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

Plan for Lecture 28:

- Chap. 21 in Marder & pdf file from Bassani's text
  - Optical properties of solids
    - Interband transitions
    - Excitons

20	Mon: 03/16/2015		Review Mid-term exam	#19	03/18/2015
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				04/10/2015
30	Fri: 04/10/2015				04/13/2015
31	Mon: 04/13/2015				04/15/2015
32	Wed: 04/15/2015				04/17/2015
33	Fri: 04/17/2015				04/20/2015
34	Mon: 04/20/2015				
35	Wed: 04/22/2015				
36	Fri: 04/24/2015				
	Mon: 04/27/2015		Presentations I		
	Wed: 04/29/2015		Presentations II		
	Fri: 05/01/2015		Presentations III & Take home exam		

Treatment of electromagnetic fields in solids

Zero order Hamiltonian for electron

$$H_0 = \frac{p^2}{2m} + U(\mathbf{r})$$ ← periodic potential

Hamiltonian in the presence of an electromagnetic field

$$H = \frac{1}{2m}\left(\mathbf{p} + \frac{e}{c}\mathbf{A}\right)^2 + U(\mathbf{r}) + e\phi$$

First order perturbation

$$H_1 = \frac{e}{2mc}(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}) + e\phi$$

Treatment of electromagnetic fields in solids

First order perturbation

$$H_1 = \frac{e}{2mc}(\mathbf{A}\cdot\mathbf{p} + \mathbf{p}\cdot\mathbf{A}) + e\phi$$

Possibility #1:

$$\mathbf{A} = \Re\left(\frac{\mathbf{E}_0 c}{i\omega}e^{-i\omega t}\right) \quad \text{and} \quad \phi = 0$$

Possibility #2:

$$\mathbf{A} = 0 \quad \text{and} \quad \phi = \Re\left(\mathbf{r}\cdot\mathbf{E}_0 e^{-i\omega t}\right)$$

Treatment of electromagnetic fields in solids
using possibility #1 and following Bassani's text

Fermi Golden Rule:

$$\mathscr{P}_{i\to f} = \frac{2\pi}{\hbar}\,|\langle f|\mathscr{L}|i\rangle|^2\,\delta(E_f - E_i \mp \hbar\omega).$$

In this case: $\mathbf{e}A_0 \equiv \dfrac{\mathbf{E}_0 c}{i\omega}$

$$\mathscr{P}_{v\mathbf{k}s\to c\mathbf{k}s} = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 |\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k})|^2\,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega),$$

$$\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k}) = \langle\psi_{c\mathbf{k}}|\,\mathbf{e}\cdot\mathbf{p}\,|\psi_{v\mathbf{k}}\rangle$$
$$= \mathbf{e}\cdot\int_{\substack{\text{crystal}\\\text{volume}}} \psi_c^*(\mathbf{k},\mathbf{r})\,(-i\hbar\nabla)\,\psi_v(\mathbf{k},\mathbf{r})\,d\mathbf{r}.$$

Treatment of electromagnetic fields in solids
using possibility #1 and following Bassani's text

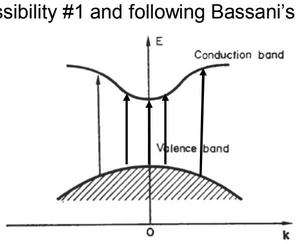

FIG. 5-1. Schematic representation in an energy band diagram of vertical transitions produced by a radiation field.

Treatment of electromagnetic fields in solids
using possibility #1 and following Bassani's text

spin

$$W(\omega) = \frac{2\pi}{\hbar}\left(\frac{eA_0}{mc}\right)^2 \sum_{v,c} \int_{BZ} \frac{2d\mathbf{k}}{(2\pi)^3} |\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k})|^2 \,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega),$$

Normalizing the result in terms of imaginary part of dielectric constant:

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{m^2\omega^2} \sum_{v,c} \int_{BZ} \frac{2\,d\mathbf{k}}{(2\pi)^3} |\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k})|^2 \,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega).$$

Treatment of electromagnetic fields in solids
using possibility #1 and following Bassani's text

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{m^2\omega^2} \sum_{v,c} \int_{BZ} \frac{2\,d\mathbf{k}}{(2\pi)^3} |\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k})|^2 \,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega).$$

From Kramers-Kronig transform:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi} P \int_0^\infty \omega' \varepsilon_2(\omega') \frac{1}{\omega'^2 - \omega^2}\, d\omega',$$

Special results:

$$\int_0^\infty \omega \varepsilon_2(\omega)\, d\omega = \frac{\pi}{2}\omega_p^2, \qquad \omega_p = \left(\frac{4\pi n e^2}{m}\right)^{1/2}$$

$$\varepsilon_1(0) = 1 + \frac{2}{\pi}\int_0^\infty \frac{\varepsilon_2(\omega)}{\omega}\, d\omega.$$

Treatment of electromagnetic fields in solids
using possibility #1 and following Bassani's text

$$\varepsilon_2(\omega) = \frac{4\pi^2 e^2}{m^2\omega^2} \sum_{v,c} \int_{BZ} \frac{2\,d\mathbf{k}}{(2\pi)^3} |\mathbf{e}\cdot\mathbf{M}_{cv}(\mathbf{k})|^2 \,\delta(E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega).$$

Sometimes can use group theory to determine "forbidden" transitions

When matrix elements are constant; structure depends sensitively on joint density of states

$$J_{cv}(\hbar\omega) = \int_{BZ} \frac{2d\mathbf{k}}{(2\pi)^3} \delta[E_c(\mathbf{k}) - E_v(\mathbf{k}) - \hbar\omega],$$

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Electronic Spectra of Crystalline Germanium and Silicon*†

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(Received 9 December 1963)

A detailed calculation of the energy bands of germanium and silicon has been performed by use of the pseudopotential method. The first three potential coefficients have been determined empirically, and all higher ones set equal to zero. This potential was used to compute the energy eigenvalues at ~50 000 points throughout the Brillouin zone. By use of this sample, we calculated the imaginary part of the dielectric constant in the optical and near ultraviolet where direct transitions between the valence and low-lying conduction bands dominate the response. Photoelectric yield curves were obtained for comparison with recent experiments. In all cases agreement of theory and experiment was reasonable. Energy contours were constructed in several of the principal symmetry planes. These were used to explain the structure in the optical properties of Ge and Si in terms of transitions near certain important critical points. Effective masses and the static dielectric constant were also computed.

Band structure of Si (as calculated by Brust)

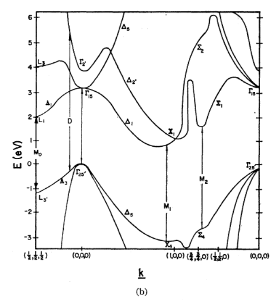
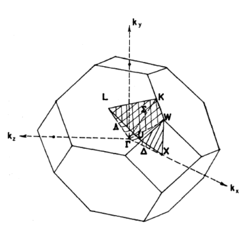
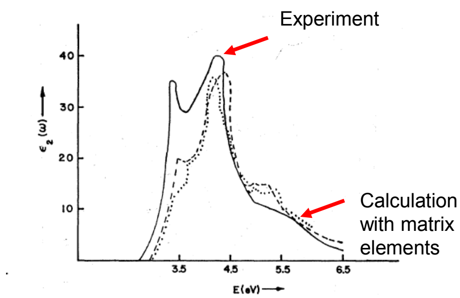


FIG. 6. Pseudopotential energy bands along Δ, Λ, and Σ symmetry directions. Some of the principal transitions have been marked.

Integration region of Brillouin zone





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First principles calculation

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Electron-hole excitations and optical spectra from first principles

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(Received 13 April 2000)

We present a recently developed approach to calculate electron-hole excitations and the optical spectra of condensed matter from first principles. The key concept is to describe the excitations of the electronic system by the corresponding one- and two-particle Green's function. The method combines three computational techniques. First, the electronic ground state is treated within density-functional theory. Second, the single-particle spectrum of the electrons and holes is obtained within the *GW* approximation to the electron self-energy operator. Finally, the electron-hole interaction is calculated and a Bethe-Salpeter equation is solved, yielding the coupled electron-hole excitations. The resulting solutions allow the calculation of the entire optical spectrum. This holds both for bound excitonic states below the band gap, as well as for the resonant spectrum above the band gap. We discuss a number of technical developments needed for the application of the method to real systems. To illustrate the approach, we discuss the excitations and optical spectra of spatially isolated systems (atoms, molecules, and semiconductor clusters) and of extended, periodic crystals (semiconductors and insulators).

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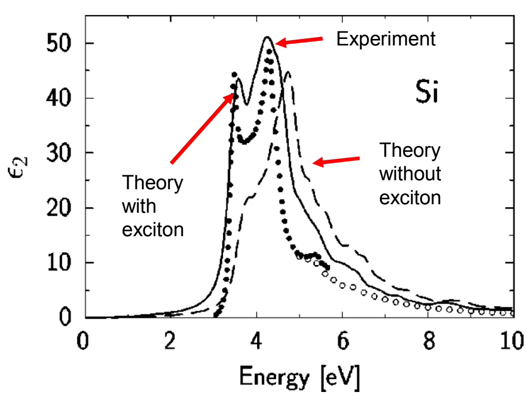

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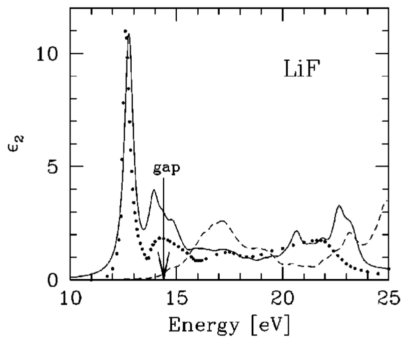
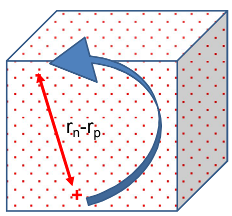


Exciton effects



Exciton effects (using Marder's materials)

Wannier approximation

$$\left[\frac{-\hbar^2}{2m_n^\star}\nabla^2_{\vec{r}_n} + \frac{-\hbar^2}{2m_p^\star}\nabla^2_{\vec{r}_p} - \frac{e^2}{\epsilon^0|\vec{r}_n - \vec{r}_p|} - \mathcal{E}\right]\Psi(\vec{r}_n, \vec{r}_p) = 0.$$

$$\begin{aligned}
\vec{R} &= \frac{m_n^\star \vec{r}_n + m_p^\star \vec{r}_p}{m_n^\star + m_p^\star} \\
\vec{r} &= \vec{r}_n - \vec{r}_p \\
0 &= \left[\frac{-\hbar^2}{2(m_n^\star + m_p^\star)}\nabla^2_{\vec{R}} - \mathcal{E}_{\rm cm}\right]\Psi_{\rm cm}(\vec{R}) \\
0 &= \left[\frac{-\hbar^2}{2\mu}\nabla^2_{\vec{r}} - \frac{e^2}{\epsilon^0 r} - \mathcal{E}_{\rm b}\right]\Psi_{\rm b}(\vec{r}), \\
\mu &= \frac{m_n^\star m_p^\star}{m_n^\star + m_p^\star}.
\end{aligned}$$

$$\mathcal{E}_l = -\frac{\mu e^4}{2\hbar^2 \epsilon^{0^2} l^2} = -\frac{\mu}{m\epsilon^{0^2} l^2}\cdot 13.6\text{eV}$$

Self-trapped excitons (RT Williams) NaCl