University of Anbar
College of Science
Department of Physics

فيزياء الحالة الصلبة

Solid State Physics

المرحلة الرابعة
الكورس الثاني
صلبة2

الدكتور قيس عبدالله عباس

Lecture2

1. Nearly free electron model.

On the free electron model the allowed energy values are distributed essentially continuously from zero to infinity.

في نموذج الإلكترون الحر ، يتم توزيع قيم الطاقة المسموح بها بشكل أساسي من الصفر إلى ما لا نهاية.

$$\varepsilon_k = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2) \quad ,$$

where, for periodic boundary conditions over a cube of side L,

$$k_x, k_y, k_z = 0, \ \mp\frac{2\pi}{L} ; \mp\frac{4\pi}{L} ; \ldots\ldots\ldots$$

The free electron wavefunctions are of the form

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

What happens when we add a periodic lattice of lattice constant a?

ماذا يحدث عندما نضيف دورية الشبيكة لثابت الشبيكة؟

Effect of the periodic potential: particles (behaving like waves) which are moving through a lattice spaced by lattice constant a.

تأثير الجهد الدوري: الجسيمات (تتصرف مثل الأمواج) التي تتحرك من خلال الشبيكة متباعدة بواسطة ثابت الشبيكة

Electrons diffract from the periodic lattice.

الالكترونات تحيد من دورية الشبيكة

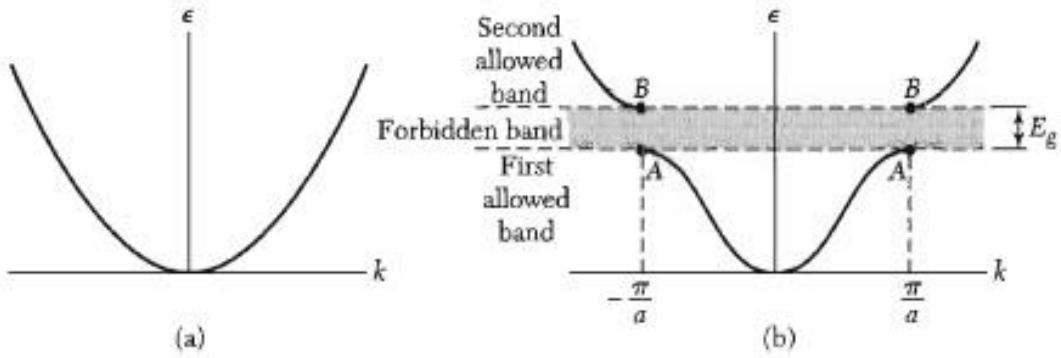
This is the physical origin of the band gap. There are some electron energy levels which are forbidden because the electron waves cancel themselves out of these wavelengths.

هذا هو الأصل الفيزياوي لفجوة الحزمة. هناك بعض مستويات الطاقة الإلكترونية المحظورة لأن موجات الإلكترون تلغي نفسها عند هذه الأطوال الموجية..

What wavelengths are these? وما هذه الاطوال الموجية

At zone boundary k=$\mp\frac{\pi}{a}$

Figure Free electron model, Nearly free electron model



We explain physically the origin of energy gaps in the simple problem of a linear solid of lattice constant a. The low energy portions of the band structure are shown qualitatively, in figure (a) for entirely free electrons and in figure (b) for electrons that are nearly free, but with an energy gap at $k = \pm\pi/a$. The Bragg condition $(k+G)^2 = k^2$ for diffraction of a wave of wavevector **k** becomes in one dimension

$$k = \pm\frac{1}{2}G = \pm n\pi/a$$

where $G = 2\pi n/a$ is a reciprocal lattice vector and **n** is an integer. The first reflections and the first energy gap occur at $\boldsymbol{k} = \pm\pi/a$. The region in **k** space between $-\pi/a$ and π/a is the **first Brillouin zone** of this lattice. Other energy gaps occur for other values of the integer **n**.

1.1 Bragg reflection and energy gap.

There is an analogy between electron waves and lattice waves (phonons), For most value of the dispersion curve, the electron move freely throughout the lattice (there is a group velocity that is)

هناك تماثل بين موجات الإلكترون وموجات الشبيكة (الفونونات) ، بالنسبة لمعظم قيمة منحنى التشتت ، يتحرك الإلكترون بحرية في جميع أنحاء الشبيكة (هناك سرعة جماعية غير صفرية)

At the zone boundary ($k = \pm\pi/a$), there are only standing waves $(d\omega/dk = 0)$.
عند حدود النطاق يوجد فقط موجات واقفة

What standing wave solutions are stable with these k- values?

The time-independent state is represented by standing waves. We can form:

$$exp^{(\pm i\pi x/a)} = \cos(\pi x/a) \pm i\, sin\,(\pi x/a)$$

The simplest solution is a combination of wave function of the electrons,

$$\Psi_1 = exp^{(ik.x)} = exp^{(i\,\pi x/a)}$$

$$\Psi_2 = exp^{(-ik.x)} = exp^{(-i\,\pi x/a)}$$

The two different standing waves from the two traveling waves:

$$\Psi^{+} = \Psi_1 + \Psi_2 = exp^{(ik.x)} + exp^{(-ik.x)} = 2\cos(\pi x/a)$$

$$\Psi^{-} = \Psi_1 - \Psi_2 = exp^{(ik.x)} - exp^{(-ik.x)} = 2\,i\sin(\pi x/a)$$

The standing waves are labelled (+) or (-) according to whether or not they change sign when -x is substituted for x. Both standing waves are composed of equal parts of right and left-directed traveling waves.

The combination of these two traveling waves $exp^{(ik.x)}$ give standing wave solutions (sin and cos).

The two standing waves Ψ^+ and Ψ^- pile up electrons at different regions, and therefore the two waves have different values of the potential energy in the field of the ions of the lattice. This is the origin of the energy gap.

The probability density p of a particle is $\Psi^*\Psi = |\Psi|^2$. For a pure traveling wave $exp^{(ik.x)}$, we have, $p = exp^{(-ik.x)}exp^{(ik.x)} = 1$, so that the charge density is constant.

The charge density is not constant for linear combinations of plane waves. Consider the standing wave Ψ (+) for this we have

$$p(+) = |\Psi(+)|^2 \propto cos^2 \pi x/a$$

This function piles up electrons (negative charge) on the positive ions centred at x = 0, a, 2a, . . . in Figure below, where the potential energy is lowest.

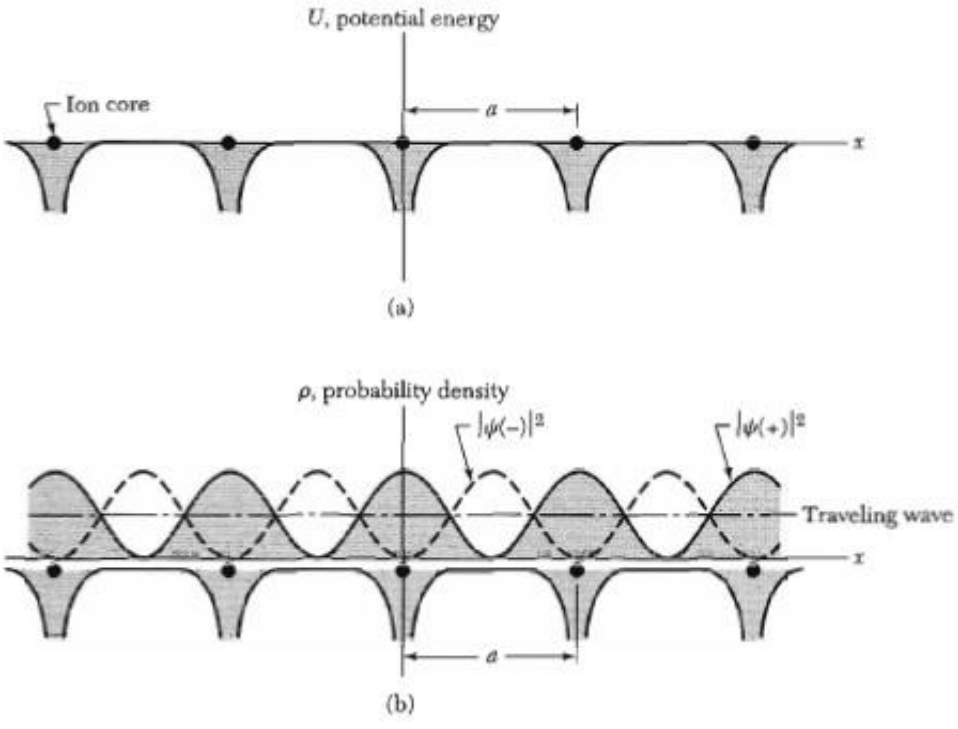


Figure (a) the variation of the potential energy of a conduction electron in the field of the positive ion cores.

The potential energy of an electron in the field of a positive ion is negative, so that the force between them is attractive.

For the other standing wave $\Psi(-)$ the probability density is

$$p(-) = |\Psi(-)|^2 \propto sin^2 \pi x/a$$

which concentrates electrons away from the ion cores.

In Figure (b) we show the electron concentration for the standing waves $\Psi(+)$, $\Psi(-)$, and for a traveling wave.

References

1- Charles Kittel - Introduction to Solid State Physics-Wiley (2005)

2- J. S. Blakemore - Solid State Physics-Cambridge University Press (1985)

3- M. A. OMAR Elementary-solid-state-physics