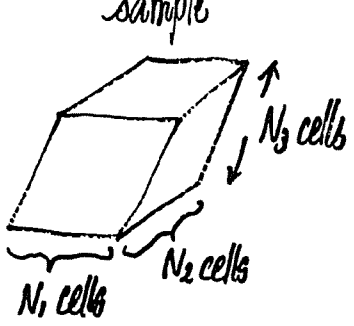
## H. Periodic B.C.[†] [Revisited] (General 3D case)

- Let $\vec{a}_1$, $\vec{a}_2$, $\vec{a}_3$ be the primitive vectors of the crystal.
- Consider a "big" crystal with:

  $N_1$ unit cells in $\vec{a}_1$-direction
  $N_2$ unit cells in $\vec{a}_2$-direction
  $N_3$ unit cells in $\vec{a}_3$-direction




$N_1, N_2, N_3 \gg 1$

Total number of unit cells $= N = N_1 \cdot N_2 \cdot N_3$

Impose periodic B.C. on $\vec{u}(\vec{R})$:

$$\vec{u}(\vec{R}) = \vec{u}(\vec{R}+N_1\vec{a}_1) = \vec{u}(\vec{R}+N_2\vec{a}_2) = \vec{u}(\vec{R}+N_3\vec{a}_3)$$

Since $\vec{u}(\vec{R}) \sim e^{i\vec{q}\cdot\vec{R}}$,

$$\text{B.C.} \Rightarrow \underbrace{e^{iN_1\vec{q}\cdot\vec{a}_1} = e^{iN_2\vec{q}\cdot\vec{a}_2} = e^{iN_3\vec{q}\cdot\vec{a}_3} = 1}_{\text{allowed } \vec{q}\text{'s}}$$

- At this point, it is useful to recall $\vec{a}_i \cdot \vec{b}_j = 2\pi\delta_{ij}$

[†] This generalizes the discussion on periodic B.C. to 3D.



Requires that:

$$\left.\begin{aligned} N_1\vec{q}\cdot\vec{a}_1 &= 2\pi\cdot(\text{integer}) = 2\pi h \\ N_2\vec{q}\cdot\vec{a}_2 &= 2\pi\cdot(\text{integer}) = 2\pi k \\ N_3\vec{q}\cdot\vec{a}_3 &= 2\pi\cdot(\text{integer}) = 2\pi l \end{aligned}\right\} \begin{array}{l} h,k,l \\ \text{are} \\ \underline{\text{integers}} \end{array}$$

$\therefore$ B.C. implies that $\vec{q}$ must be of the form:

$$\vec{q} = \frac{h}{N_1}\vec{b}_1 + \frac{k}{N_2}\vec{b}_2 + \frac{l}{N_3}\vec{b}_3$$

where $\vec{b}_1, \vec{b}_2, \vec{b}_3$ are the primitive vectors generating the reciprocal lattice.

- Since $N_1, N_2, N_3 \gg 1$ ($\sim 10^8$), the allowed $\vec{q}$'s are densely populated in the reciprocal space.

How dense?

Each allowed $\vec{q}$-point occupies

$$\frac{|\vec{b}_1\cdot(\vec{b}_2\times\vec{b}_3)|}{N_1\cdot N_2\cdot N_3} = \frac{v_G}{N}$$

($v_G$: volume of primitive cell in reciprocal space; $N$: Total # unit cells)

$$= \frac{1}{N}\frac{(2\pi)^3}{\Omega_c}$$

($V = N\Omega_c$: volume of a cell = volume of crysta)

$$= \frac{(2\pi)^3}{V}$$

$\therefore$ Each allowed $\vec{q}$ occupies $\frac{(2\pi)^3}{V}$ in reciprocal space.

In a "volume" $v_G$ of reciprocal space, there are $N$ allowed $\vec{q}$'s.

$\therefore$ **There are $N$ allowed $\vec{q}$'s in 1st B.Z.**

**Number of allowed $\vec{q}$'s in one unit volume of reciprocal space$^{+}$ $= \frac{V}{(2\pi)^3}$**

**$=$ "Density of states in q-space"**

Since $\vec{q}'$ and $\vec{q}$ differ by a reciprocal lattice vector $\vec{G}$ give the same normal mode oscillation, it is sufficient to consider $\vec{q}$ in 1st B.Z.

$^{+}$ This result is also useful in electron band theory. The density of states in q-space is uniform.



## A short summary:

- A sample of $N$ primitive cells + periodic B.C.
  $\Rightarrow$ $N$ allowed $\vec{q}$'s in 1st B.Z. (true for 1D, 2D, 3D)
- 1D: sample of length $L$
  # of allowed $\vec{q}$'s in a unit length of reciprocal space $= \frac{L}{2\pi}$

  2D: sample of area $A$
  # of allowed $\vec{q}$'s in a unit area of reciprocal space $= \frac{A}{(2\pi)^2}$

  3D: sample of volume $V$
  # of allowed $\vec{q}$'s in a unit volume of reciprocal space $= \frac{V}{(2\pi)^3}$
- $N \gg 1$ $\Rightarrow$ allowed $\vec{q}$'s in B.Z. are densely packed
  $\therefore$ When we see $\sum_{\vec{q} \text{ in 1st B.Z.}} (\cdots)$, we may replace the sum by an integral, i.e.

1D $\quad \sum_{q \in \text{1st B.Z.}} (\cdots) \rightarrow \frac{L}{2\pi} \int_{\text{1st B.Z.}} dq \, (\cdots)$

2D $\quad \sum_{\vec{q} \in \text{1st B.Z.}} (\cdots) \rightarrow \frac{A}{(2\pi)^2} \int_{\text{1st B.Z.}} d^2q \, (\cdots)$

3D $\quad \sum_{\vec{q} \in \text{1st B.Z.}} (\cdots) \rightarrow \frac{V}{(2\pi)^3} \int_{\text{1st B.Z.}} d^3q \, (\cdots)$

- Dispersion relation)

p atoms in basis and N primitive cells in sample

$\Rightarrow$ 3pN normal modes $\Rightarrow$ 3p branches

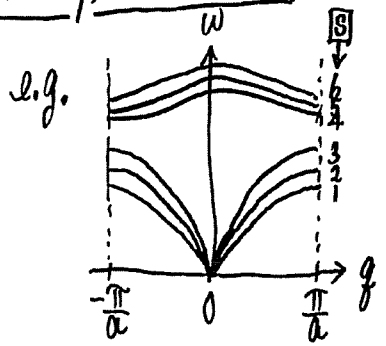
3 acoustic branches
3p-3 optical branches

$\Rightarrow$ a total of 3pN eigen-frequencies $\omega$'s.

These eigen-frequencies can be labelled by:

$\omega_s(\vec{q})$

$s$: branch index ($s = 1, 2, \cdots, 3p$)

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In energy band theory, we will use an analogous label $E_n(\vec{k})$, where $\vec{k} \in 1^{st}$ B.Z. and "n" is the band index.



# I. The Notion of "Phonons"

- Always remember that:
  - each normal mode involves all atoms
  - normal modes are independent of each other
- It turns out that in considering the physical consequences (and mathematics) of these normal mode oscillations, a "particle" viewpoint emerges. These particles are not matter particles.

With Harmonic Approximation, we have

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{ij} \frac{1}{2} K (u_i - u_j)^2$$

that gives the eq. of motion. (only carry quadratic terms $\sim uu$)

Solving for normal mode frequencies, we have in general

$\omega_s(\vec{q})$ , $\vec{q} \in 1^{st}$ B.Z. (N of them)

$s$: branch index
(3p branches, for p atoms/ basis)

- Using the eigenvectors to perform a transformation of coordinates, the Hamiltonian has the form of a collection of independent (uncoupled) harmonic oscillators, each for a normal mode eigenfrequency.

$$H = \sum_{\text{eigenfrequencies}} \frac{1}{2m_i} p_i^2 + \frac{1}{2} m_i \underbrace{\omega_i^2}_{\uparrow} x_i^2$$

from solving dispersion relation

i.e. $3pN$ independent harmonic oscillators

- Each oscillator can be labelled by $(s,\vec{q})$ based on its angular frequency, $\omega_s(\vec{q})$.

$$H = \sum_s \sum_{\vec{q}} h_{s,\vec{q}}$$

$$h_{s,\vec{q}} \equiv \frac{1}{2m_{s,\vec{q}}} p_{s,\vec{q}}^2 + \frac{1}{2} m_{s,\vec{q}}\, \omega_s^2(\vec{q})\, x_{s,\vec{q}}^2$$

- Do quantum mechanics on <u>each oscillator</u>

$\Rightarrow$ energy spectrum of

$$\left(n_s(\vec{q}) + \frac{1}{2}\right)\hbar\omega_s(\vec{q}) \quad , \quad n_s(\vec{q}) = 0, 1, 2, \cdots$$

for oscillator of angular frequency $\omega_s(\vec{q})$



<u>Consider the mode $\omega_s(\vec{q})$:</u>

$$\hat{h}_{s,\vec{q}} \underbrace{|n_s(\vec{q})\rangle}_{\text{energy eigenstate}} = \left(n_s(\vec{q}) + \frac{1}{2}\right)\hbar\omega_s(\vec{q})$$

$\uparrow$ a number

$|0\rangle$ "no" phonon in the mode $(s,\vec{q})$

$|1\rangle$ 1 phonon in the mode $(s,\vec{q})$

$|2\rangle$ 2 phonons in the mode $(s,\vec{q})$

$\vdots$ $\vdots$

$|n_s(\vec{q})\rangle$ $n_s(\vec{q})$ phonons in the mode $(s,\vec{q})$

$\vdots$ $\vdots$

Each phonon in the mode $(s,\vec{q})$:
- has energy $\hbar\omega_s(\vec{q})$
- has wavevector $\vec{q}$
- has a <u>quasi-momentum</u> or "<u>crystal momentum</u>" $\hbar\vec{q}$

Thus, $\hat{h}_{s,\vec{q}}$ can be written as

$$\hat{h}_{s,\vec{q}} = \left(\hat{n}_s(\vec{q}) + \frac{1}{2}\right)\hbar\omega_s(\vec{q})$$

$\hat{n}_s(\vec{q})$: number (of excitations) operator

$$= \left(\hat{a}_s^\dagger(\vec{q})\,\hat{a}_s(\vec{q}) + \frac{1}{2}\right)\hbar\omega_s(\vec{q})$$

with $[\hat{a}_s(\vec{q}), \hat{a}_s^\dagger(\vec{q})] = 1$

$\hat{a}_s(\vec{q})$: destruction operator; $\hat{a}_s^\dagger(\vec{q})$: creation operator

Treating each mode $(s,\vec{q})$ in this way, the total Hamiltonian becomes:

$$\hat{H} = \sum_s \sum_{\vec{q}} \left( \hat{a}_s^\dagger(\vec{q})\, \hat{a}_s(\vec{q}) + \frac{1}{2} \right) \hbar\omega_s(\vec{q})$$

($\sum_s$: over branches; $\sum_{\vec{q}}$: over all allowed $\vec{q}$'s in 1st BZ)

$$= \sum_s \sum_{\vec{q}} \left( \hat{n}_s(\vec{q}) + \frac{1}{2} \right) \hbar\omega_s(\vec{q})$$

An eigenstate of $\hat{H}$ can be written as:

$$| n_{s_1}(\vec{q}_1), n_{s_1}(\vec{q}_2), \cdots; n_{s_2}(\vec{q}_1)\, n_{s_2}(\vec{q}_2) \cdots \rangle$$

3pN numbers (each can be 0, 1, 2, ···) specifying the number of phonons $n_s(\vec{q})$ in the mode $(s,\vec{q})$

and the total vibrational energy of this state is

$$\underbrace{\sum_s \sum_{\vec{q}} \left( n_s(\vec{q}) + \frac{1}{2} \right) \hbar\omega_s(\vec{q})}$$

sum of amount of excitations (# phonons) in each mode $(s,\vec{q})$

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The commutators are: $[\hat{a}_s(\vec{q}), \hat{a}_{s'}^\dagger(\vec{q}')] = \delta_{ss'}\delta_{\vec{q}\vec{q}'}$

$[\hat{a}_s(\vec{q}), \hat{a}_{s'}(\vec{q}')] = 0 = [\hat{a}_s^\dagger(\vec{q}), \hat{a}_{s'}^\dagger(\vec{q}')]$



- The form of $\hat{H} = \sum_s \sum_{\vec{q}} \left( \hat{n}_s(\vec{q}) + \frac{1}{2} \right) \hbar\omega_s(\vec{q})$

$$= \text{zero point energy} + \sum_s \sum_{\vec{q}} \hat{n}_s(\vec{q}) \hbar\omega_s(\vec{q})$$

is convenient in many ways.

For example, for a solid at equilibrium at temperature T, we could ask:

(i) what is the mean excitation $\langle n_s(\vec{q}) \rangle$ of a mode $(s,\vec{q})$ at temp. T?

(ii) what is the internal energy and heat capacity contributed by lattice vibrations at temp. T?

These are easy!

We know how to do Statistical Mechanics of a system of collection of independent harmonic oscillators!

- # phonons in mode $(s,\vec{q})$ depends on temperature, i.e., phonons are NOT real matter particles.

## A brief summary on "phonons":

- We solved the classical H for normal modes $\omega_s(\vec{q})$.
- After doing that, $H = \sum_s \sum_{\vec{q}}$ (SHO of frequency $\omega_s(\vec{q})$)

  ↓ QM says eigenenergies are $(n_s(\vec{q}) + \frac{1}{2})\hbar\omega_s(\vec{q})$
- Total vibrational energy $= \sum_s \sum_{\vec{q}} (n_s(\vec{q}) + \frac{1}{2})\hbar\omega_s(\vec{q})$

  for a state with $n_s(\vec{q})$ phonons in the mode $(s,\vec{q})$
- A phonon in mode $(s,\vec{q})$ has { energy $\hbar\omega_s(\vec{q})$, wave vector $\vec{q}$, crystal momentum $\hbar\vec{q}$ } — like a particle†
- Crystal momentum is not the physical momentum. It is useful in considering "conservation laws" in scattering processes.

† Phonon, in many-body physics, belongs to a type of excitations called collective excitations, as each $(s,\vec{q})$ mode is related to motions of all atoms.



## J. Inelastic Scattering by Lattice Vibrations

- Neutron scattering involving phonons
- Inelastic neutron scattering can probe $\omega(\vec{q})$

### A quick review on (X-ray) elastic scattering†

$\vec{6} \rightarrow \bigcirc \nearrow \vec{s}'$ $\quad |\vec{s}| = |\vec{s}'|$ a result of periodicity

Laue condition: $\Delta\vec{s} = \vec{s}' - \vec{s} = \vec{G}$ for constructive interference

X-rays (EM waves)

$\hbar\vec{s}$ = momentum of photon (incident)

$\hbar\vec{s}'$ = momentum of photon (scattered)

$\Delta\vec{s} = \vec{G}$ implies $\hbar\vec{s}' - \hbar\vec{s} = \hbar\vec{G}$

or $\hbar\vec{s}' = \hbar\vec{s} + \hbar\vec{G}$

$\vec{G}$ could be written as $-\vec{G}'$ (just a reciprocal lattice vector), then $\hbar\vec{s}' = \hbar\vec{s} - \hbar\vec{G}$

Key Point: In scatterings off a periodic system (crystal), the system plays a role in giving or taking a momentum $\hbar\vec{G}$, where $\vec{G}$ is a reciprocal lattice vector.

† See Ch. V on elastic scattering of waves in SSP.

Incident neutron: momentum $\hbar\vec{k}$, energy $\frac{\hbar^2 k^2}{2M}$

Idea: In a solid (there are excitations related to $\omega_s(\vec{q})$), an electron can interact with the quantized vibrations (i.e., creates/destroys phonons) and exchange energy (thus inelastic) with them.
[electron-phonon interaction]†

Elastic Scattering:

- Similar to X-rays
- $|\hbar\vec{k}| = |\hbar\vec{k}'|$ and $E = E'$ (energy of scattered particle)
- Following discussion in Ch.V, we require

$$\Delta\hbar\vec{k} = \hbar\vec{k}' - \hbar\vec{k} = \vec{G}$$

or $\underbrace{\hbar\vec{k}' - \hbar\vec{k}}_{\text{difference in momentum}} = \hbar\vec{G}$

† Electron-phonon interaction is a key process of why a metal has an increasing resistivity with temperature. Surprisingly, it is also the key to understand superconductivity.



Inelastic Scattering

- The "momentum conservation" rule




We start with an equation that we obtained in the last chapter.

Remark: There is a factor of $\left(A\frac{e^{ikR}}{R}e^{-i\omega t}\right)$ in front (c.f. Ch.V)

The scattered wave amplitude has a factor:

$$F = \sum_j f_j e^{-i\Delta\vec{k}\cdot\vec{r}_j}$$ (see p.II-⑧-⑫)

$\vec{r}_j$: where the atoms are; $\Delta\vec{k} = \vec{k}' - \vec{k}$

$\sum_j$: over all atoms

$$= \sum_{\vec{R}} \sum_{\ell} f_\ell e^{-i\Delta\vec{k}\cdot(\vec{R} + \vec{\rho}_\ell + \vec{u}(\vec{R},\ell))}$$

- $\sum_{\vec{R}}$: over lattice points
- $\sum_{\ell}$: over basis atoms $\ell$ decorating each lattice point
- $\vec{\rho}_\ell$: equilibrium position of the $\ell^{th}$ atom in the basis in the cell at $\vec{R}$ [included in discussion of elastic scattering]
- $\vec{u}(\vec{R},\ell)$: displacement of the $\ell^{th}$ atom in the basis in the cell at $\vec{R}$ [needed for considering inelastic scattering]
- $\vec{u}$: atom vibration

Remark: We ignored the small displacements $\vec{u}(\vec{R},\ell)$ in the discussion in Ch.V on X-ray diffraction.

For small displacements,

$$F = \sum_{\vec{R}} \sum_{\ell} f_\ell \, e^{-i\Delta\vec{k}\cdot(\vec{R}+\vec{\rho}_\ell)} \, e^{-i\Delta\vec{k}\cdot\vec{u}(\vec{R},\ell)}$$

($e^{-i\Delta\vec{k}\cdot\vec{u}(\vec{R},\ell)}$: small oscillations)

$$\approx \sum_{\vec{R}} \sum_{\ell} f_\ell \, e^{-i\Delta\vec{k}\cdot(\vec{R}+\vec{\rho}_\ell)} \left(1 - i\Delta\vec{k}\cdot\vec{u}(\vec{R},\ell)\right)$$

($1$: 1st term gives)

$F = a(\Delta\vec{k}) \cdot \mathcal{S}(\Delta\vec{k})$

and thus the Laue condition $\Delta\vec{k} = \vec{G}$ for a non-vanishing $F$

- $\vec{u}(\vec{R},\ell)$ can be written in terms of the normal mode eigenvectors (amplitudes) as: (schematic) [Bloch's theorem + normal mode]

$$u(\vec{R},\ell) \sim \frac{\vec{A}_\ell}{\sqrt{M_\ell}} \, e^{i\vec{q}\cdot\vec{R}} e^{-i\omega(q)t} + \frac{\vec{A}_\ell^*}{\sqrt{M_\ell}} \, e^{-i\vec{q}\cdot\vec{R}} e^{+i\omega(q)t}$$

$$F \approx \left(\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}}\right)\left(\sum_\ell f_\ell e^{-i\Delta\vec{k}\cdot\vec{\rho}_\ell}\right) \leftarrow \text{elastic scattering}$$

$$- \left(\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} e^{i\vec{q}\cdot\vec{R}}\right)\left(\sum_\ell f_\ell \, i\Delta\vec{k}\cdot\frac{\vec{A}_\ell}{\sqrt{M_\ell}} e^{-i\Delta\vec{k}\cdot\vec{\rho}_\ell}\right) e^{-i\omega(q)t}$$

$$- \left(\sum_{\vec{R}} e^{-i\Delta\vec{k}\cdot\vec{R}} e^{-i\vec{q}\cdot\vec{R}}\right)\left(\sum_\ell f_\ell \, i\Delta\vec{k}\cdot\frac{\vec{A}_\ell^*}{\sqrt{M_\ell}} e^{-i\Delta\vec{k}\cdot\vec{\rho}_\ell}\right) e^{+i\omega(q)t}$$



- The 2nd term has a factor:

$$\sum_{\vec{R}} e^{-i(\Delta\vec{k}-\vec{q})\cdot\vec{R}}$$

| Recall: $e^{i\vec{G}\cdot\vec{R}} = 1$

∴ 2nd term will be non-vanishing if $\Delta\vec{k} - \vec{q} = \vec{G}$ ← a reciprocal lattice vector

OR $\Delta\vec{k} = \vec{q} + \vec{G}$ "conservation of wave vector"

OR $\boxed{\hbar\vec{k}' = \hbar\vec{k} + \hbar\vec{q} + \hbar\vec{G}}$ "conservation of momentum"

(single phonon absorption)

- Similarly, the 3rd term has a factor:

$$\sum_{\vec{R}} e^{-i(\Delta\vec{k}+\vec{q})\cdot\vec{R}}$$

∴ 3rd term will be non-vanishing if $\Delta\vec{k} + \vec{q} = \vec{G}$

OR $\Delta\vec{k} = -\vec{q} + \vec{G}$

OR $\boxed{\hbar\vec{k}' = \hbar\vec{k} - \hbar\vec{q} + \hbar\vec{G}}$

(single phonon creation)

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Remark: The treatment here is general, and can be applied to other inelastic scattering (different source / different excitations)

- If we include a factor $e^{-i\omega t}$ into F, then we will have a factor

$$e^{-i(\omega+\omega(\vec{q}))t} = e^{-i\omega' t} \quad \text{in the } \underline{2^{nd} \text{ term}}$$

or $\omega' = \omega + \omega(\vec{q})$

$\hbar\omega' = \hbar\omega + \hbar\omega(\vec{q})$ (single phonon absorption)

↑ outgoing ↑ incident ↑ phonon energy

and a factor

$$e^{-i\omega t}\, e^{+i\omega(\vec{q})t} = e^{-i\omega' t} \quad \text{in the } \underline{3^{rd} \text{ term}}$$

or $\hbar\omega' = \hbar\omega - \hbar\omega(\vec{q})$ (single phonon creation)

- These energy and momentum conservation laws indicate that the particle viewpoint of lattice vibrations is useful and makes good physical sense.



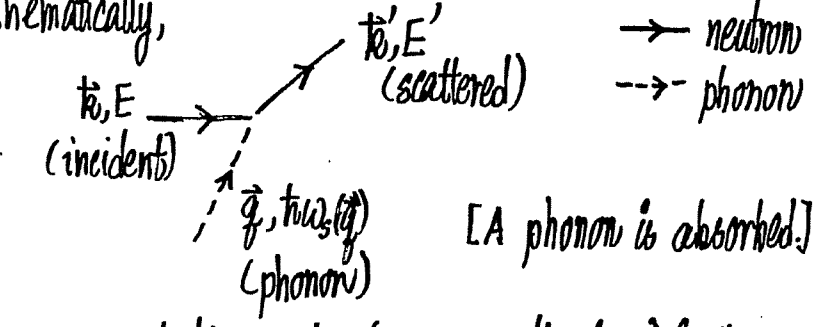
Inelastic Scattering: (diagramatic)

- Neutron exchanges energy/momentum with crystal

The simplest processes are: (besides elastic scattering)

(a) Absorption (Destroying) of a single phonon

Schematically,




[A phonon is absorbed.]

There are selection rules (or conservation laws) for the proce

$E' = E + \hbar\omega_s(\vec{q})$ [energy conservation]

and $\hbar\vec{k}' = \hbar\vec{k} + \hbar\vec{q} + \hbar\vec{G}$ ← can be regarded as a form of "momentum conservation"

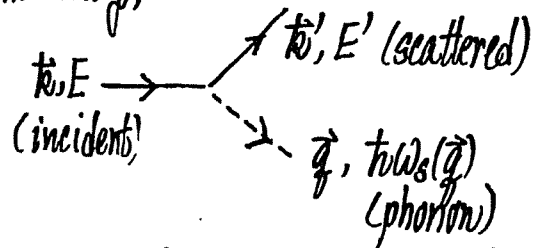
or $\Delta\vec{k} = \vec{q} + \vec{G}$

↑ due to phonon ↑ due to periodicity

Thus, "$\hbar\vec{q}$" behaves as if it is the momentum of a phonon. To distinguish it from the physical momentum, it is called the crystal momentum.

(b) Emission (Creation) of a single phonon

Schematically,††




[A phonon is created.]

The selection rules (conservation laws) are:

$$E' = E - \hbar\omega_s(\vec{q}) \qquad \text{[energy conservation]}$$

and

$$\hbar\vec{k}' = \hbar\vec{k} - \hbar\vec{q} + \hbar\vec{G} \qquad \text{["momentum conservation"]}$$

or $\Delta\hbar\vec{k} = -\vec{q} + \vec{G}$

† This kind of diagram, while treated as schematic here, could be turned into serious business! In many-body physics, such diagram is called Feynman diagram. The lines are free propagators or Green's functions for neutron and phonon. The vertex, where the lines meet, represents the interaction. There are (simple) rules to calculate the probability amplitude for such neutron-phonon process.

‡ If the particle is not neutron but electron, then we are dealing with electron-phonon scattering, which is important in the understanding of resistivity of solids, and superconductivity.

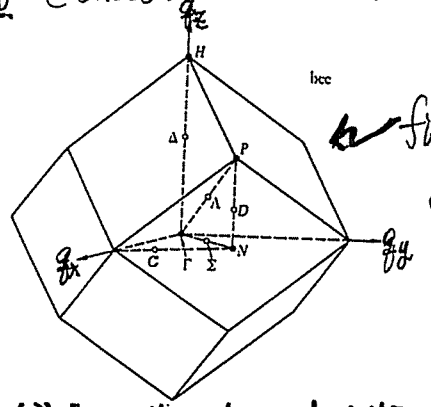


• Here by measuring $E'$ and $\hbar\vec{k}'$ of neutrons in inelastic neutron scattering off a solid, we can probe $\omega(\vec{q})$, the phonon dispersion relation.

probing solid excitations


$\Delta E$ and $\Delta\hbar\vec{k}$ $\Rightarrow \omega_s(\vec{q})$

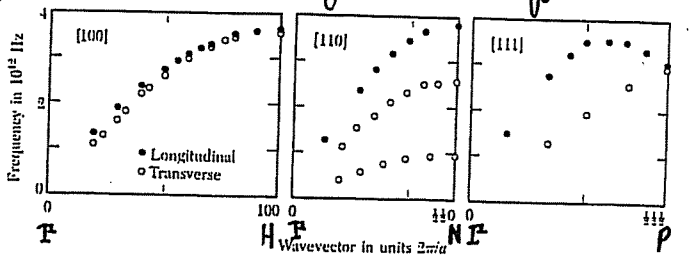
e.g. Sodium (direct lattice is bcc)




Reciprocal lattice is fcc

← first Brillouin zone

With measured $\omega_s(\vec{q})$ [usually only part of it], one could fit the "spring constants" (derivatives of V) and to study atomic interactions.†




Neutron diffraction measurements of $\omega_s(\vec{q})$

The dispersion curves of sodium for phonons propagating in the [001], [110], and [111] directions at 90 K, as determined by inelastic scattering of neutrons

† It is still an active research area. For more information, see M. Finnis, "Interatomic forces in condensed matter", Oxford U. Press (2003).

- If the inelastic scattering involves EM waves (visible or near UV), then $q \approx 0$ modes are involved (Raman Scattering, Brillouin scattering).

Applications

Lattice vibrations or phonons are important in considering:

- thermal properties
  - heat capacity, thermal conductivity, expansion, etc.
- electrical / transport properties
  - resistivity
  - superconductivity
- optical / dielectric properties in IR range.



References:

- Kittel: Ch.4; Christman: Ch.6; 黃昆: 第三章
- Ashcroft and Mermin: Appendix L (p.780-783)
  - gives the mathematics of quantising the displacement fields and how the Hamiltonian can be diagonalized.
- "Physics World" (December, 1997): articles on neutron scattering and its applications in solid state physics
- Books/Articles specifically on lattice vibrations:
  - M. Born and K. Huang, "Dynamical theory of crystal lattices" (1954).
  - J. Ziman, "Electrons and Phonons" (1960).
  - W. Cochran, "Dynamics of atoms in crystals" (1973).
  - A.A. Maradudin et. al., "Theory of lattice dynamics in the harmonic approximation", Solid State Physics, Supp. 3 (1971); see also Rev. Mod. Phys. 40, 1 (1968).