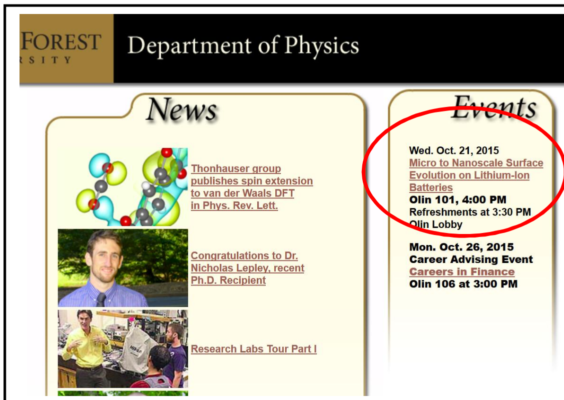
PHY 752 Solid State Physics
11-11:50 AM MWF Olin 103

Plan for Lecture 22:

- **Scattering of particles by crystals (Chap. 10 in GGGPP)**
  - **Photon scattering**
  - **Electron scattering**
  - **Neutron scattering**
  - **Effects of lattice vibrations**

8	Fri, 9/11/2015	Chap. 2	Group theory	#7
9	Mon, 9/14/2015	Chap. 2.4-2.7	Densities of states	#8`
10	Wed, 9/16/2015	Chap. 3	Free electron model	#9
11	Fri, 9/18/2015	Chap. 4	One electron approximations to the many electron problem	#10
12	Mon, 9/21/2015	Chap. 4	One electron approximations to the many electron problem	#11
13	Wed, 9/23/2015	Chap. 4	Density functional theory	#12
14	Fri, 9/25/2015	Chap. 5	Implementation of density functional theory	#13
15	Mon, 9/28/2015	Chap. 5	Implementation of density functional theory	#14
16	Wed, 9/30/2015	Chap. 5	First principles pseudopotential methods	#15
17	Fri, 10/02/2015	Chap. 6	Example electronic structures	#16
18	Mon, 10/05/2015	Chap. 6	Ionic and covalent crystals	#17
19	Wed, 10/07/2015	Chap. 6	More examples of electronic structures	#18
20	Fri, 10/09/2015	Chap. 1-6	Review	Start exam
	Mon, 10/12/2015		No class	Take-home exam
	Wed, 10/14/2015		No class	Exam due before 10/19/2015
	Fri, 10/16/2015		Fall break -- no class	
21	Mon, 10/19/2015	Chap. 10	X-ray and neutron diffraction	#HW19
22	Wed, 10/21/2015	Chap. 10	Scattering of particles by crystals	#HW20
	Wed, 12/02/2015		Student presentations I	
	Fri, 12/04/2015		Student presentations II	
	Mon, 12/07/2015		Begin Take-home final	



WFU Physics Colloquium

TITLE: Micro to Nanoscale Surface Evolution on Lithium-Ion Batteries

SPEAKER: Sung-Jin Cho,

Department of Nano Engineering,
Joint School of Nanoscience and Nanoengineering,
North Carolina A&T State University,
Greensboro, NC

TIME: Wednesday October 21, 2015 at 4:00 PM

PLACE: Room 101 Olin Physical Laboratory

Refreshments will be served at 3:30 PM in the Olin Lounge. All interested persons are cordially invited to attend.

ABSTRACT

Two ongoing research projects related to energy storage materials and devices such as lithium-ion batteries will be described. First, we report a thoroughly new concept applied to the design and synthesis of a multifunctional, nanoscale interface and multi-phase

General considerations of particle scattering experiments

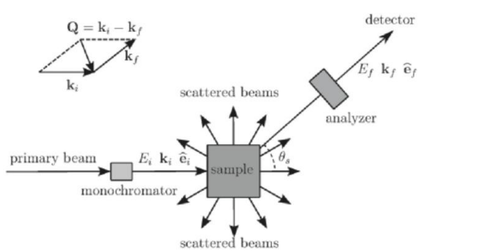


Figure 10.1 Schematic experimental set-up for scattering measurements. The momentum transfer to the target is $\hbar\mathbf{Q} = \hbar\mathbf{k}_i - \hbar\mathbf{k}_f$, and the energy transfer to the target is $E = E_i - E_f$.

Photon scattering

$$\text{photons}: \quad \lambda = \frac{12398.5}{\hbar\omega} \quad (\lambda \text{ in Å and } \hbar\omega \text{ in eV}).$$

$$\hbar\omega \approx 10-50 \text{ keV}$$

Elastic scattering of X-rays proceeds primarily by Thompson scattering by "free" electrons

Consider incident electric field of X-ray:

$$\mathbf{E}(\mathbf{r}, t) = \widehat{\mathbf{e}}_i \, E_0 \, e^{i(\mathbf{k}_i \cdot \mathbf{r} - \omega t)}.$$

Response by electron:

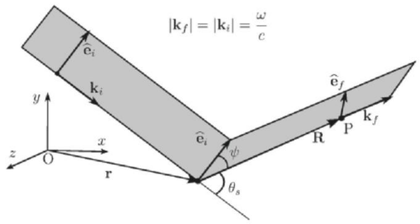
$$\ddot{\mathbf{u}}(\mathbf{r}, t) = \frac{(-e)}{m} \widehat{\mathbf{e}}_i \, E_0 \, e^{i(\mathbf{k}_i \cdot \mathbf{r} - \omega t)}.$$

Photon scattering -- continued

Radiation by excited electron:

$$\mathbf{E}_d(\mathbf{r},\mathbf{R},t) = \frac{-e}{c^2 R}\left\{\ddot{\mathbf{u}}(\mathbf{r},t-R/c) - \left[\widehat{\mathbf{k}}_f \cdot \ddot{\mathbf{u}}(\mathbf{r},t-R/c)\right]\widehat{\mathbf{k}}_f\right\}$$
$$= \frac{1}{R}\frac{e^2}{mc^2}E_0\, e^{i\mathbf{k}_i\cdot\mathbf{r}}e^{-i\omega(t-R/c)}\left[\widehat{\mathbf{e}}_i - (\widehat{\mathbf{k}}_f\cdot\widehat{\mathbf{e}}_i)\widehat{\mathbf{k}}_f\right],$$

$$|\mathbf{k}_f| = |\mathbf{k}_i| = \frac{\omega}{c}$$



Photon scattering -- continued

Intensity of scattered $I_s(\mathbf{R}) = I_0\frac{1}{R^2}\left(\frac{e^2}{mc^2}\right)^2(\widehat{\mathbf{e}}_i\cdot\widehat{\mathbf{e}}_f)^2,$

Corresponding scattering cross section averaging over polarizations of incident radiation:

$$\left(\frac{d\sigma}{d\Omega}\right)^{(\text{unpol})}_{\text{Th}} = \left(\frac{e^2}{mc^2}\right)^2\frac{1+\cos^2\theta_s}{2},$$

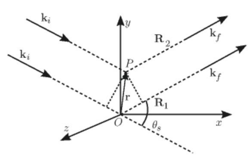
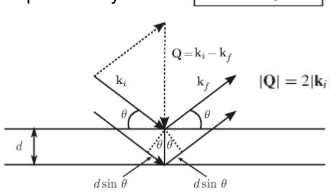


Figure 10.3 Schematic geometry of an electromagnetic field scattered from one electron at the origin O and one electron at the point P; the difference in optical path length between the wave scattered from O and the wave scattered from P is $\mathbf{k}_i\cdot\mathbf{r} - \mathbf{k}_f\cdot\mathbf{r} = \mathbf{Q}\cdot\mathbf{r}$, where $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$ is the momentum transfer in units $\hbar$.

Extending analysis to scattering by many electrons characterized by electron density $n_{el}(\mathbf{r})$

$$\frac{d\sigma}{d\Omega} = \left(\frac{d\sigma}{d\Omega}\right)_{\text{Th}}\left|\int n_{\text{el}}(\mathbf{r})e^{i\mathbf{Q}\cdot\mathbf{r}}\,d\mathbf{r}\right|^2 = \left(\frac{d\sigma}{d\Omega}\right)_{\text{Th}}|F(\mathbf{Q})|^2$$

For periodic system $\boxed{\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f \equiv \mathbf{G}}$,



$$|\mathbf{Q}| = 2|\mathbf{k}_i|\sin\theta = 2\frac{2\pi}{\lambda}\sin\theta = n\frac{2\pi}{d},$$

Figure 10.4 Waves reflected from successive planes reinforce if $2d\sin\theta$ equals an integer number $n\lambda$ of wavelengths. The geometrical construction of $\mathbf{Q} = \mathbf{k}_i - \mathbf{k}_f$ is also provided.

Corrections to Thompson scattering –

Compton scattering – correction for electron recall

Can be important if photon energy $\hbar\omega$ is comparable to rest mass energy of electron mc^2.

Other competing effects

Photon excitation processes

Phonons

Neutron scattering

Effective potential for interaction of neutron with nucleus:

$$V_p(\mathbf{r}-\mathbf{R}) = \frac{2\pi\hbar^2}{M_n} b\,\delta(\mathbf{r}-\mathbf{R}),$$

neutron scattering length

Probability of neutron interaction with nuclei at positions R_m:

$$P_{\mathbf{k}_f \leftarrow \mathbf{k}_i} = b^2 \frac{8\pi^3\hbar^3}{M_n^2} \frac{1}{V^2} \sum_{F,I} p_I \left| \langle \Phi_F | \sum_m e^{i\mathbf{Q}\cdot\mathbf{R}_m} | \Phi_I \rangle \right|^2 \delta(E_F - E_I - E).$$

In terms of scattering cross section:

$$\frac{d^2\sigma}{dE_f\, d\Omega} = \frac{V^2}{(2\pi)^3} \frac{M_n^2}{\hbar^3} \frac{k_f}{k_i} P_{\mathbf{k}_f \leftarrow \mathbf{k}_i} = \underline{b^2 \frac{k_f}{k_i} S(\mathbf{Q}, E)}$$

Neutron scattering --- continued

$$\frac{d^2\sigma}{dE_f\, d\Omega} = b^2 \frac{k_f}{k_i} S(\mathbf{Q}, E)$$

$$S(\mathbf{Q}, E) = \frac{1}{\hbar} \int_{-\infty}^{+\infty} \frac{dt}{2\pi} e^{-iEt/\hbar} \sum_{m\,n} \langle e^{-i\mathbf{Q}\cdot\mathbf{R}_m} e^{i\mathbf{Q}\cdot\mathbf{R}_n(t)} \rangle$$

Some details –

Effects of lattice vibrations

Zero phonon contributions; elastic scattering

$$S_0(\mathbf{Q}, E) = N e^{-2W} \sum_{\mathbf{t}_n} e^{i\mathbf{Q}\cdot\mathbf{t}_n} \delta(E).$$

Debye-Waller factor

Digression on analysis of thermal averages of lattice vibrations (Appendix A of Chapter 9 in GGGPP)

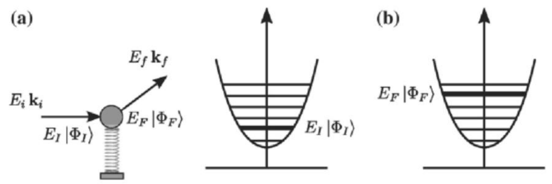


Figure 10.14 (a) Diffusion of particles by a scatterer, represented by an elastically bound nucleus of mass M and frequency $\hbar\omega_0$. (b) Schematic representation of initial and final energy levels and states of the harmonic oscillator scatterer, of given frequency ω_0.

$$\boxed{S(\mathbf{Q}, E) = \frac{1}{\hbar}\int_{-\infty}^{+\infty}\frac{dt}{2\pi}\, e^{-iEt/\hbar}\langle e^{-i\mathbf{Q}\cdot\mathbf{R}}\, e^{i\mathbf{Q}\cdot\mathbf{R}(t)}\rangle},$$

Convenient identity: $\langle e^{A} e^{B}\rangle = e^{\langle A^2 + 2AB + B^2\rangle/2}$,

We use the above expression with $A = -i\mathbf{Q}\cdot\mathbf{u}$ and $B = i\mathbf{Q}\cdot\mathbf{u}(t)$ (without loss of generality, whenever useful, we can suppose that $\mathbf{Q}$ is in the x-direction). Equation (10.48) thus takes the form

$$\boxed{S(\mathbf{Q}, E) = e^{-2W}\,\frac{1}{\hbar}\int_{-\infty}^{+\infty}\frac{dt}{2\pi}\, e^{-iEt/\hbar} e^{\langle \mathbf{Q}\cdot\mathbf{u}\;\mathbf{Q}\cdot\mathbf{u}(t)\rangle}}, \qquad (10.51a)$$

where

$$2W = \langle(\mathbf{Q}\cdot\mathbf{u})^2\rangle. \qquad (10.51b)$$

The quantity $\exp(-2W)$ is called the *Debye-Waller factor*; its physical consequences will be apparent soon.

Using Eq. (10.49b), the explicit expression of $2W$ reads

$$2W = \frac{\hbar^2 Q^2}{2M}\frac{1}{\hbar\omega_0}\left(\frac{2}{e^{\hbar\omega_0/k_BT} - 1} + 1\right).$$

Some steps:

$$u_x = \sqrt{\frac{\hbar}{2M\omega_0}}\left[a_x + a_x^\dagger\right], \qquad (10.49a)$$

and similar expressions for u_y and u_z. From elementary properties of harmonic oscillators (see Appendix 9.A) we obtain

$$\langle u_x^2\rangle = \frac{\hbar}{2M\omega_0}\langle(a_x + a_x^\dagger)(a_x + a_x^\dagger)\rangle = \frac{\hbar}{2M\omega_0}\left(2\langle n\rangle + 1\right),$$

where the average number of phonons $\langle n\rangle = \langle a_x^\dagger a_x\rangle$ is given by the Bose-Einstein distribution function $1/(\exp(\hbar\omega_0/k_BT) - 1)$. Then

$$\langle u_x^2\rangle = \frac{\hbar}{2M\omega_0}\left(\frac{2}{e^{\hbar\omega_0/k_BT} - 1} + 1\right). \qquad (10.49b)$$

Averaging over lattice vibrations at constant T:

$$\langle A \rangle = \sum_{n=0}^{\infty} P_n \langle n|A|n \rangle,$$

where

$$P_n = \frac{e^{-\left(n+\frac{1}{2}\right)\hbar\omega/k_B T}}{\sum_m e^{-(m+\frac{1}{2})\hbar\omega/k_B T}} = \frac{e^{-n\hbar\omega/k_B T}}{\sum_m (e^{-\hbar\omega/k_B T})^m}.$$

Some clever tricks:

$$\boxed{\langle A \rangle = (1-z) \sum_{n=0}^{\infty} z^n \langle n|A|n \rangle \quad \text{with} \quad z = \exp\left(-\hbar\omega/k_B T\right)}.$$

Example:

$$\langle a^\dagger a \rangle = (1-z) \sum_{n=0}^{\infty} z^n \langle n|a^\dagger a|n \rangle = (1-z) \sum_{n=0}^{\infty} n\, z^n$$

$$= (1-z) z \frac{\partial}{\partial z} \sum_{n=0}^{\infty} z^n = \frac{z}{1-z} = \frac{1}{e^{\hbar\omega/k_B T} - 1},$$

Harmonic oscillator operators:

$$[a, a^\dagger] = aa^\dagger - a^\dagger a = 1.$$

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right).$$

Eigenstates:

$$a^\dagger a|n\rangle = n|n\rangle.$$

$$a|n\rangle = \sqrt{n}|n-1\rangle, \quad a^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle.$$