University of Anbar College of Science Department of Physics



فيزياء الحالة الصلبة Solid state Physics

المرحلة الرابعة الكورس الثاني

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Magnitude of the Energy Gap:

The wavefunctions at the Brillouin zone boundary $k = \pi/a$ are $\sqrt{2} \cos \pi x/a$ and $\sqrt{2} \sin \pi x/a$, normalized over unit length or line. Let us suppose that the potential energy of an electron in the crystal at point x is

 $U(x) = U\cos 2\pi x/a$

The first-order energy difference between the two standing wave states is

$$E_g = \int_0^1 dx \ U(x) \left[|\Psi(+)|^2 - |\Psi(-)|^2 \right]$$

=
$$\int dx \ U \cos(2\pi x/a) \left(\cos^2 \pi x/a - \sin^2 \pi x/a \right) = U$$

We see that the gap is equal to the Fourier component of the crystal potential.

Bloch function.

Bloch considered the total potential of crystal (crystal potential) [V(r)] is the sum of two parts:

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لقد اعتبر بلوخ أن إجمالي الجهد للبلورة (الجهد البلوري)[(V (r)] هو مجموع جز أين:
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1- The electrostatic potential $[V_i(r)]$ due to the array of atomic cores. For a perfect lattice (i.e., one with no phonons), this contribution to V(r) should have the translational periodicity of the lattice.

ان الجهد الالكتروستاتيكي ناتج عن ترتيب من النوى الذرية, للحصول على شبيكة مثالية (واحدة بدون فونون) ، يجب أن يكون لهذا التوزيع المساهمة الدورية الانتقالية لشبيكة .

2- The potential $[V_e(r)]$ due to all other outer electrons. Bloch assumed that the charge density from this source would have the same long-term average value in every unit cell of the crystal and would thus also be periodic. Such an assumption certainly satisfies the requirements of electrical neutrality and crudely takes account of electron-electron repulsion.

$$V(r) = V_i(r) + V_e(r)$$

From Schrodinger equation in 3-dimension for one electron

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + U(r)\right]\Psi = E \Psi$$

Where U(r) = -eV(r) has the periodicity of the lattice

He calculated that the wave function which satisfies this equation subject to each potential must be of the form:

$$\Psi_k(r) = U_k(r) \ e^{ik.r}$$

Where $U_k(r)$ is a function (independent on the time and it is depending on the value of the wave vector k) also, it has the complete periodicity of the lattice.

هذه الدالة لاتعتمد على الزمن ولكن تعتمد على متجه الموجة
$$U_k(r) = U_k(r+T)$$

Where T is translation vector.

$$\Psi_k(r+T) = U_k(r+T) e^{ik.(r+T)}$$
$$\Psi_k(r+T) = \Psi_k(r) e^{ik.T}$$

This is the equation of Block function.

Bloch theorem: states that the eigen function of the wave equation for a periodic potential are of the form of the product of a plane wave $e^{ik.r}$ times a function $U_k(r)$ with the periodicity of the crystal lattice.

Kronig-Penney model.

A periodic for which the wave equation can be solved in terms of elementary functions is the square-well array of Figure The wave equation is

where U(x) is the potential energy and \mathcal{E} is the energy eigenvalue. In the region 0 < x < a in which U = 0, the eigenfunction is a linear combination,

of plane waves traveling to the right and to the left, with energy

In the region -b < x < 0 within the barrier the solution is of the form



Figure (1) Square-well periodic potential as introduced by Kronig and Penney.

we want the complete solution to have the Bloch form

$$(\Psi_k(r) = U_k(r)exp^{(ik.r)})$$

Thus, the solution in the region n < x < a + b must be related to the solution (4) in the region -b < r < 0 by the Bloch theorem:

$$\Psi(a < x < a + b) = \Psi(-b < x < 0) e^{ik(a+b)} \dots (6)$$

The constants A, B, C, D are chosen so that Ψ and $d\Psi/dx$ are continuous at x = 0 and x = a. These are the usual quantum mechanical boundary conditions in problems that involve square potential wells. At x = 0,

$$ik(A - B) = Q(C - D)$$
(8)

with Q from (4). At x = a, with the use of (6) for $\Psi(a)$ under the barrier in terms of $\Psi(-b)$,

$$Ae^{ika} + Be^{-ika} = (Ce^{-Qb} + De^{Qb}) e^{ik(a+b)} \dots (9)$$
$$ik(Ae^{ika} - Be^{-ika}) = Q(Ce^{-Qb} - De^{Qb}) e^{ik(a+b)} \dots (10)$$

The four equations (7) to (10) have a solution only if the determinant of the coefficients of A, B, C, D vanishes, yielding

$$\left[\frac{Q^2 - k^2}{2Qk}\right] \sinh Qb \, \sin ka + \cosh Qb \cos ka = \cos k(a+b) \dots \dots \dots (11)$$

when we pass to the limit b = 0 and $U_o = \infty$ in such a way that $Q^2ba/2 = P$, a finite quantity. In this limit $Q \gg k$ and $Qb \ll 1$. Then equation (11) reduces to:

 $(P/ka) \sin ka + \cos ka = \cos ka$ (12) The ranges of K for which this equation has solutions are plotted in Fig below:



Figure 2 Plot of the function $(P/ka) \sin ka + \cos ka$, for $P = 3\pi/2$. The allowed values of the energy e are given by those ranges of $ka = (2m\epsilon/\hbar^2)^{1/2} a$ for which the function lies between ± 1 . For other values of the energy there are no traveling wave or Bloch-like solutions to the wave equation, so that forbidden gaps in the energy spectrum are formed.



Figure 3 Plot of energy vs. wavenumber for the Kronig-Penney potential, with $P = 3\pi/2$. Notice the energy gaps at $ka = \pi, 2\pi, 3\pi, \dots$...

Number of orbitals in a band

Consider a linear crystal constructed of an even number N of primitive cells of lattice constant a. In order to count states, we apply periodic boundary conditions to the wavefunctions over the length of the crystal. The allowed values of the electron wavevector k in the first Brillouin zone are given by:

$$k = 0; \pm \frac{2\pi}{L}; \pm \frac{4\pi}{L}; \dots; \frac{N\pi}{L}$$

We cut the series off at $N\pi/L = \pi/a$, for this is the zone boundary. The point $-N\pi/L = -\pi/a$, is not to be counted as an independent point because it is connected by a reciprocal lattice vector with π/a . The total number of points is exactly N, the number of primitive cells.

Each primitive cell contributes exactly one independent value of \mathbf{k} to each energy band. This result carries over into three dimensions. With account taken of the two independent orientations of the electron spin, there are 2N independent orbitals in each energy band.

If there is a single atom of valence, one in each primitive cell, the band can be half filled with electrons. If each atom contributes two valence electrons to the band, the band can be exactly filled. If there are two atoms of valence, one in each primitive cell, the band can also be exactly filled.