University of Anbar

College of Science

Department of Physics

فيزياء الحالة الصلبة

Solid state Physics

المرحلة الرابعة

الكورس الاول

صلبة 1

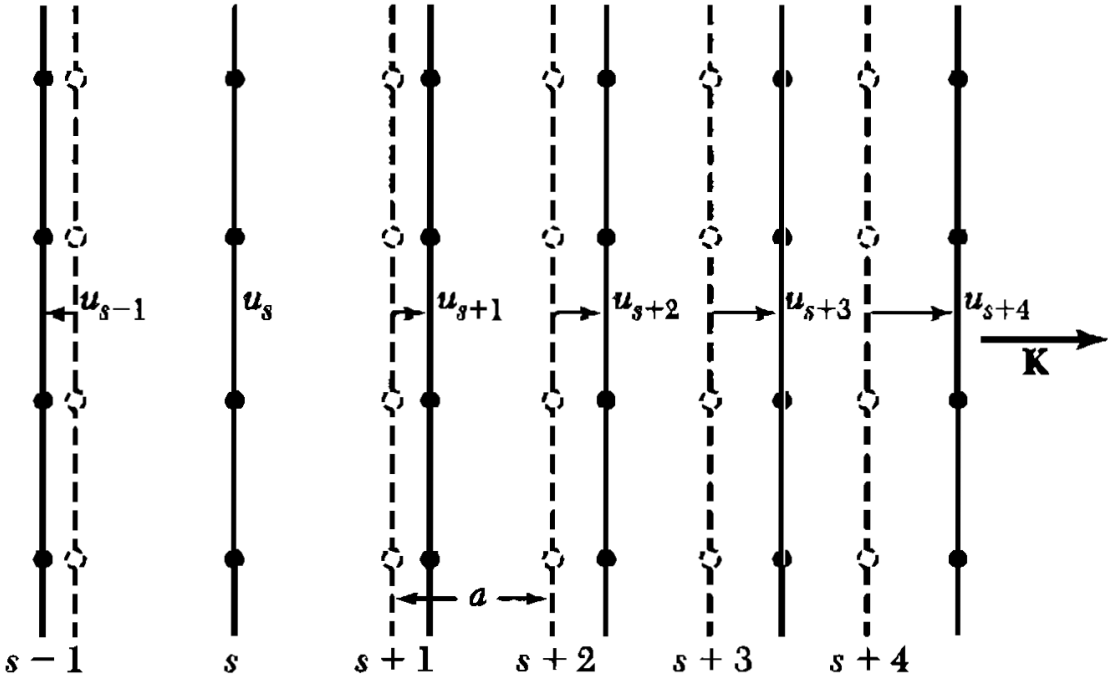
Syllabus of this course مفردات الكور س

1- crystal structure
2- x-ray diffraction
3- lattice vibration
4- thermal properties in solids
5- free electron model

4. Lattice or Crystal Vibrations اهتزاز الشبيكة او البلورة

4.1 Vibrations Of Crystals With Monatomic احادية الذرة Basis

- Consider نعتبر the elastic vibrations الاهتزاز مرن of a crystal with one atom in the primitive cell. We want to find the frequency of an elastic wave in terms of the wavevector that describes لوصف the wave الموجة and in terms of the elastic constants.
- Assume لنفرض that the elastic response الاستجابة مرنة of the crystal is a linear function دالة خطية of the forces.
- We assume that the force on the planes caused by the displacement الازاحة of the plane s + p is proportional تتناسب to the difference u_s+, -u_s of their displacements.



- we consider only nearest-neighbor الجار الاقرب interactions تتفاعل, with p ±1, the total force on s from plane s ±1.

$$F_s = C(u_{s+1} - u_s) + C(u_{s-1} - u_s) \ . \qquad (1)$$

This expression التعبير is linear خطية in the displacements الازاحات and is of the form وبصيغة of Hook's low قانون هوك.

The constant C is the force constant between nearest-neighbor planes.

The equation of motion of an atom in the plane s is

$$M\frac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s) \ , \qquad (2)$$

where M is the mass of an atom.

We look for solutions with all displacements having the time dependence $exp(-i\omega t). then\ d^2u_s/dt^2 = -\omega^2 u_s,$ and equation (2) becomes

$$-M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s) \ . \qquad (3)$$

This is a difference equation in the displacements u and has traveling wave solutions of the form:

$$u_{s\pm1} = u \exp(isKa) \exp(\pm iKa) \ , \qquad (4)$$

where a is the spacing between planes and K is the wavevector. The value to use for a will depend on the direction of K.

From equations 3, 4 we have

$$-\omega^2 Mu \exp(isKa) = Cu\{\exp[i(s+1)Ka] + \exp[i(s-1)Ka] - 2\exp(isKa)\} \quad . \qquad (5)$$

We cancel $u \exp(isKa)$ from both sides, to leave

$$\omega^2 M = -C[\exp(iKa) + \exp(-iKa) - 2] \quad . \qquad (6)$$

With the identity $2\cos Ka = \exp(iKa) + \exp(-iKa)$, we have the **dispersion relation** $\omega(K)$.

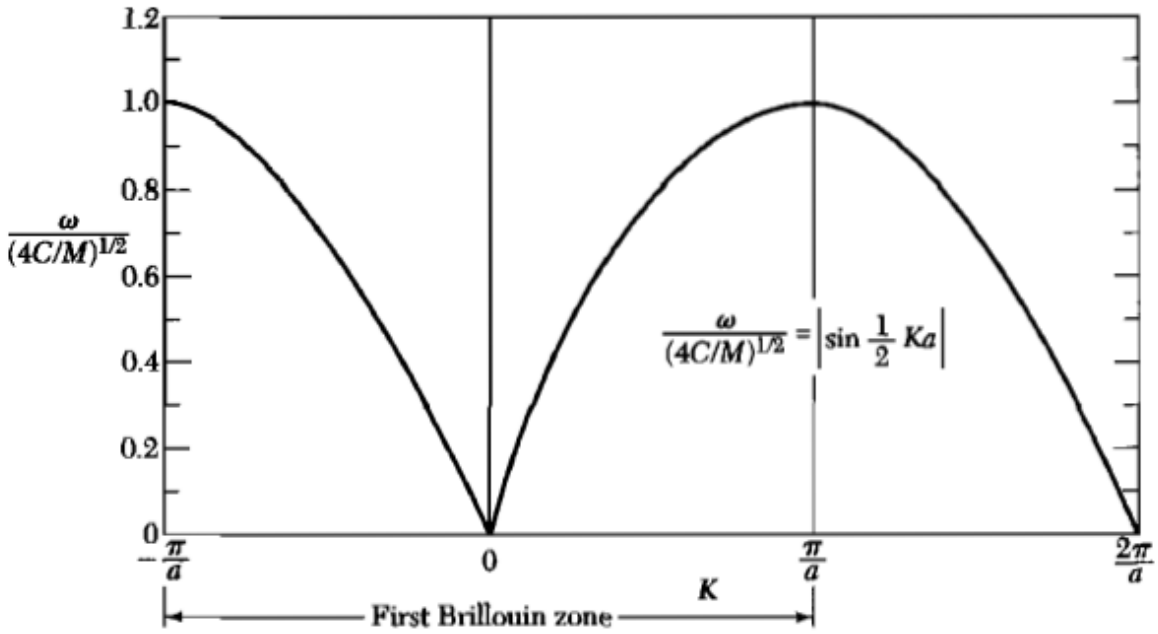
$$\omega^2 = (2C/M)(1 - \cos Ka) \quad . \qquad (7)$$

The boundary of the first Brillouin zone lies at $K = \pm\pi/a$. We show from (7) that the slope of ω versus K is zero at the zone boundary:

$$d\omega^2/dK = (2Ca/M)\sin Ka = 0 \qquad (8)$$

at $K = \pm\pi/a$, for here $\sin Ka = \sin(\pm\pi) = 0$.

$$-\pi < Ka \leq \pi \quad , \qquad \text{or} \qquad -\frac{\pi}{a} < K \leq \frac{\pi}{a} \quad .$$



Group velocity:

The transmission velocity of a wave packet is the **group velocity**, given as

$$v_g = d\omega/dK$$

4.2 Vibrations Of Crystals With Two Atoms per primitive Basis

We consider a cubic crystal where atoms of mass M1 lie on one set of planes and atoms of mass M2, lie on planes interleaved between those of the first

$$M_1 \frac{d^2u_s}{dt^2} = C(v_s + v_{s-1} - 2u_s) \ ;$$
$$M_2 \frac{d^2v_s}{dt^2} = C(u_{s+1} + u_s - 2v_s) \ . \qquad (10)$$

The solutions of these equations are:

$$u_s = u \exp(isKa) \exp(-i\omega t) \ ; \qquad v_2 = v \exp(isKa) \exp(-i\omega t) \ . \qquad (11)$$

From equations 10, 11

$$-\omega^2 M_1 u = Cv[1 + \exp(-iKa)] - 2Cu \ ;$$
$$-\omega^2 M_2 v = Cu[\exp(iKa) + 1] - 2Cv \ .$$

$$\begin{vmatrix} 2C - M_1\omega^2 & -C[1 + \exp(iKa)] \\ -C[1 + \exp(iKa)] & 2C - M_2\omega^2 \end{vmatrix} = 0 \ ,$$

or

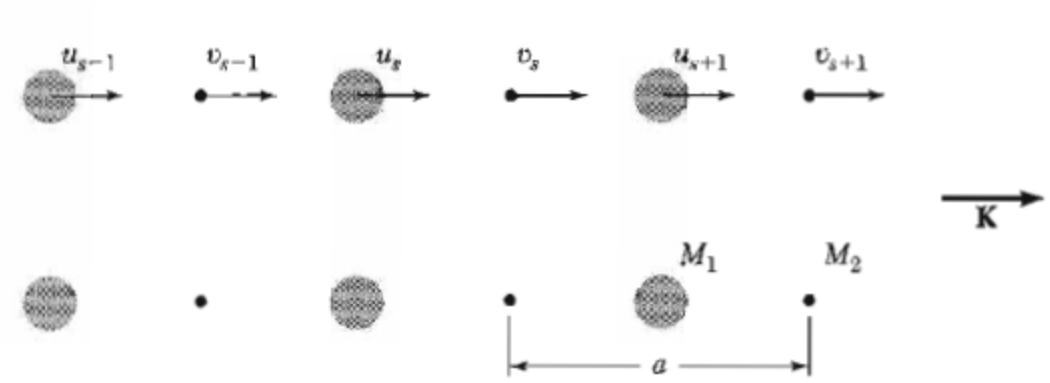
$$M_1M_2\omega^4 - 2C(M_1 + M_2)\omega^2 + 2C^2(1 - \cos Ka) = 0 \ .$$

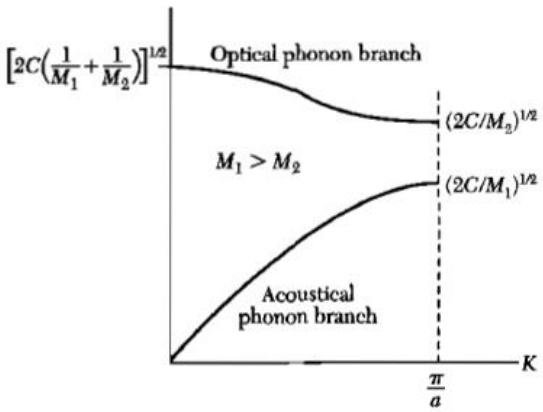
$$\omega^2 \cong 2C\left(\frac{1}{M_1}+\frac{1}{M_2}\right) \qquad \text{(optical branch)} \ ;$$

$$\omega^2 \cong \frac{\frac{1}{2}C}{M_1+M_2}K^2a^2 \qquad \text{(acoustical branch)} \ .$$

The extent of the first Brillouin zone is $-\pi/a \leq K \leq \pi/a$, where a is the repeat distance of the lattice. At $K_{max} = \pm\pi/a$ the roots are

$$\omega^2 = 2C/M_1 \ ; \qquad \omega^2 = 2C/M_2 \ .$$





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**