# Lecture 6
# Bloch's Theorem, Crystal Momentum Conservation, Phonon Scattering

Symmetry!

# Bloch's Theorem

Chapter 8, A&M; Should be viewed as describing wave function of any particles, not only electrons.

- The crystal translation operator can be defined as $T_{\mathbf{R}}\, f(\mathbf{x}) = f(\mathbf{x}+\mathbf{R})$, where **R** is a Bravais lattice vector.
- Bloch's Theorem is simply a statement that if H is invariant under translation by all **R**'s then the eigenfunction of H can be written as eigenstates of $T_{\mathbf{R}}$: $T_{\mathbf{R}}\, \psi(\mathbf{x}) = \exp(i\mathbf{k}\cdot\mathbf{R})\ \psi(\mathbf{x})$
- Staring point to prove it is that $T_R$ is diagonalizable using the complete basis of plane waves $\exp(i\mathbf{k}\cdot\mathbf{x})$ with eigenvalue $\exp(i\mathbf{k}\cdot\mathbf{R})$.

# Bloch's Theorem

Chapter 8, A&M; Should be viewed as describing wave function of any particles, not only electrons.

Form 1

$$\psi_{n\mathbf{k}}(\mathbf{x}) = \exp(i\mathbf{k}\cdot\mathbf{x})\, u_{n\mathbf{k}}(\mathbf{x}),$$

$$u_{n\mathbf{k}}(\mathbf{x}+\mathbf{R}) = u_{n\mathbf{k}}(\mathbf{x})$$

n includes all other quantum #'s
(spin, polarization, orbital …)

Form 2

$$\psi_{n\mathbf{k}}(\mathbf{x}+\mathbf{R}) = \exp(i\mathbf{k}\cdot\mathbf{R})\, \psi_{n\mathbf{k}}(\mathbf{x})$$

What is u for the normal mode problem of the lattice?

# Crytal Momentum and its Conservation

- The eigenvalue of $T_{\mathbf{R}}$, $\exp(i\mathbf{k}\cdot\mathbf{R})$, defines $\mathbf{k}$ only up to $\mathbf{K}$.
- $\hbar\mathbf{k}$ is the "crystal momentum."
- The form $\exp(i\mathbf{k}\cdot\mathbf{R})$ suggests that the operator that has eigenvalues $\hbar\mathbf{k}$ is the generator of the crystal translation – crystal momentum operator.
- Crystal momentum conservation

$$\Sigma_{\text{initial}}\,\mathbf{k} = \Sigma_{\text{final}}\,\mathbf{k} + \mathbf{K}$$

(any reciprocal lattice vector $\mathbf{K}$ is a new "zero" in crystal)

Holds however many (different kinds of) particles are involved or elastic/inelastic scatterings.

# Neutron Scattering of Phonons

- 0 phonon scattering:

neutron init: $\mathbf{p} = \hbar\mathbf{q}$, neutron final: $\mathbf{p}' = \hbar\mathbf{q}'$,

$$q' = q, \quad \mathbf{q}' = \mathbf{q} + \mathbf{K}.$$

- 1 phonon scattering:

$$E' = E + \hbar\omega_s(\mathbf{k}), \qquad \mathbf{p}' = \mathbf{p} + \hbar\mathbf{k} + \hbar\mathbf{K},$$

$$E' = E - \hbar\omega_s(\mathbf{k}), \qquad \mathbf{p}' = \mathbf{p} - \hbar\mathbf{k} + \hbar\mathbf{K},$$

$$\frac{p'^2}{2M_n} = \frac{p^2}{2M_n} + \hbar\omega_s\left(\frac{\mathbf{p}'-\mathbf{p}}{\hbar}\right), \quad \text{phonon absorbed,}$$

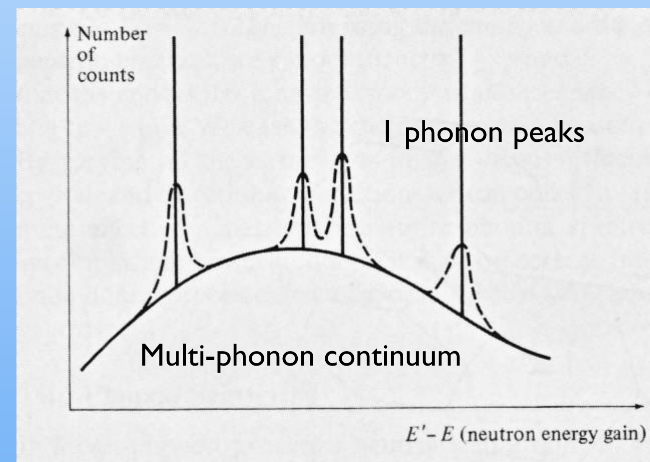
$$\frac{p'^2}{2M_n} = \frac{p^2}{2M_n} - \hbar\omega_s\left(\frac{\mathbf{p}-\mathbf{p}'}{\hbar}\right), \quad \text{phonon emitted.}$$

- Multi-phonon scattering

$$E' = E + \hbar\omega_s(\mathbf{k}) + \hbar\omega_{s'}(\mathbf{k}'), \qquad \mathbf{p}' = \mathbf{p} + \hbar\mathbf{k} + \hbar\mathbf{k}' + \hbar\mathbf{K}.$$

2 phonon absorption

$$E' = E + \hbar\omega_s(\mathbf{k}) + \hbar\omega_{s'}\left(\frac{\mathbf{p}'-\mathbf{p}}{\hbar} - \mathbf{k}\right).$$



# Energy, momentum conservation

$$\frac{E_N}{k_B} = 24(q[\text{Å}^{-1}])^2\ \text{K}.$$

$$E_N = 2.1(q[\text{Å}^{-1}])^2 \times 10^{-3}\ \text{eV},$$

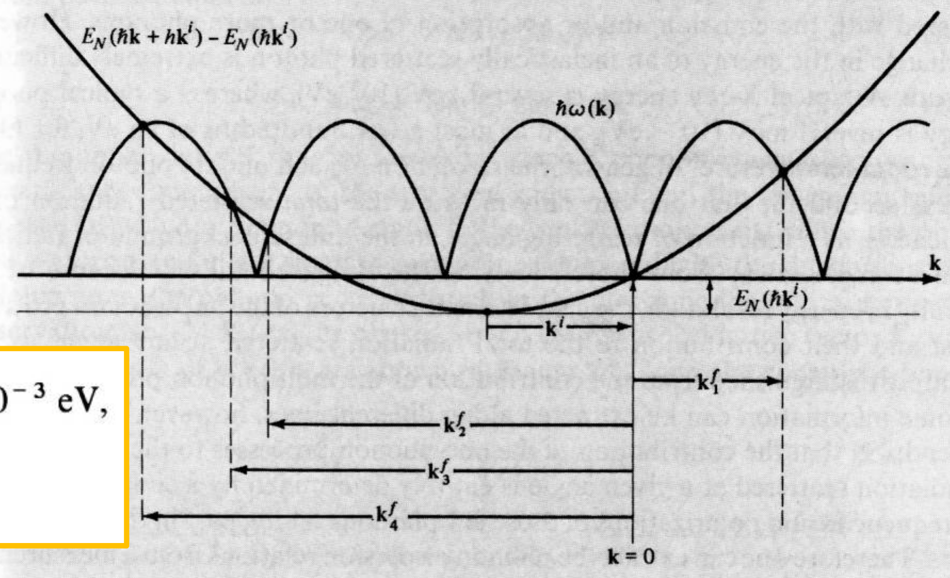



**Figure 24.6**

Graphical solution to the one-phonon conservation laws when the incident neutron has wave vector $\mathbf{k}^i$. The conservation law for phonon absorption can be written

$$E_N(\hbar\mathbf{k} + \hbar\mathbf{k}^i) - E_N(\hbar\mathbf{k}^i) = \hbar\omega(\mathbf{k}),$$

where $\hbar\mathbf{k}$ is the momentum of the scattered neutron, and $E_N(\mathbf{p}) = p^2/2M_N$. To draw the left-hand side of this equation, one displaces the neutron energy-momentum curve horizontally so that it is centered at $\mathbf{k} = -\mathbf{k}^i$ rather than $\mathbf{k} = 0$, and displaces it downward by an amount $E_N(\hbar\mathbf{k}^i)$. Solutions occur wherever this displaced curve intersects the phonon dispersion curve $\hbar\omega(\mathbf{k})$. In the present case there are solutions for four different scattered neutron wave vectors, $\mathbf{k}_1{}^f \cdots \mathbf{k}_4{}^f$.

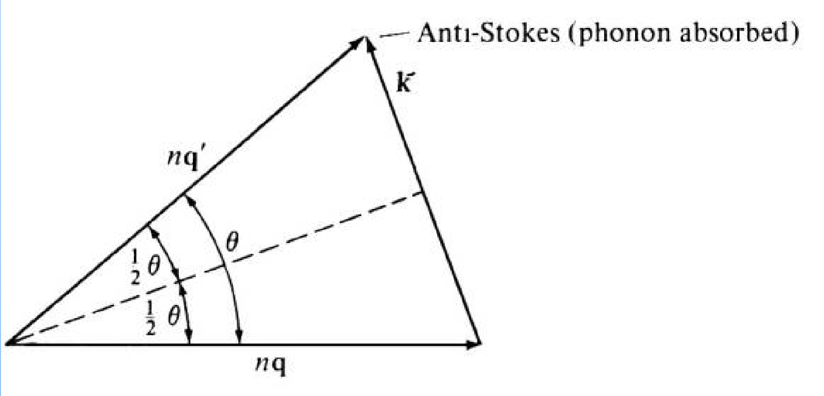
# Optical or X-Ray Measurement

$$\hbar\omega' = \hbar\omega \pm \hbar\omega_s(\mathbf{k})$$

$$\hbar n\mathbf{q}' = \hbar n\mathbf{q} \pm \hbar\mathbf{k} + \hbar\mathbf{K}.$$

Optical Phonons – Raman Scattering
Acoustic Phonons – Brillouin Scattering

Laser light is used (~ a few 1000 Å wavelength with ~ eV energy)
$|\mathbf{q}'| \approx |\mathbf{q}|$
**k** ~ 0 is probed




Raman, Brillouin

$$k = 2nq \sin \tfrac{1}{2}\theta = (2\omega n/c) \sin \tfrac{1}{2}\theta.$$

Brillouin

$$c_s(\hat{\mathbf{k}}) = \frac{\Delta\omega}{2\omega}\frac{c}{n}(\csc \tfrac{1}{2}\theta).$$

It is also possible to probe phonons using High energy X-ray (10 keV) using modern synchrotrons (such as ESRF, APS).

# Wave Picture of Neutron Scattering

Diffraction by a moving grating – Convenient to use the moving frame

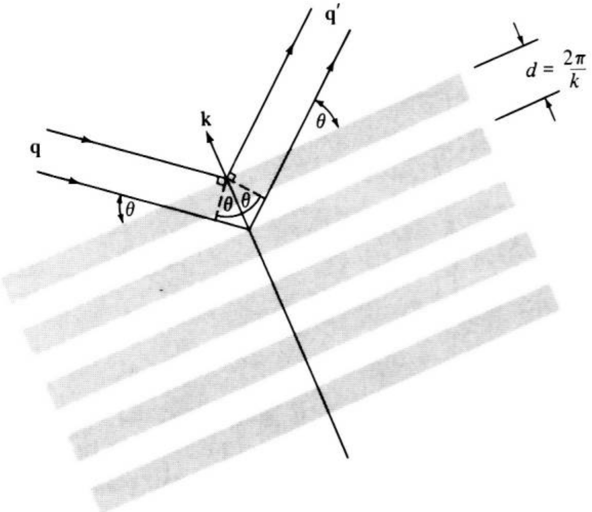



**Figure 24.10**
Scattering of a neutron by a phonon in a frame of reference in which the phonon phase velocity is zero. The phonon appears as a static diffraction grating; i.e., it results in regions of alternating high and low ionic density. The Bragg condition (p. 97), $m\lambda = 2d \sin\theta$ ($m$ an integer) can be written as

$$\frac{2\pi m}{q} = \frac{4\pi}{k} \sin\theta$$

or

$$mk = 2q \sin\theta$$

or

$$mk = (\mathbf{q}' - \mathbf{q}) \cdot \hat{\mathbf{k}}.$$

Since Bragg reflection is specular (angle of incidence equals angle of reflection) and since the magnitude $q'$ equals the magnitude $q$, it follows that $\mathbf{q}' - \mathbf{q}$ must be parallel to $\mathbf{k}$ and therefore $\mathbf{q}' - \mathbf{q} = m\mathbf{k}$.

Phase velocity of phonon $\mathbf{v} = \frac{\omega}{k}\hat{\mathbf{k}}.$

$$\bar{\omega} = \omega - \mathbf{k} \cdot \mathbf{v},$$
$$\frac{\bar{E}}{\hbar} = \frac{E}{\hbar} - \mathbf{q} \cdot \mathbf{v},$$
$$\frac{\bar{E}'}{\hbar} = \frac{E'}{\hbar} - \mathbf{q}' \cdot \mathbf{v}.$$

same

$$\frac{E'}{\hbar} = \frac{E}{\hbar} + (\mathbf{q}' - \mathbf{q}) \cdot \mathbf{v}.$$

$$\boxed{\mathbf{q}' = \mathbf{q} + m\mathbf{k},}$$

$$\frac{E'}{\hbar} = \frac{E}{\hbar} + m\mathbf{k} \cdot \mathbf{v}.$$

$$\boxed{E' = E + m\hbar\omega.}$$