictly positive as well. Similarly, the lowest value of the B is strictly larger than $\pi/2$, and so on.

A closer inspection shows that in the intervals $n\pi < u < (n+1/2)\pi$, with $n = 0, 1, 2, \dots$, the first inequality in (13.4) is always fulfilled; in such intervals, the value of u corresponding to the upper edge E_U of the band is $(n+1/2)\pi$ whence, using the second of (13.1) and $h = 2\pi\bar{h}$, one finds $E_U = [(n+1/2)h/a]^2/(2m)$. To find the lower edge E_L of the band in the same intervals, one must find the corresponding value u_L by solving $2u_L/\vartheta = \cot(u_L)$. In the same manner, the second inequality in (13.4) is always fulfilled in the intervals $(n+1/2)\pi < u < (n+1)\pi$, whence $E_U = [(n+1)h/a]^2/(2m)$; to find the lower edge of the band in the same intervals,

one must solve $2u_L/\vartheta = -\tan(u_L)$. As mentioned above, the limiting value of the range of u is $\pi/2$; it follows that in this model the high-energy limit of the band extension, in both intervals $n\pi < u < (n + 1/2)\pi$ and $(n + 1/2)\pi < u < (n + 1)\pi$, is

$$E_U - E_L \approx n \frac{(h/a)^2}{2m}. \quad (13.5)$$

To calculate, e.g., the shape of the lowest band, one must find the solution of $2u/\vartheta = \cot(u)$ in the interval $0 < u < \pi/2$; taking $\vartheta = 0.4$ for consistency with Fig. 13.1, the outcome is $u_L \simeq 0.43284$. Defining the normalized energy $\eta = E/E_0$, with $E_0 = 2\hbar^2/(ma^2)$, and using (13.1), it follows

$$ka = \arccos[2 \cos^2(\sqrt{\eta}) - 1 + \vartheta \sin(\sqrt{\eta}) \cos(\sqrt{\eta})/\sqrt{\eta}], \quad (13.6)$$

where the limits of η are $u_L^2 \simeq 0.18735$ and $\pi^2/4 \simeq 2.4674$. The inverse function of (13.6), namely, $\eta = \eta(ka)$ in the interval¹ $-\pi \leq ka \leq +\pi$, is shown in Fig. 13.2;

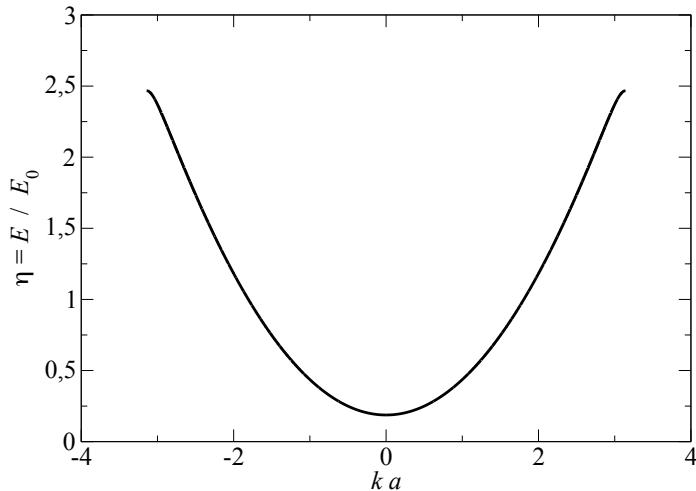


Fig. 13.2 The inverse function $\eta(ka)$ of (13.6), with $\vartheta = 0.4$.

the same function is shown in Fig. 13.3, where the first two bands are considered.

13.2 Solution in the Forbidden Gap

Still considering the lowest band, it has been observed above that the first inequality in (13.4) is always fulfilled in the interval $0 < u < \pi/2$, whereas the second one is

¹ Apart from the scaling factor a , this interval coincides with the Brillouin zone.

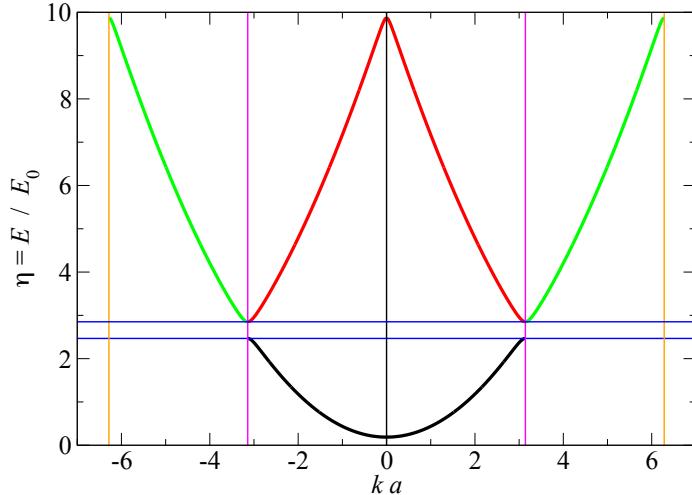


Fig. 13.3 The first two bands derived as the inverse function $\eta(ka)$ of (13.6), with $\vartheta = 0.4$. The lower band (black curve) is the same as in Fig. 13.2. The two vertical, magenta lines denote the first Brillouin zone in normalized units ($-\pi \leq ka \leq +\pi$). The green curves represent the second band; the second Brillouin zone is made of the two disjoint intervals $\pi \leq ka \leq 2\pi$ and $-2\pi \leq ka \leq -\pi$, whose boundaries are the pairs of magenta and orange lines. Folding the second band into the first Brillouin zone yields the red curve. The horizontal, blue lines are the limit of the forbidden gap between the first and second band, $\eta_1 \simeq 2.48$ and $\eta_2 \simeq 2.85$, respectively.

fulfilled only in the subinterval $u_L < u < \pi/2$; in the other subinterval $0 < u < u_L$, instead, there are no real solutions of (13.1) because its left hand side λ is larger than unity. It follows that the interval of energies corresponding to $0 < u < u_L$ is a forbidden band. As observed in Sect. D.9, the values of k that solve (13.1) with $\lambda > 1$ are imaginary: letting $ka = i\kappa a$, whence $\cos(ka) = \cosh(\kappa a)$, transforms (13.1) into $\exp(\kappa a) + \exp(-\kappa a) = 2\lambda$, whence $\exp(\kappa a) = \lambda \pm \sqrt{\lambda^2 - 1}$. Taking the logarithm and observing that $\lambda - \sqrt{\lambda^2 - 1} = (\lambda + \sqrt{\lambda^2 - 1})^{-1}$ finally yields

$$k = \pm \frac{i}{a} \log(\lambda + \sqrt{\lambda^2 - 1}), \quad \lambda = 2 \cos^2(\sqrt{\eta}) - 1 + \vartheta \frac{\sin(\sqrt{\eta}) \cos(\sqrt{\eta})}{\sqrt{\eta}}. \quad (13.7)$$

One notes that also in this case the dependence of η on k is even, as should be. The form of $\eta \kappa a$ for $\kappa \leq 0$ is shown in Fig. 13.4 (red curve), together with the right half of the curve of Fig. 13.2 (black curve).

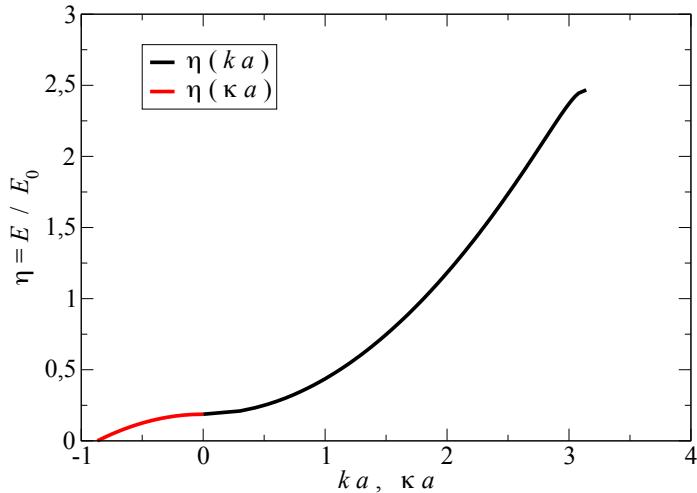


Fig. 13.4 The black curve shows the inverse function $\eta(ka)$ of (13.6), with $\vartheta = 0.4$ and $ka \geq 0$ (it coincides with the right half of the curve of Fig. 13.2). The red curve shows the inverse function $\eta(\kappa a)$ of (13.7), still with $\vartheta = 0.4$ and with $\kappa a \leq 0$.

13.3 Group Velocity and Effective Mass

The dispersion relation (13.1), still with $2u = \alpha a$, can also be used to calculate the group velocity v and the effective mass m^* . Using the definition $E_0 = 2\hbar^2/(ma^2)$ introduced in Sect. 13.1, the group velocity is found from

$$v = \frac{1}{\hbar} \frac{dE}{dk} = \frac{a}{\hbar} \frac{dE}{d(ka)} = \frac{a}{\hbar} \frac{dE}{du} \frac{du}{d(ka)} = \frac{a}{\hbar} \frac{2E_0 u}{d(ka)/du}. \quad (13.8)$$

Letting $F(u) = \vartheta \sin(2u)/(2u) + \cos(2u)$ transforms (13.1) into $\cos(ka) = F(u)$; to proceed, one uses primes to indicate derivatives with respect to u , this yielding $F' = -\sin(ka)d(ka)/du$, whence $d(ka)/du = \pm F'/\sqrt{1-F^2}$. In conclusion, letting $v_0 = 4\hbar/(ma)$ transforms (13.8) into

$$v = \pm v_0 u \frac{\sqrt{1-F^2}}{F'}, \quad F' = \vartheta \frac{2u \cos(2u) - \sin(2u)}{2u^2} - 2 \sin(2u). \quad (13.9)$$

To simplify the notation one lets $D = du/d(ka)$, whence

$$\frac{d^2u}{d(ka)^2} = \frac{dD}{d(ka)} = \frac{dD}{du} \frac{du}{d(ka)} = \frac{1}{2} \frac{dD^2}{du}. \quad (13.10)$$

From $D = du/d(ka) = \pm\sqrt{1-F^2}/F'$ it follows

$$\frac{d^2u}{d(ka)^2} = \frac{1}{2} \frac{d}{du} \left[\frac{1-F^2}{(F')^2} \right] = -\frac{F}{F'} - \frac{(1-F^2)F''}{(F')^3}. \quad (13.11)$$

In turn, the inverse effective mass is given by

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2E}{dk^2}, \quad \frac{\hbar^2}{a^2 m^*} = \frac{d^2E}{d(ka)^2}. \quad (13.12)$$

On the other hand,

$$\frac{d^2E}{d(ka)^2} = \frac{d}{d(ka)} \left[\frac{dE}{du} \frac{du}{d(ka)} \right] = D \frac{d}{du} (2E_0 u D), \quad (13.13)$$

whence

$$\frac{1}{2E_0} \frac{d^2E}{d(ka)^2} = D^2 + u \frac{1}{2} \frac{dD^2}{du} = \frac{1-F^2}{(F')^2} - u \left[\frac{F}{F'} + \frac{(1-F^2)F''}{(F')^3} \right]. \quad (13.14)$$

It is of interest to specify the above findings for the lowest band at, e.g., the Γ point $k = 0$. There, the relation $\cos(ka) = F(u)$ yields $F = 1$; also, from the discussion of Sect. 13.1 one finds that $F = 1$ implies $\cot(u) = 2u/\vartheta$, so that the value of u corresponding to the Γ point in the lowest band is u_L . Finally, from $\cot(u_L) = 2u_L/\vartheta > 0$ one draws

$$F'(u_L) = -\frac{2}{\cot(u_L)} - \frac{2/u_L}{1+\cot^2(u_L)} < 0. \quad (13.15)$$

Inserting (13.15), along with $F(u_L) = 1$, into the fist relation of (13.9), yields $v(u_L) = 0$ as should be; in turn, the right hand side of (13.14) at the Γ point becomes $-u_L/F'(u_L)$: combining the latter with (13.14) and (13.12) yields

$$\frac{m^*}{m} = -\frac{F'(u_L)}{4u_L} > 0. \quad (13.16)$$

13.4 Dependence of $E(\mathbf{k})$ on the Lattice Parameters

Consider the simple case where the characteristic vectors $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ of the Bravais lattice are mutually orthogonal, so that $\mathbf{a}_2 \wedge \mathbf{a}_3 = c_1 \mathbf{a}_1$, with $c_1 \neq 0$ a constant; the other two vector products fulfill similar relations. From the definition D.5 of the characteristic vectors of the reciprocal lattice one then finds

$$\mathbf{b}_1 = \frac{\mathbf{a}_1}{a_1^2}, \quad \mathbf{b}_2 = \frac{\mathbf{a}_2}{a_2^2}, \quad \mathbf{b}_3 = \frac{\mathbf{a}_3}{a_3^2}, \quad (13.17)$$

namely, each vector \mathbf{b}_i is parallel to the corresponding vector \mathbf{a}_i , and $b_i = 1/a_i$. The volumes of the lattice cells turn out to be $\tau_l = a_1 a_2 a_3$, $\tau_G = b_1 b_2 b_3$. In a cubic

lattice it is $a_1 = a_2 = a_3$, whence $b_1 = b_2 = b_3$; indicating with a and, respectively, $b = 1/a$ the common lengths, it follows $\tau_l = a^3$, $\tau_G = b^3$.

If an external cause makes the volume of the Bravais lattice to change, that of the reciprocal lattice changes as well: a change in the characteristic vectors \mathbf{a}_i makes the characteristic vectors \mathbf{b}_i to change, this modifying the shape of the Brillouin zone; as a consequence, each branch $E_r(\mathbf{k})$ of the dispersion relation (Sect. D.6) suffers a deformation.

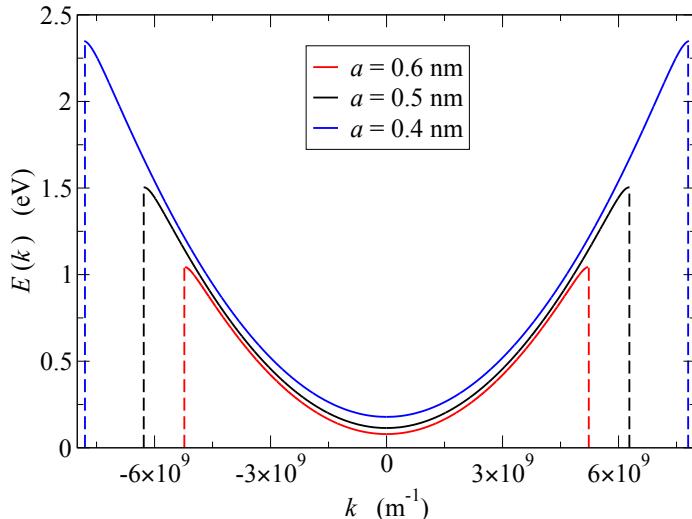


Fig. 13.5 Dispersion relation $E(k)$ of a one-dimensional lattice calculated from (13.6) for different lattice constants: $a = 4$ nm (blue curve), $a = 5$ nm (black curve), $a = 6$ nm (red curve). The vertical, dashed lines mark the boundaries of the Brillouin zone.

In the one-dimensional case considered here, the deformation in the dispersion relation can easily be visualized by calculating (13.6) at different values of a ; Fig. 13.5 shows the $E(k)$ relations obtained from (13.6), still with $\vartheta = 0.4$, by letting $a = 4, 5, 6$ nm and using the free-electron mass for m . In the calculation one must avoid using the normalized parameters ka and $\eta = E/E_0$ because a is embedded in the normalization factors. When $a = 4$ nm, the boundaries of the Brillouin zone are $\pm\pi/a \simeq \pm7.85 \times 10^9$ m $^{-1}$; when, instead, $a = 5$ nm, the boundaries are $\pm6.28 \times 10^9$ m $^{-1}$; finally, when $a = 6$ nm the boundaries are $\pm5.24 \times 10^9$ m $^{-1}$.

From the findings of Sect. 13.1 one notes that the minimum of each branch in Fig. 13.5 corresponds to $k = 0$; the energy corresponding to the minimum then reads

$$E_{\min} = E_0 u_L^2 = \frac{2\hbar^2 u_L^2}{m} \frac{1}{a^2}, \quad \frac{E_{\min}(5)}{E_{\min}(6)} = 1.44, \quad \frac{E_{\min}(5)}{E_{\min}(4)} = 0.64, \quad (13.18)$$

where symbol $E_{\min}(5)$ indicates the minimum when $a = 5$ nm, and the like for the other symbols. Remembering that for $\vartheta = 0.4$ it is $u_L^2 \simeq 0.18735$, one obtains $E_{\min}(5) \simeq 0.11422$ eV, $E_{\min}(6) \simeq 0.07932$ eV, and $E_{\min}(4) \simeq 0.17847$ eV, whence $E_{\min}(5) - E_{\min}(6) \simeq 35$ meV and $E_{\min}(4) - E_{\min}(5) \simeq 64$ meV. Considering an equilibrium condition, and assuming that the minimum of the branch is sufficiently close to the Fermi level, one finds that a change in the lattice constant may affect significantly the electron population of the branch.

In contrast, one notes from (13.16) that the effective mass, which in this model depends on u_L only, is left unaltered by a change in the lattice constant.

Revanth Reddy Pannala
EBIT, Unibio
కుంటర్ రెడ్డి పన్లా