PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 36:

Review
- Comment on Kramers-Kronig transforms
- Some equations worth knowing
- Course assessment forms

21	Wed: 03/18/2015	Chap. 16	Electron Transport	#20	03/20/2015
22	Fri: 03/20/2015	Chap. 16	Electron Transport	#21	03/23/2015
23	Mon: 03/23/2015	Chap. 17	Electron Transport	#22	03/25/2015
24	Wed: 03/25/2015	Chap. 17 & 18	Electron Transport		
25	Fri: 03/27/2015	Chap. 18	Microscopic picture of transport	#23	03/30/2015
26	Mon: 03/30/2015	Chap. 19	Semiconductor devices	#24	04/01/2015
27	Wed: 04/01/2015	Chap. 20	Models of dielectric functions	#25	04/06/2015
	Fri: 04/03/2015	Good Friday	No class		
28	Mon: 04/06/2015	Chap. 21	Optical properties of solids	#26	04/08/2015
29	Wed: 04/08/2015	Chap. 22	Modern theory of polorization	#27	04/10/2015
30	Fri: 04/10/2015		Surface properties of solids	#28	04/13/2015
31	Mon: 04/13/2015		X-ray and neutron diffraction in solids	#29	04/15/2015
32	Wed: 04/15/2015	Chap. 26	The Hubbard model	#30	04/17/2015
33	Fri: 04/17/2015	Chap. 26	The Hubbard Model		
34	Mon: 04/20/2015	Chap. 26	The Hubbard Model		
35	Wed: 04/22/2015	Chap. 26	The Hubbard Model		
36	Fri: 04/24/2015		Review		
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

Schedule for PHY 752 Presentations

Monday 4/27/2015

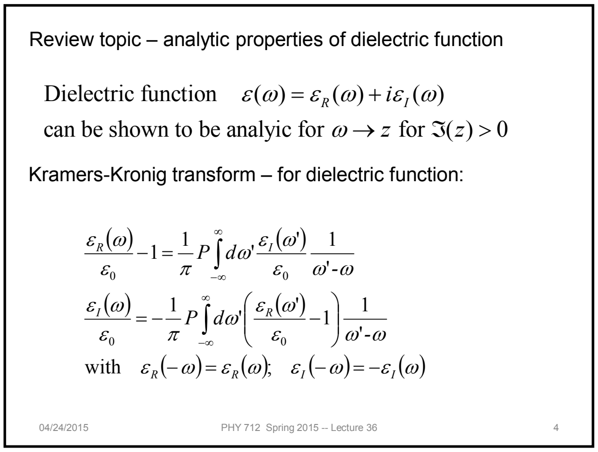
	Presenter	Topic
11:00 -11:25 AM	David Montgomery	Phonon models
11:25-11:50 AM	Ahmad Al Qawasmeh	Electronic and structural properties of graphite and graphene

Wednesday 4/29/2015

	Presenter	Topic
11:00 -11:25 AM	Drew Onken	"Treating Crystal Defects and Dislocations"
11:25-11:50 AM	Calvin Arter	Van der Waals density exchange functionals with spin effects

Friday 5/1/2015

	Presenter	Topic
11:00 -11:25 AM	Evan Welchman	“How and why structure searches work”
11:25-11:50 AM	Jason Howard	"Using C++ to translate and compare lattice coordinates"



Review topic – analytic properties of dielectric function

Dielectric function $\varepsilon(\omega)=\varepsilon_R(\omega)+i\varepsilon_I(\omega)$

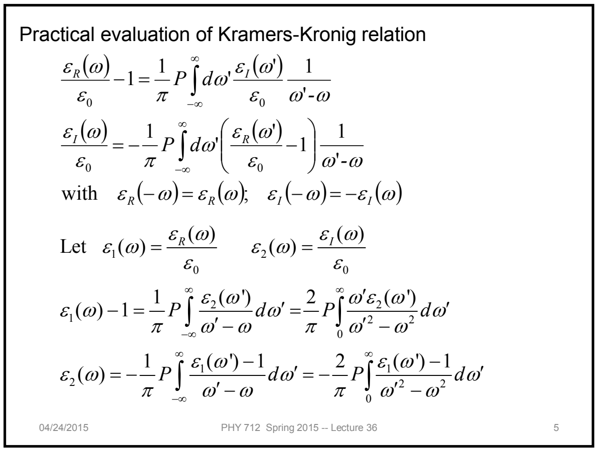
can be shown to be analytic for $\omega \rightarrow z$ for $\Im(z)>0$

Kramers-Kronig transform – for dielectric function:

$$\frac{\varepsilon_R(\omega)}{\varepsilon_0}-1=\frac{1}{\pi}P\int_{-\infty}^{\infty}d\omega'\frac{\varepsilon_I(\omega')}{\varepsilon_0}\frac{1}{\omega'-\omega}$$

$$\frac{\varepsilon_I(\omega)}{\varepsilon_0}=-\frac{1}{\pi}P\int_{-\infty}^{\infty}d\omega'\left(\frac{\varepsilon_R(\omega')}{\varepsilon_0}-1\right)\frac{1}{\omega'-\omega}$$

with $\varepsilon_R(-\omega)=\varepsilon_R(\omega);\quad \varepsilon_I(-\omega)=-\varepsilon_I(\omega)$



Practical evaluation of Kramers-Kronig relation

$$\frac{\varepsilon_R(\omega)}{\varepsilon_0}-1=\frac{1}{\pi}P\int_{-\infty}^{\infty}d\omega'\frac{\varepsilon_I(\omega')}{\varepsilon_0}\frac{1}{\omega'-\omega}$$

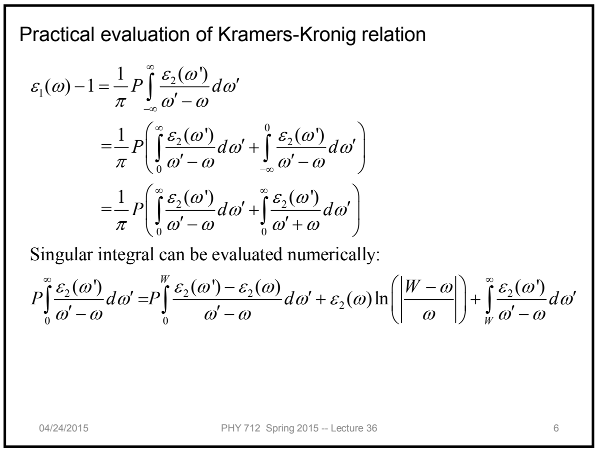
$$\frac{\varepsilon_I(\omega)}{\varepsilon_0}=-\frac{1}{\pi}P\int_{-\infty}^{\infty}d\omega'\left(\frac{\varepsilon_R(\omega')}{\varepsilon_0}-1\right)\frac{1}{\omega'-\omega}$$

with $\varepsilon_R(-\omega)=\varepsilon_R(\omega);\quad \varepsilon_I(-\omega)=-\varepsilon_I(\omega)$

Let $\varepsilon_1(\omega)=\dfrac{\varepsilon_R(\omega)}{\varepsilon_0}\qquad \varepsilon_2(\omega)=\dfrac{\varepsilon_I(\omega)}{\varepsilon_0}$

$$\varepsilon_1(\omega)-1=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'=\frac{2}{\pi}P\int_{0}^{\infty}\frac{\omega'\varepsilon_2(\omega')}{\omega'^2-\omega^2}d\omega'$$

$$\varepsilon_2(\omega)=-\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\varepsilon_1(\omega')-1}{\omega'-\omega}d\omega'=-\frac{2}{\pi}P\int_{0}^{\infty}\frac{\varepsilon_1(\omega')-1}{\omega'^2-\omega^2}d\omega'$$

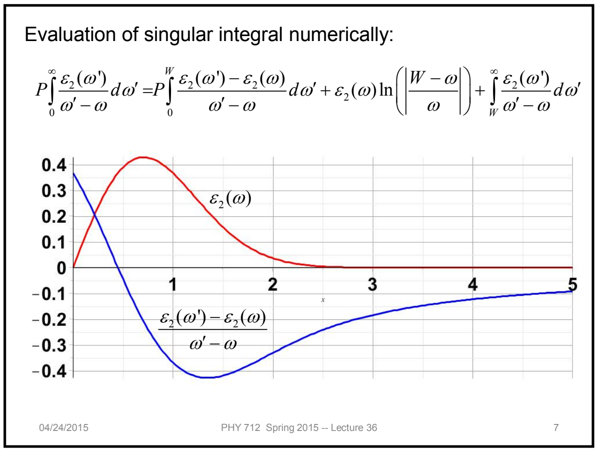


Practical evaluation of Kramers-Kronig relation

$$\begin{aligned}\varepsilon_1(\omega)-1&=\frac{1}{\pi}P\int_{-\infty}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'\\&=\frac{1}{\pi}P\left(\int_{0}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'+\int_{-\infty}^{0}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'\right)\\&=\frac{1}{\pi}P\left(\int_{0}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'+\int_{0}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'+\omega}d\omega'\right)\end{aligned}$$

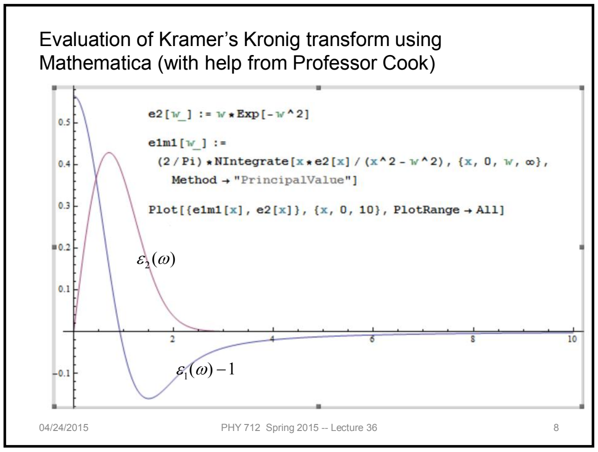
Singular integral can be evaluated numerically:

$$P\int_{0}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'=P\int_{0}^{W}\frac{\varepsilon_2(\omega')-\varepsilon_2(\omega)}{\omega'-\omega}d\omega'+\varepsilon_2(\omega)\ln\left(\left|\frac{W-\omega}{\omega}\right|\right)+\int_{W}^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'$$



Evaluation of singular integral numerically:

$$P\int_0^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega' = P\int_0^{W}\frac{\varepsilon_2(\omega')-\varepsilon_2(\omega)}{\omega'-\omega}d\omega' + \varepsilon_2(\omega)\ln\left(\left|\frac{W-\omega}{\omega}\right|\right) + \int_W^{\infty}\frac{\varepsilon_2(\omega')}{\omega'-\omega}d\omega'$$

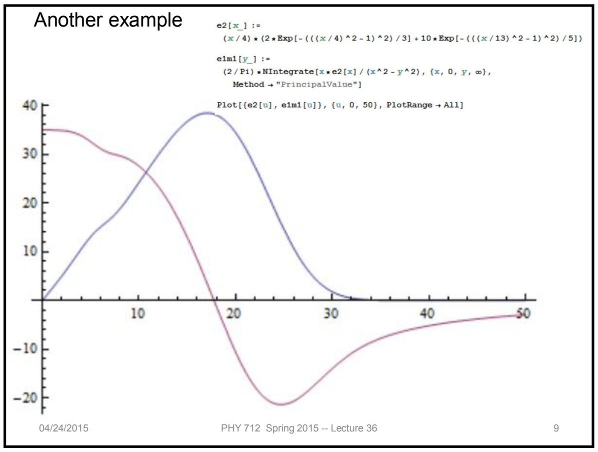


Evaluation of Kramer’s Kronig transform using Mathematica (with help from Professor Cook)

```
e2[w_] := w * Exp[-w^2]

e1m1[w_] :=
 (2 / Pi) * NIntegrate[x * e2[x] / (x^2 - w^2), {x, 0, w, ∞},
   Method → "PrincipalValue"]

Plot[{e1m1[x], e2[x]}, {x, 0, 10}, PlotRange → All]
```



Another example

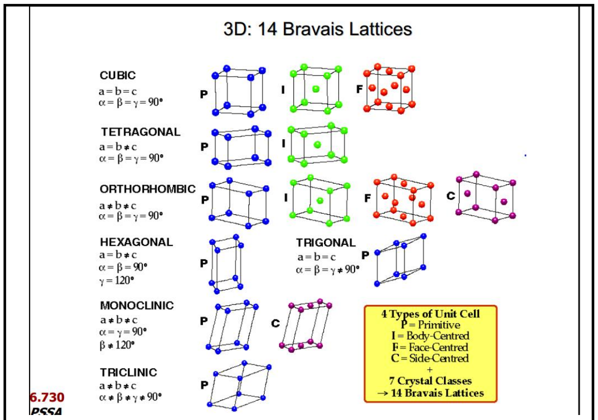
```
e2[x_] :=
 (x / 4) * (2 * Exp[- (((x / 4)^2 - 1)^2) / 3] + 10 * Exp[- (((x / 13)^2 - 1)^2) / 5])

e1m1[y_] :=
 (2 / Pi) * NIntegrate[x * e2[x] / (x^2 - y^2), {x, 0, y, ∞},
   Method → "PrincipalValue"]

Plot[{e2[u], e1m1[u]}, {u, 0, 50}, PlotRange → All]
```

Some equations worth remembering --

3D: 14 Bravais Lattices



CUBIC
$a = b = c$
$\alpha = \beta = \gamma = 90°$

TETRAGONAL
$a = b \neq c$
$\alpha = \beta = \gamma = 90°$

ORTHORHOMBIC
$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$

HEXAGONAL
$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$

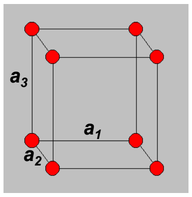
TRIGONAL
$a = b = c$
$\alpha = \beta = \gamma \neq 90°$

MONOCLINIC
$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$

TRICLINIC
$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$

4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices

Bravais lattice vectors:



Atomic basis vectors:

$$\boldsymbol{\tau}_a = x_a \mathbf{a}_1 + y_a \mathbf{a}_2 + z_a \mathbf{a}_3$$

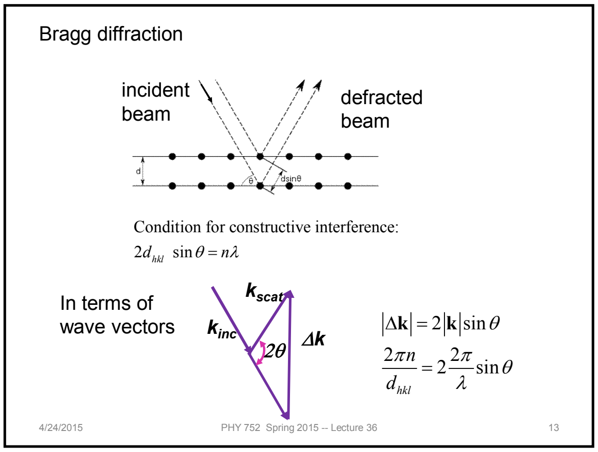
Reciprocal lattice (modulo 2 π)

$$\mathbf{b}_i = \frac{\mathbf{a}_j \times \mathbf{a}_k}{\mathbf{a}_i \cdot \left(\mathbf{a}_j \times \mathbf{a}_k\right)}$$

Note that $\mathbf{b}_i \cdot \mathbf{a}_j = \delta_{ij}$

Distance between diffracting planes

$$d_{hkl} = \frac{1}{\left|h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3\right|}$$



Bragg diffraction

Condition for constructive interference:

$2d_{hkl}\ \sin\theta = n\lambda$

In terms of wave vectors

$$|\Delta\mathbf{k}| = 2|\mathbf{k}|\sin\theta$$

$$\frac{2\pi n}{d_{hkl}} = 2\frac{2\pi}{\lambda}\sin\theta$$

Single particle wavefunction in a periodic system

Bloch wave: periodic function

$$\Psi_{n\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{n\mathbf{k}}(\mathbf{r})$$

Eigenfunctions of the periodic Hamiltonian are Bloch states with eigenvalues E_{nk} and electron velocity $\Leftrightarrow \frac{1}{\hbar}\nabla_k E_{nk}$

Wannier representation of electronic states -- continued

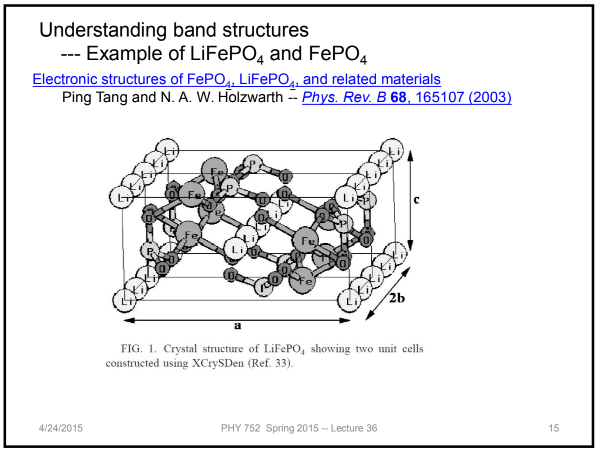
Wannier function in lattice cell **T**, associated with band n is given by:

$$\mathrm{W}_n(\mathbf{r}-\mathbf{T}) = \frac{V}{(2\pi)^3}\int d^3k\ e^{-i\mathbf{k}\cdot\mathbf{T}}\Psi_{n\mathbf{k}}(\mathbf{r})$$

Note that:

$$\langle W_n(\mathbf{r}-\mathbf{T})|W_{n'}(\mathbf{r}-\mathbf{T}')\rangle = \delta_{nn'}\delta_{\mathbf{TT}'}$$

Comment: Wannier functions are not unique since the the Bloch function may be multiplied by a **k**-dependent phase, which may generate a different function W_n(**r**-**T**).

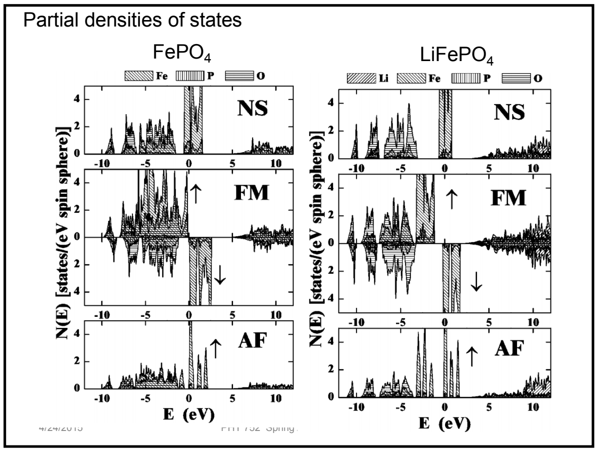


Understanding band structures
--- Example of $LiFePO_4$ and $FePO_4$

Electronic structures of $FePO_4$, $LiFePO_4$, and related materials

Ping Tang and N. A. W. Holzwarth -- *Phys. Rev. B* **68**, 165107 (2003)

FIG. 1. Crystal structure of $LiFePO_4$ showing two unit cells constructed using XCrySDen (Ref. 33).



Partial densities of states

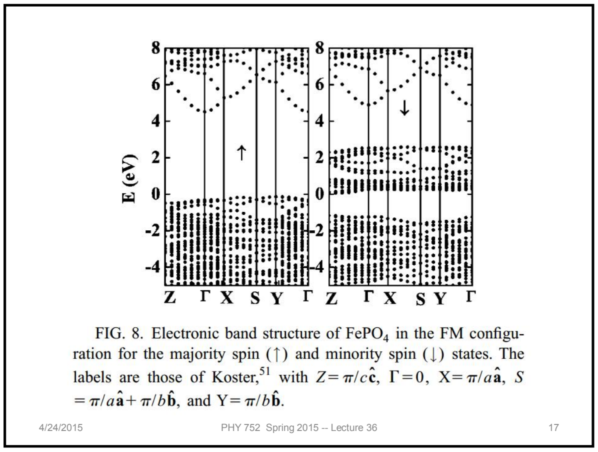


FIG. 8. Electronic band structure of FePO$_4$ in the FM configuration for the majority spin (↑) and minority spin (↓) states. The labels are those of Koster,[51] with $Z=\pi/c\hat{\mathbf{c}}$, $\Gamma=0$, $X=\pi/a\hat{\mathbf{a}}$, $S=\pi/a\hat{\mathbf{a}}+\pi/b\hat{\mathbf{b}}$, and $Y=\pi/b\hat{\mathbf{b}}$.

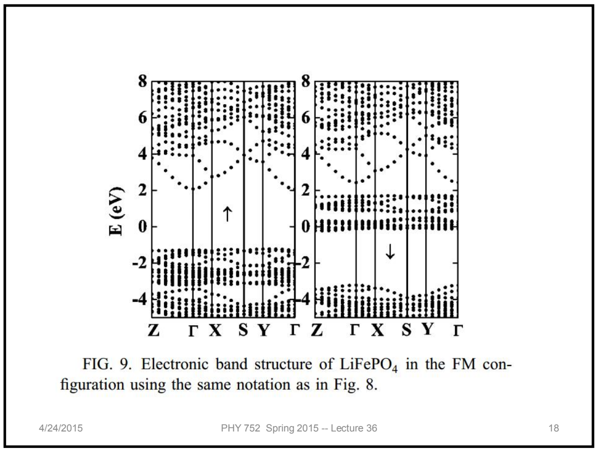


FIG. 9. Electronic band structure of LiFePO$_4$ in the FM configuration using the same notation as in Fig. 8.