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

Plan for Lecture 20:

1. Discussion of Mid-Term Exam
2. Course topics
3. Electronic transport (Marder Chapter 16-18)

9	Wed: 02/04/2015	Chap. 8	Electronic structure; LCAO and tight binding	#9	02/06/2015
10	Fri: 02/06/2015	Chap. 8	Band structure examples	#10	02/09/2015
11	Mon: 02/09/2015	Chap. 9	Electron-electron interactions	#11	02/11/2015
12	Wed: 02/11/2015	Chap. 9	Electron-electron interactions	#12	02/13/2015
13	Fri: 02/13/2015	Chap. 9	Electron-electron interactions	#13	02/16/2015
14	Mon: 02/16/2015	Chap. 10	Electronic structure calculation methods	#14	02/18/2015
15	Wed: 02/18/2015	Chap. 10	Electronic structure calculation methods	#15	02/20/2015
16	Fri: 02/20/2015	Chap. 10	Electronic structure calculation methods	#16	02/23/2015
17	Mon: 02/23/2015	Chap. 10	Electronic structure calculation methods	#17	02/25/2015
18	Wed: 02/25/2015	Chap. 10	Electronic structure calculation methods	#18	02/27/2015
19	Fri: 02/27/2015	Chap. 1-3,7-10	Review; Take-home exam distributed		
	Mon: 03/02/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Wed: 03/04/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Fri: 03/06/2015	*APS Meeting*	Take-home exam (no class meeting)		
	Mon: 03/09/2015	*Spring break*			
	Wed: 03/11/2015	*Spring break*			
	Fri: 03/13/2015	*Spring break*			
20	Mon: 03/16/2015			#19	03/18/2015

1. Consider the group C_4 corresponding to the following transformations of a general point xyz, $y\bar{x}z$, $\bar{y}xz$, and $\bar{x}\bar{y}z$ or equivalently the identity (E), rotation about the z-axis by 90^o (C_4), rotation about the z axis by -90^o ($C_{\bar{4}}$), and rotation about the z-axis by 180^o (C_2).
   (a) Find the multiplication table for this group.
   (b) Find the classes for this group.
   (c) Verify that in terms of the classes $\mathcal{C}_1$, $\mathcal{C}_2$, $\mathcal{C}_3$, $\mathcal{C}_4$, the character table for this group can be written as follows. (Associate the classes you find with the $\mathcal{C}_i$ labels.)

	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$
χ_1	1	1	1	1
χ_2	1	1	-1	-1
χ_3	1	-1	i	$-i$
χ_4	1	-1	$-i$	i

   (d) Analyze the spherical harmonic functions $Y_{lm}(\theta, \phi)$ for $l = 0, 1$, and 2 for this group and find the "compatible" representations.

Group multiplication table:

	xyz	$y\bar{x}z$	$\bar{y}xz$	$\bar{x}\bar{y}z$
xyz	xyz	$y\bar{x}z$	$\bar{y}xz$	$\bar{x}\bar{y}z$
$y\bar{x}z$	$y\bar{x}z$	$\bar{x}\bar{y}z$	xyz	$\bar{y}xz$
$\bar{y}xz$	$\bar{y}xz$	xyz	$\bar{x}\bar{y}z$	$y\bar{x}z$
$\bar{x}\bar{y}z$	$\bar{x}\bar{y}z$	$\bar{y}xz$	$y\bar{x}z$	xyz

Note that group is *abelian.*

$xyz \equiv E \qquad \theta = 0$

$y\bar{x}z = C_4 \qquad \theta = 90^o$

$\bar{y}xz = C'_4 \qquad \theta = -90^o$

$\bar{x}\bar{y}z = C_2 \qquad \theta = 180^o$

θ	0	180	90	-90
	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$
χ_1	1	1	1	1
χ_2	1	1	-1	-1
χ_3	1	-1	i	$-i$
χ_4	1	-1	$-i$	i
l=0	*1*	*1*	*1*	*1*
l=1	*3*	*-1*	*1*	*1*
l=2	*5*	*1*	*-1*	*-1*

Recall that the character for rotation of spherical harmonics l by angle θ is:

$$\chi_l^{rot}(\theta) = \frac{\sin\left(\left(l+\frac{1}{2}\right)\theta\right)}{\sin(\theta/2)}$$

Projection of rotation representations onto representations of 4-fold group:

$$\chi_l^{rot}(\mathcal{C}) = \sum_{i=1}^{4} c_i \chi_i(\mathcal{C})$$

where $c_i = \sum_{\mathcal{C}} \left\langle \chi_l^{rot}(\mathcal{C}) \middle| \chi_i(\mathcal{C}) \right\rangle$

2. The following band structure diagrams are taken from the literature. For each case, find the approximate location of the last occupied energy level and explain your reasoning.

   (a) The following band structure is for the valence states ($3s^2 3p^1$) of Al in the fcc structure. The figure is taken from a paper by Walter Harrison, Phys. Rev. **118** 1182 (1960).

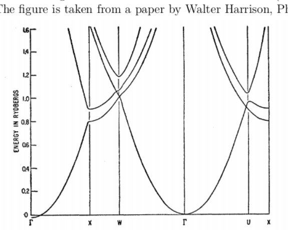


FIG. 2. Energy versus wave number along various symmetry lines, obtained using a four-OPW approximation and fitting Heine's values at W. The curves ΓX were obtained using only two OPW's, giving rise to the discrepancy at Γ on the left.

Need to accommodate 3 electrons; 1.5 bands

(b) The following band structure is for the valence states ($6s^2 6p3$) of Bi in the so-called A7 structure which a distorted cubic structure with two atoms in a unit cell. The Figure is taken from a paper by Stuart Golin, Phys. Rev. **166** 643 (1968). The author has indicated the Fermi level on the diagram. You should explain the reasoning behind this location and indicate whether the material is a metal or insulator.

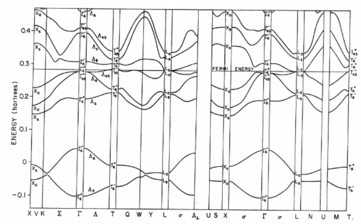


FIG. 2. The band structure of bismuth along various lines and planes. [The direction L-$\Lambda_\perp$ is perpendicular to the trigonal axis ($\Lambda_\perp$ is on that axis) and is of interest in interpreting tunneling measurements. See C. B. Duke (private communication); see also D. J. BenDaniel and C. B. Duke, Phys. Rev. Letters 14, 902 (1965).]

Need to accommodate 10 electrons; 5 bands

(c) The Following band structure is for the valence states of InN with In having the valence states ($5s^2 5p^1$) and N having the valence states ($2p^3$) in the so-called wurtzite structure having a hexagonal bravais lattice and two InN units in each primitive cell. The figure is taken from a paper by Foley and Tansley, Phys. Rev. B **33** 1430 (1986).

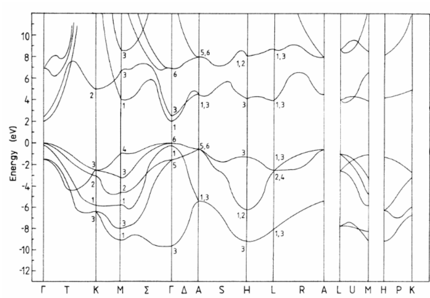


FIG. 2. The energy bands of indium nitride.

Need to accommodate 12 electrons; 6 bands

4. In class, we discussed the simple tight-binding model of a body-centered cubic lattice (with lattice constant a) and showed that the band dispersion has the form:

$$E(k_x, k_y, k_z) = \alpha + 8\beta \left(\cos\left(\frac{k_x a}{2}\right) \cos\left(\frac{k_y a}{2}\right) \cos\left(\frac{k_z a}{2}\right) \right).$$

For the following, assume that $\alpha = 0$ and $\beta = -1$ in Rydberg units.

(a) Express the band energy about its minimum at $\mathbf{k} = 0$ to quadratic order in $k^2 = k_x^2 + k_y^2 + k_z^2$.

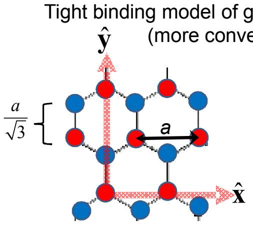
(b) Note that the quadradic expansion of the band dispersion is related to the band dispersion of a 3-dimensional free electron and use this form to approximate the density of states and the Fermi energy of the system assuming that there are two electrons within the cube of volume a^3.

$$E(k_x,k_y,k_z) = -8\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y a}{2}\right)\cos\left(\frac{k_z a}{2}\right)$$
$$\approx -8\left(1-\frac{1}{2}\left(\frac{k_x a}{2}\right)^2\right)\left(1-\frac{1}{2}\left(\frac{k_y a}{2}\right)^2\right)\left(1-\frac{1}{2}\left(\frac{k_z a}{2}\right)^2\right)$$
$$\approx -8\left(1-\frac{a^2}{8}\left(k_x^2+k_y^2+k_z^2\right)\right) = -8 + a^2k^2$$

$$E_F \approx -8 + \left(6\pi^2\right)^{2/3}$$

3. This problem concerns the tight-binding Hamiltonian for a 2-dimensional graphene lattice as shown on slide 21 of Lecture 10 and is similar to assignment # 10. Assume the tight binding atomic basis consists of a single C π orbital on each site (blue and red sites are identical). Consider the nearest neighbor matrix elements $(pp\pi)_1$ and next nearest neighbor matrix elements $(pp\pi)_2$ only and assume that the basis functions are orthonormal. Your results should be expressed in terms of these parameters.
   (a) Find the forms of the 4 matrix elements $H_{rr}(k_x,k_y)$, $H_{bb}(k_x,k_y)$,$H_{rb}(k_x,k_y)$, and $H_{br}(k_x,k_y)$.
   (b) Find the forms of the eigenvalues of the tight binding matrix.
   (c) Now assume that $(pp\pi)_2 << (pp\pi)_1$. Let $(pp\pi)_1 = 1$ and plot the bands for several directions in the hexagonal Brillouin zone.
   (d) Examine the form of the bands near the K point of the Brillouin zone, finding the eigenstates at the K point. Also show that for a state near the K point ($\mathbf{k} = \frac{4\pi}{3a}\hat{\mathbf{x}} + \kappa$, where the vector κ is assumed to be small, the band dispersion is approximately linear in κ.

Tight binding model of graphene π bands
(more conventional notation than Lect. 8.)



red atoms:
$$\mathbf{r}_i = \boldsymbol{\tau}_{\text{red}} + n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$
blue atoms:
$$\mathbf{r}_i = \boldsymbol{\tau}_{\text{blue}} + n_{1i}\mathbf{a}_1 + n_{2i}\mathbf{a}_2$$

$$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$
$$\boldsymbol{\tau}_{\text{red}} = 0 \qquad \boldsymbol{\tau}_{\text{blue}} = \frac{a}{\sqrt{3}}\hat{\mathbf{y}}$$

$$H = \begin{pmatrix} H_{rr}(\mathbf{k}) & H_{rb}(\mathbf{k}) \\ H_{br}(\mathbf{k}) & H_{bb}(\mathbf{k}) \end{pmatrix}$$

Guide to k-points – hcp lattice

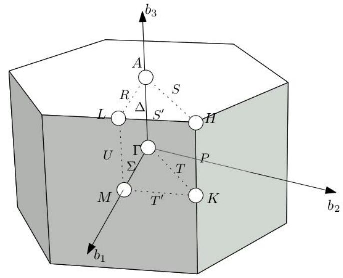
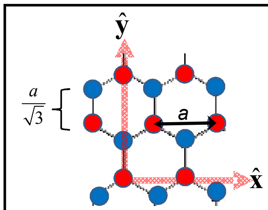


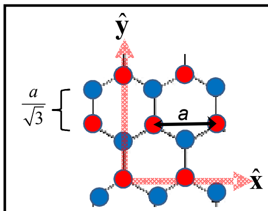
Figure 7.10: First Brillouin zone of the hexagonal lattice. Using coordinates $\vec{b}_1 = 4\pi/a\sqrt{3}(\sqrt{3}/2\ \ -1/2\ \ 0)$, $\vec{b}_2 = 4\pi/a\sqrt{3}(\sqrt{3}/2\ \ 1/2\ \ 0)$ and $2\pi/c(0\ \ 0\ \ 1)$; $\Gamma = (0\,0\,0)$, $A = (0\ \ 0\ \ 1/2)$, $M = (1/2\ \ 0\ \ 0)$, $K = (1/3\ \ 1/3\ \ 0)$, $H = (1/3\ \ 1/3\ \ 1/2)$, and $L = (1/2\ \ 0\ \ 1/2)$.



$$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

$$\mathbf{b}_1 = \frac{4\pi}{\sqrt{3}}\left(\frac{\sqrt{3}}{2}\hat{\mathbf{x}} - \frac{1}{2}\hat{\mathbf{y}}\right) \qquad \mathbf{b}_2 = \frac{4\pi}{\sqrt{3}}\left(\frac{\sqrt{3}}{2}\hat{\mathbf{x}} + \frac{1}{2}\hat{\mathbf{y}}\right)$$

$$K \text{ point: } \mathbf{k}_K = \frac{1}{3}\mathbf{b}_1 + \frac{1}{3}\mathbf{b}_2$$
$$= \frac{4\pi}{3}\hat{\mathbf{x}}$$



$$\mathbf{a}_1 = a\hat{\mathbf{x}} \qquad \mathbf{a}_2 = a\left(\frac{1}{2}\hat{\mathbf{x}} + \frac{\sqrt{3}}{2}\hat{\mathbf{y}}\right)$$

$$\boldsymbol{\tau}_{\text{red}} = 0 \qquad \boldsymbol{\tau}_{\text{blue}} = \frac{a}{\sqrt{3}}\hat{\mathbf{y}}$$

$$H = \begin{pmatrix} H_{rr}(\mathbf{k}) & H_{rb}(\mathbf{k}) \\ H_{br}(\mathbf{k}) & H_{bb}(\mathbf{k}) \end{pmatrix}$$

$$H_{rb} = (pp\pi)_1\left(e^{ik_y a/\sqrt{3}} + e^{-ik_y a/(2\sqrt{3}) - ik_x a/2} + e^{-ik_y a/(2\sqrt{3}) + ik_x a/2}\right)$$
$$= H_{br}^{\ *}$$
$$H_{rr} = H_{bb} \equiv E_0$$

$$H = \begin{pmatrix} H_{rr}(\mathbf{k}) & H_{rb}(\mathbf{k}) \\ H_{br}(\mathbf{k}) & H_{bb}(\mathbf{k}) \end{pmatrix}$$

Eigenvalues:

$$\lambda = H_{rr}(\mathbf{k}) \pm \sqrt{|H_{rb}(\mathbf{k})|^2} = H_{rr}(\mathbf{k}) \pm |H_{rb}(\mathbf{k})|$$

$$H_{rb} = (pp\pi)_1 \left(e^{ik_y a/\sqrt{3}} + e^{-ik_y a/(2\sqrt{3}) - ik_x a/2} + e^{-ik_y a/(2\sqrt{3}) + ik_x a/2} \right)$$

$$= H_{br}{}^*$$

$$H_{rr} = H_{bb} \equiv E_0$$

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$$H_{rb} = (pp\pi)_1 \left(e^{ik_y a/\sqrt{3}} + e^{-ik_y a/(2\sqrt{3}) - ik_x a/2} + e^{-ik_y a/(2\sqrt{3}) + ik_x a/2} \right)$$

$$= (pp\pi)_1 e^{-ik_y a/(2\sqrt{3})} \left(e^{ik_y a\sqrt{3}/2} + e^{-ik_x a/2} + e^{ik_x a/2} \right)$$

$$= H_{br}{}^*$$

$$H_{rr} = H_{bb} \equiv E_0$$

$$\lambda \approx E_0 \pm |H_{rb}(\mathbf{k})|$$

Near K point: $\mathbf{k} = = \frac{4\pi}{3}\hat{\mathbf{x}} + \kappa \cos\phi\, \hat{\mathbf{x}} + \kappa \sin\phi\, \hat{\mathbf{y}}$

$$\lambda \approx (pp\pi)_1 \frac{\sqrt{3}}{2}\kappa a$$

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Tentative plan for topics

Chapter 16-18	Electronic transport
Chapter 20-23	Optical properties
Chapter 26	Hubbard model
Chapter 19	Surfaces

Chapter 16: Dynamics of Bloch Electrons

Semi-classical electron dynamics

Concerned with states near Fermi level

Electron velocity $\Leftrightarrow \frac{1}{\hbar}\nabla_k E_{nk}$

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Electron velocity for Bloch electrons

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

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\mathbf{r})\right)\psi_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}\psi_{\mathbf{k}}(\mathbf{r})$$

$$\left(-\frac{\hbar^2}{2m}(\nabla + \mathbf{k})^2 + V(\mathbf{r})\right)u_{\mathbf{k}}(\mathbf{r}) = E_{\mathbf{k}}u_{\mathbf{k}}(\mathbf{r})$$

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