FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html

Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)

Andrej Kuznetsov

delivery address: Department of Physics, PB 1048 Blindern, 0316 OSLO
Tel: +47-22857762,
e-post: andrej.kuznetsov@fys.uio.no
visiting address: MiNaLab, Gaustadaleen 23a

2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	**Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space**	**3h**
W20/1 cancelled		
M25/1: 9-12 am	**Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones**	**3h**
W27/1 cancelled		
M01/2: 10-12 am	**Elastic strain and structural defects in crystals**	**2h**
W03/2: 9-10 am	**Atomic diffusion in solids**	**1h**
M08/2: 10-12 am	**Summary of Module I**	**2h**

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	**Vibrations in monoatomic and diatomic chains of atoms**	**1h**
M15/2: 10-12am	**Periodic boundary conditions, phonons and density of states (DOS)**	**2h**
W17/2: 9-10 am	**Planck distribution**	**1h**
M22/2 : 10-12am	**Lattice heat capacity: Dulong-Petit, Einstein, and Debye models**	**2h**
W24/2 cancelled		
M29/2: 9-12am	**Comparison of different models for lattice heat capacity, thermal conductivity with phonons**	**3h**
W02/3: 9-10 am	**Thermal expansion**	**1h**
M07/3: 10-12am	**Summary of Module II.**	**2h**

Module III – Electrons (Chapters 6, 7, 18 - pp.528-530, and Appendix D)

W09/3: 9-10 am	**Free electron gas (FEG) versus free electron Fermi gas (FEFG)**	**1h**
M14/3: 10-12am	**DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution**	**2h**
W16/3: 9-10 am	**Heat capacity of FEFG in 3D**	**1h**
W30/3: 9-10 am	**DOS in 2D - quantum wells**	**1h**
M04/4: 10-12am	**DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons**	**2h**
W06/4: 9-10 am	**Origin of the energy band gap**	
M11/4: 10-12am	**Nearly free electron model. Kronig-Penney model. Empty lattice approximation.**	**2h**
W13/4: 9-10 am	**Number of orbitals in a band**	**1h**
M18/4: 10-12am	**Summary of Module III.**	**2h**

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	**Metals versus semiconductors. Surfaces and interfaces.**	**1h**
M25/4: 9-12 am	**Effective mass method.**	**3h**
W27/4: 9-10 am	**Intrinsic carrier generation – elctrons and holes.**	**1h**
M02/5: 9-12 am	**Localized levels for hydrogen-like impurities – donors and acceptors. Doping.**	**3h**
W04/5: 9-10 am	**Carrier statistics in semiconductors**	**1h**
M09/5: 9-12 am	**p-n junctions**	**3h**
W11/5: 9-10 am	**Optoelectronic semiconductor properties and devices**	**1h**
M18/5: 9-12 am	**Device demonstrations. Summary of Module IV**	**3h**

Repetition

M23/5 9-12 am	**The course in a nutshell**	**2h**

W25/5, M30/5 and W1/6 cancelled

Exam during week 22 (tentatively 30-31/5)

Lectures 5-6: Vibrations and phonons

- **Examples of phonon-assisted processes**
- **Infinite 1D lattice with one or two atoms in the basis;**
- **Examples of dispersion relations in 3D;**
- **Finite chain of atoms, Born – von Karman boundary conditions;**
- **Phonon density of states in 1-D;**
- **Collective crystal vibrations – phonons;**

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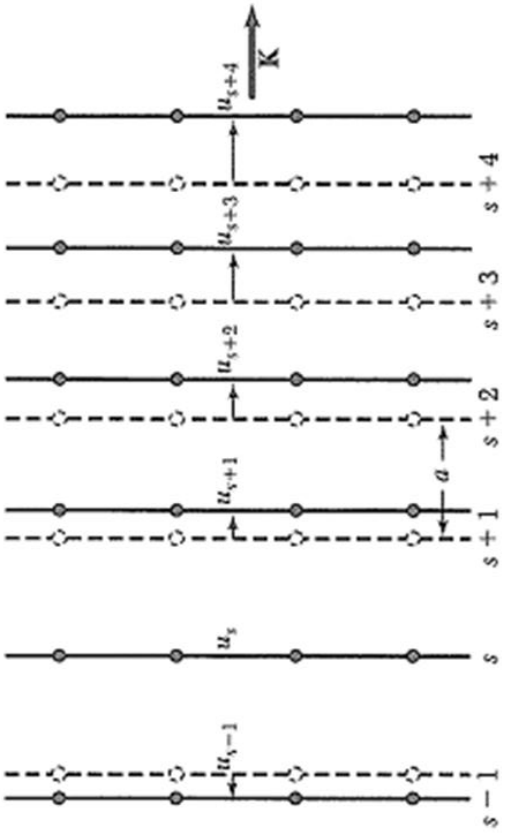
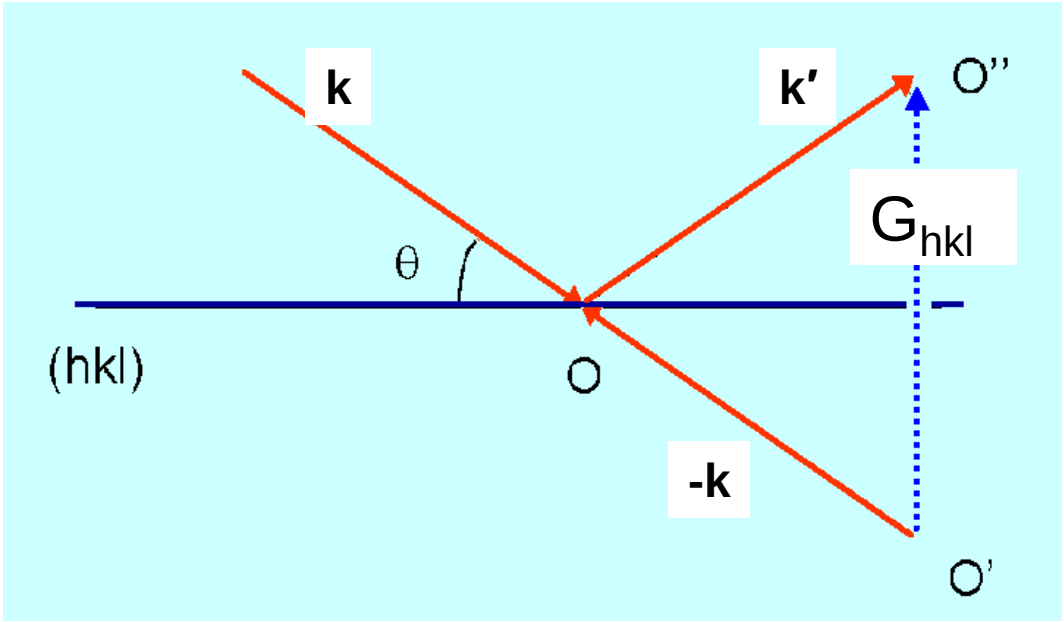
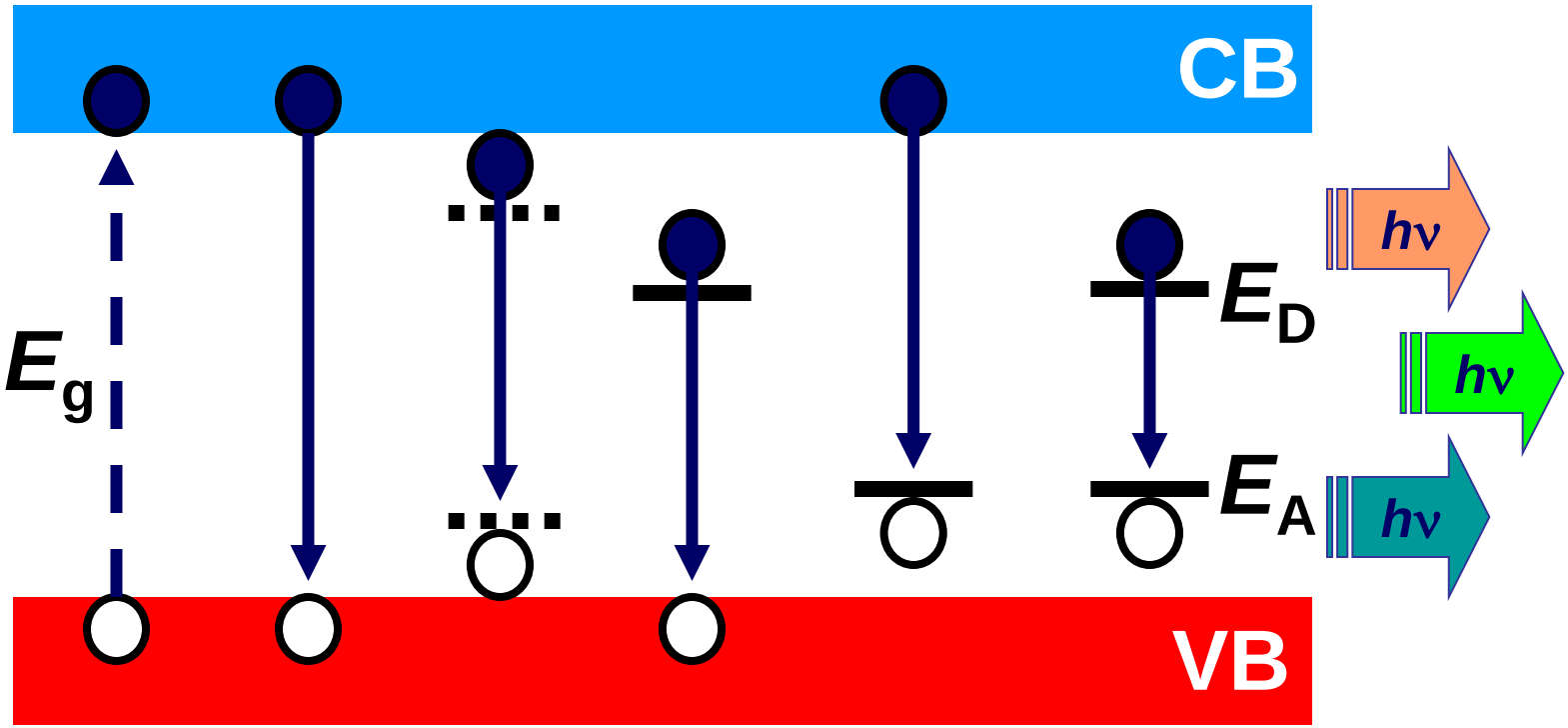
Diffraction



$$\mathbf{k}' \pm \mathbf{K} = \mathbf{k} + \mathbf{G}$$



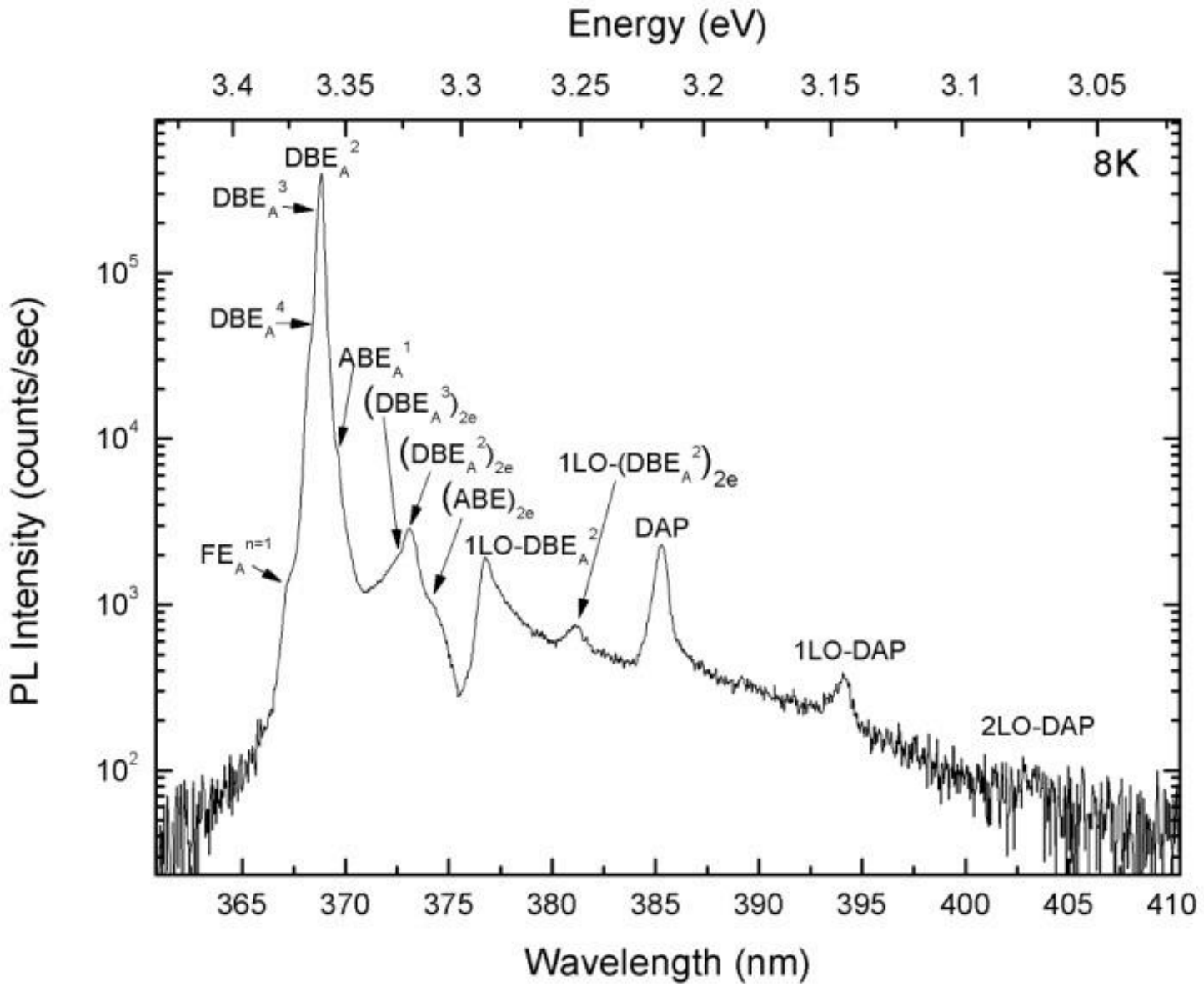
Photoluminescence



EXCITATION
- Photo generation
- Electrical injection

Photons

Photoluminescence



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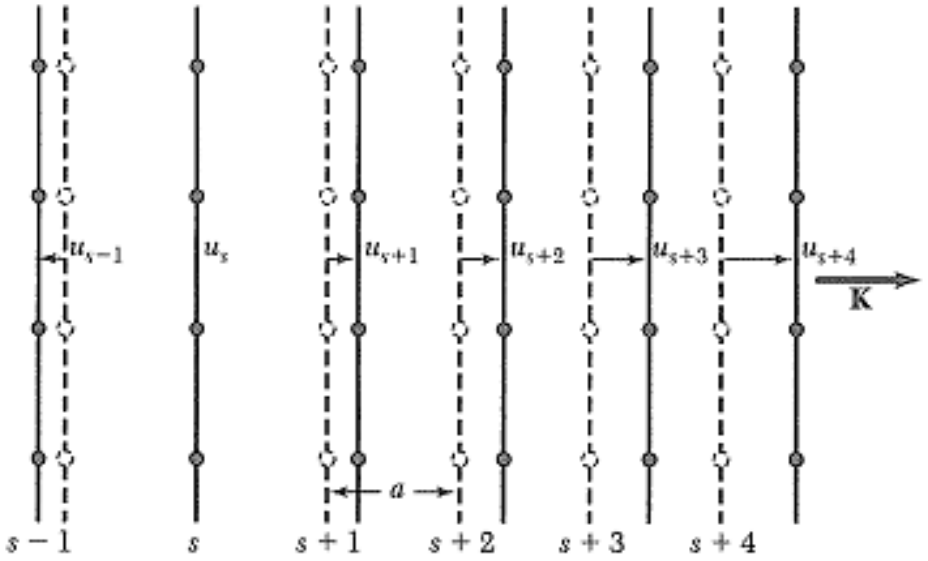
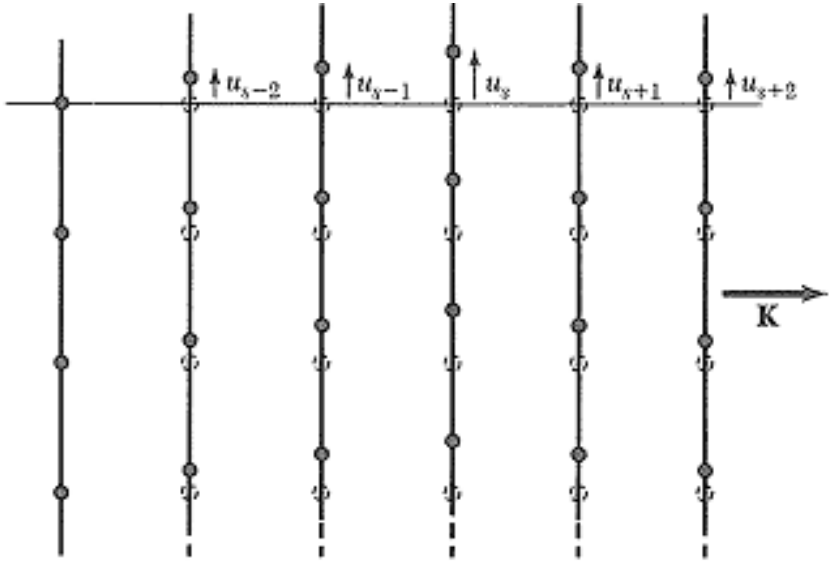
Vibrations of crystals with monatomic basis

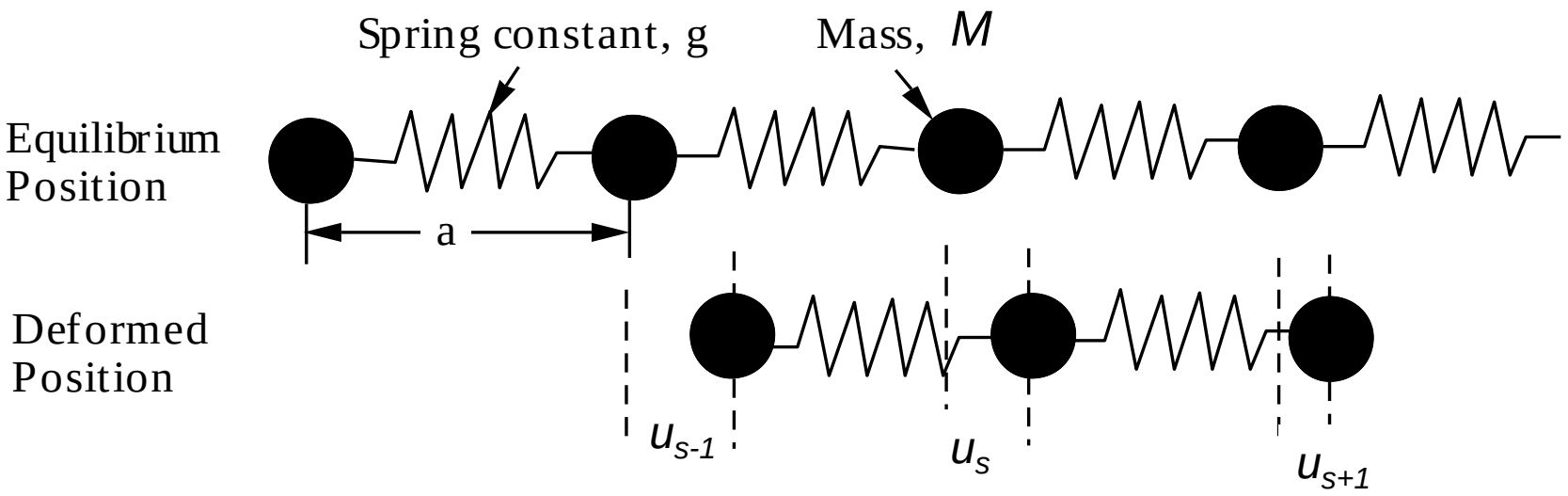


longitudinal wave



transverse wave

Vibrations of crystals with monatomic basis



u_s: displacement of the s^{th} atom from its equilibrium position

Vibrations of crystals with monatomic basis

Force on s^{th} plane = $F_s = -C(u_s - u_{s+1}) - C(u_s - u_{s-1})$ (only neighboring planes interact)

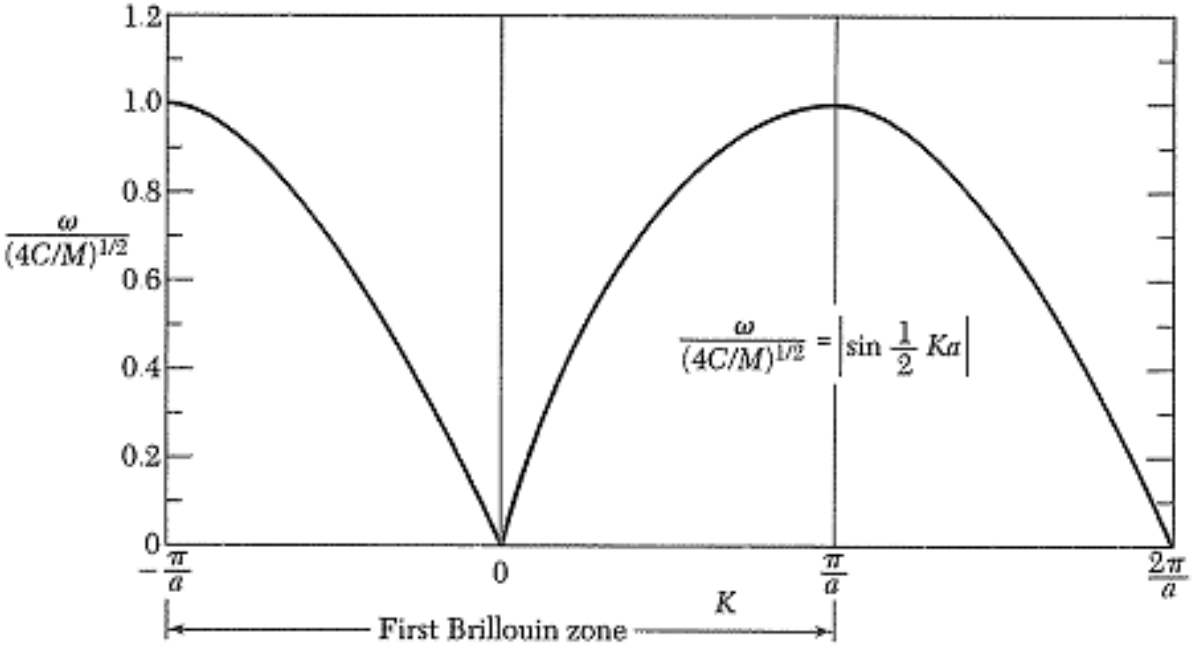
Equation of motion: $M\dfrac{d^2u_s}{dt^2} = C(u_{s+1} + u_{s-1} - 2u_s)$

$u_s(t) = u_s\, e^{-i\omega t} \quad \rightarrow \quad -M\omega^2 u_s = C(u_{s+1} + u_{s-1} - 2u_s)$

$u_s = u_0\, e^{iKas} \quad \rightarrow \quad -M\omega^2 = C(e^{iKa} + e^{-iKa} - 2)$

$$\omega^2 = \frac{2C}{M}(1 - \cos Ka)$$

Dispersion relation



$$\omega^2 = \frac{4C}{M}\sin^2\frac{1}{2}Ka$$

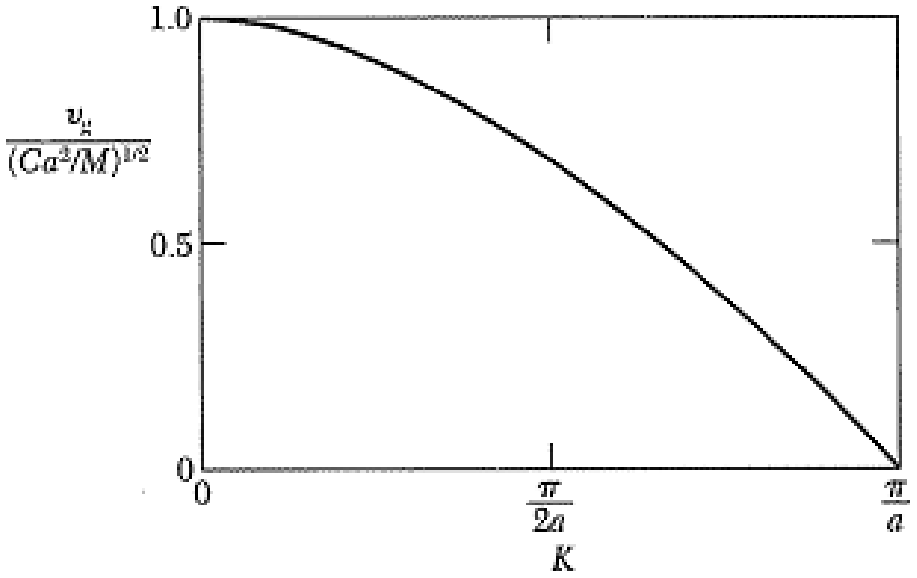
$$\omega = \sqrt{\frac{4C}{M}}\left|\sin\frac{1}{2}Ka\right|$$

Vibrations of crystals with monatomic basis

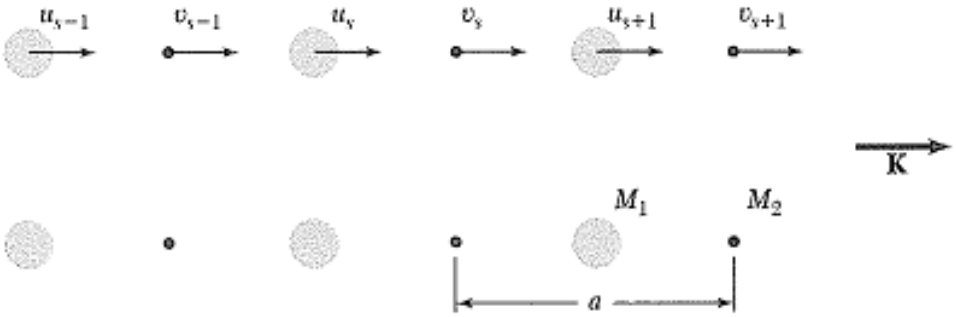
Group velocity: $\mathbf{v}_g = \nabla_{\mathbf{K}} \omega$

1-D: $v_G = \left| \frac{d\omega}{dK} \right| = \sqrt{\frac{Ca^2}{M}} \left| \cos \frac{1}{2} Ka \right|$ $\omega = \sqrt{\frac{4C}{M}} \left| \sin \frac{1}{2} Ka \right|$

$v_G = 0$ at zone boundaries



Vibrations of crystals with two atoms per basis



$$M_1 \frac{d^2 u_s}{dt^2} = C\left(v_s + v_{s-1} - 2u_s\right)$$

$$M_2 \frac{d^2 v_s}{dt^2} = C\left(u_{s+1} + u_s - 2v_s\right)$$

$$u_s = u e^{isKa - i\omega t}$$

$$v_s = v e^{isKa - i\omega t}$$

$$\rightarrow$$

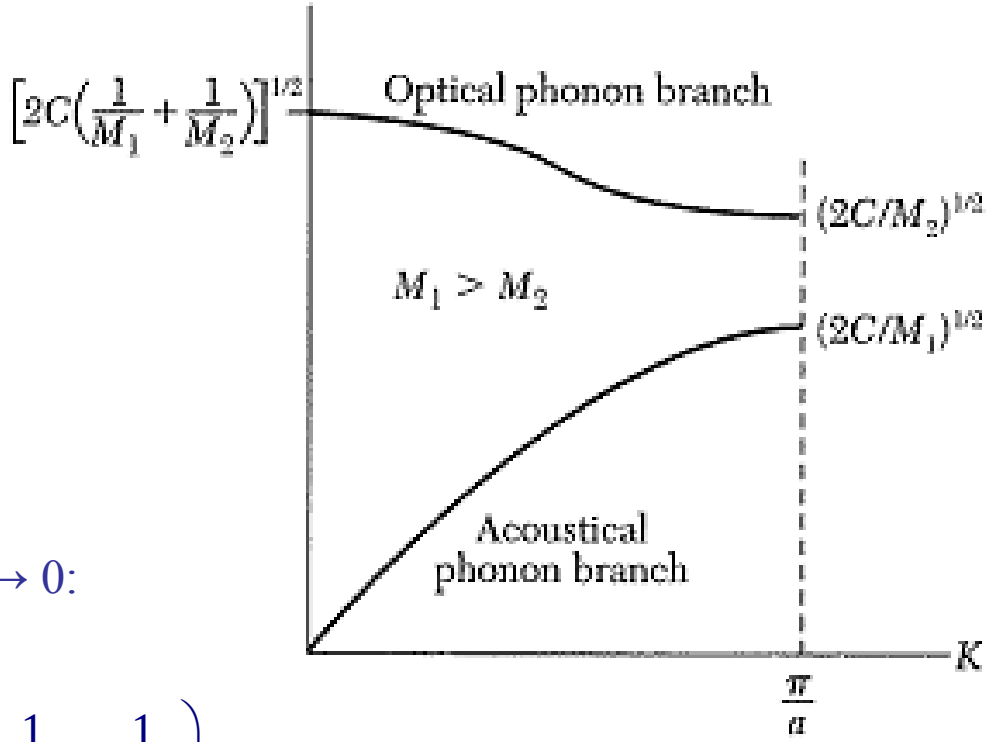
$$-M_1\omega^2 u = Cv\left(1 + e^{-iKa}\right) - 2Cu$$

$$-M_2\omega^2 v = Cu\left(1 + e^{iKa}\right) - 2Cv$$

$$\begin{vmatrix} 2C - M_1\omega^2 & -C\left(1 + e^{-iKa}\right) \\ -C\left(1 + e^{iKa}\right) & 2C - M_2\omega^2 \end{vmatrix} = 0$$

Vibrations of crystals with two atoms per basis

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



$Ka \to 0$:

$$\omega^2 = \begin{cases} 2C\left(\dfrac{1}{M_1}+\dfrac{1}{M_2}\right) & \textit{optical} \\ \dfrac{C}{2\left(M_1+M_2\right)}K^2a^2 & \textit{acoustical} \end{cases}$$

$Ka \to \pi$:
$(M_1 > M_2)$

$$\omega^2 = \begin{cases} \sqrt{2C/M_2} & \textit{optical} \\ \sqrt{2C/M_1} & \textit{acoustical} \end{cases}$$

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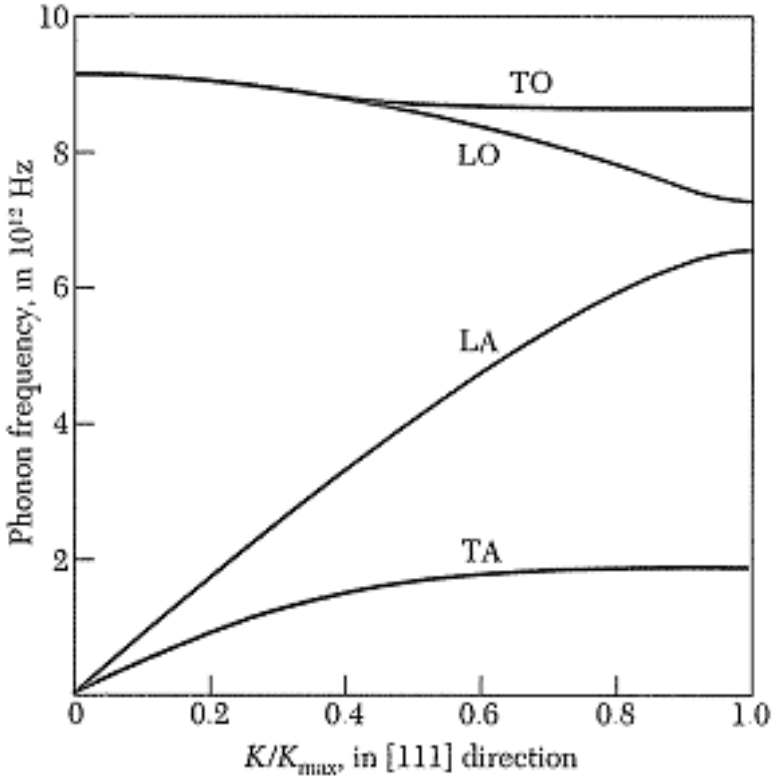
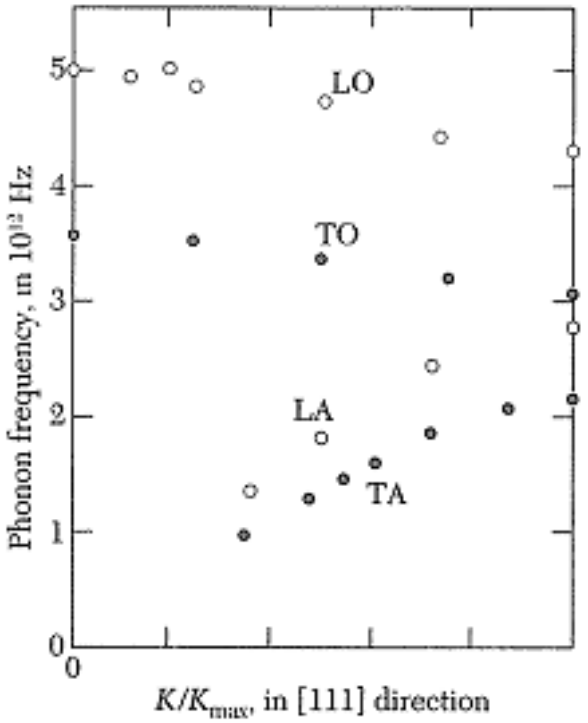
Vibrations of crystals with two atoms per basis

p atoms in primitive cell $\rightarrow$ $d\,p$ branches of dispersion.
$d = 3 \rightarrow$ 3 acoustical : 1 LA + 2 TA
$(3p - 3)$ optical: $(p-1)$ LO + $2(p-1)$ TO

E.g., Ge or KBr: $p = 2$ $\rightarrow$ 1 LA + 2 TA + 1 LO + 2 TO branches



Ge



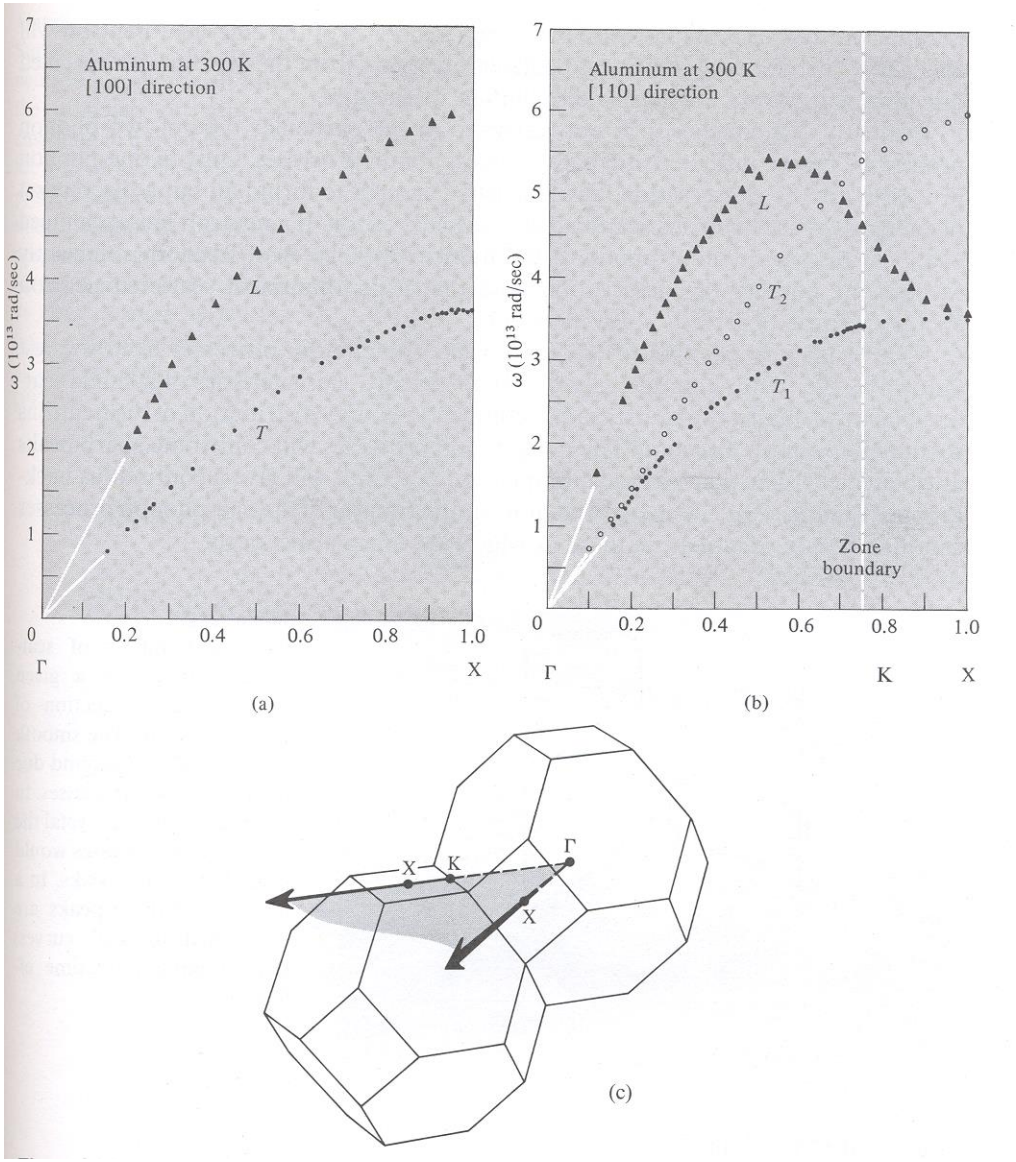
KBr

Number of allowed K in 1st BZ = N

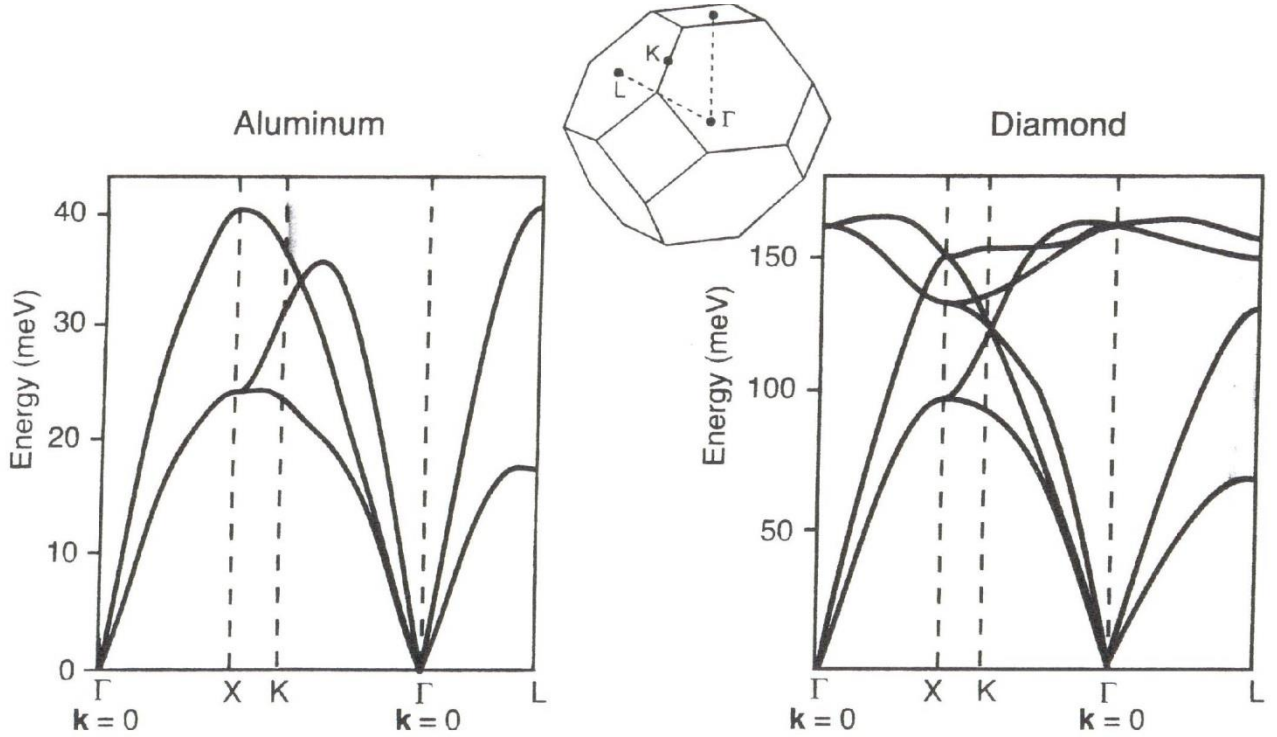
Phonon dispersion in real crystals: aluminium FCC lattice with 1 atom in the basis

In a 3-D atomic lattice we expect to observe 3 different branches of the dispersion relation, since there are two mutually perpendicular transverse wave patterns in addition to the longitudinal pattern we have considered.

Along different directions in the reciprocal lattice the shape of the dispersion relation is different. But note the resemblance to the simple 1-D result we found.



Phonon dispersion in real crystals: FCC lattice with 1 (Al) and 2 (Diamond) atoms in the basis



Characteristic points of the reciprocal space – Γ, X, K, and L points are introduced at the center and bounduries of the first Brillouin zone

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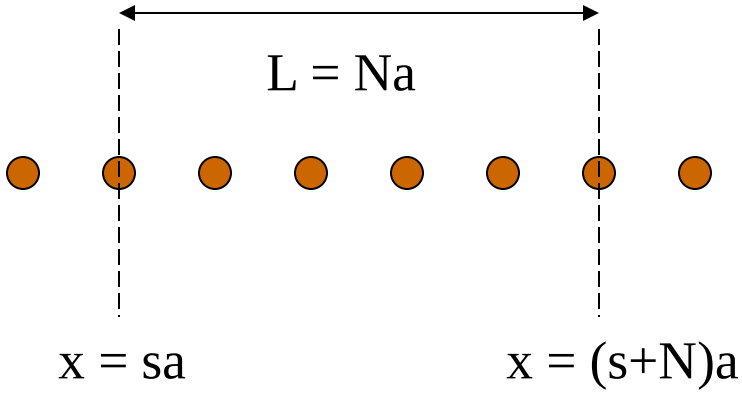
Calculating phonon density of states – DOS – in 1-D

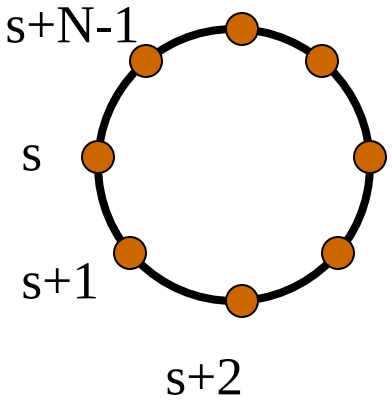
A vibrational mode is a vibration of a given wave vector $\vec{k}$ (and thus λ), frequency ω, and energy $E = \hbar\omega$. How many modes are found in the interval between $(\omega, E, \vec{k})$ and $(\omega + d\omega, E + dE, \vec{k} + d\vec{k})$?

modes $\quad dN = N(\omega)d\omega = N(E)dE = N(k)d^3\vec{k}$

We will first find N(k) by examining allowed values of k. Then we will be able to calculate N(ω) and evaluate C_V in the Debye model.

First step: simplify problem by using periodic boundary conditions for the linear chain of atoms:





We assume atoms s and s+N have the same displacement—the lattice has periodic behavior, where N is very large.

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- Collective crystal vibrations – phonons;
- Thermal equilibrium occupancy of phonons – Planck distribution.

Calculating phonon density of states – DOS – in 1-D

Since atoms s and $s+N$ have the same displacement, we can write:

$$u_s = u_{s+N} \longrightarrow ue^{i(ksa-\omega t)} = ue^{i(k(s+N)a-\omega t)} \longrightarrow 1 = e^{ikNa}$$

This sets a condition on allowed k values:

$$kNa = 2\pi n \rightarrow \quad k = \frac{2\pi n}{Na} \qquad n = 1, 2, 3, \ldots$$

So the separation between allowed solutions (k values) is:

$$\Delta k = \frac{2\pi}{Na}\,\Delta n = \frac{2\pi}{Na}$$

independent of k, so the density of modes in k-space is uniform

Thus, in 1-D:

$$\frac{\#\ of\ \ modes}{interval\ of\ \ k-space} = \frac{1}{\Delta k} = \frac{Na}{2\pi} = \frac{L}{2\pi}$$

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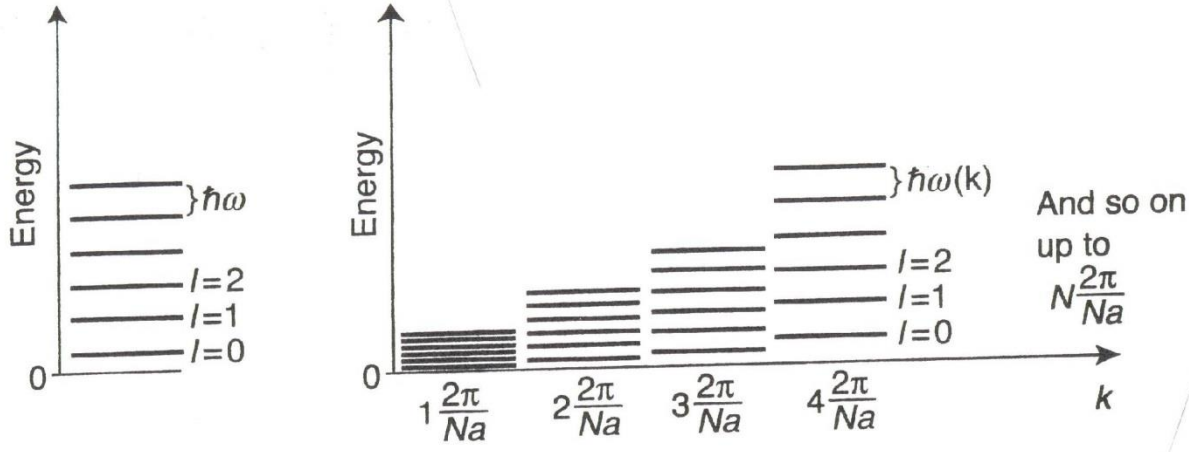
Energy level diagram for one harmonic oscillator



Energy level diagram for a chain of atoms with one atom per unit cell and a lengt of N unit cells