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

Plan for Lecture 9:

Reading: Chap. 2.4-2.7 in GGGPP;

Brillouin zones and densities of states

1. **Reciprocal lattices**
2. **k·p perturbation theory**
3. **Densities of states**

PHY 752 Solid State Physics

MWF 11 AM-11:50 PM	OPL 103	http://www.wfu.edu/~natalie/f15phy752/

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Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment
1	Wed, 8/26/2015	Chap. 1.1-1.2	Electrons in a periodic one-dimensional potential	#1
2	Fri, 8/28/2015	Chap. 1.3	Electrons in a periodic one-dimensional potential	#2
3	Mon, 8/31/2015	Chap. 1.4	Tight binding models	#3
4	Wed, 9/02/2015	Chap. 1.6, 2.1	Crystal structures	#4
5	Fri, 9/04/2015	Chap. 2	Group theory	#5
6	Mon, 9/07/2015	Chap. 2	Group theory	#6
7	Wed, 9/09/2015	Chap. 2	Group theory	#7
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			
11	Fri, 9/18/2015			

Reciprocal lattice

$$\mathbf{t}_i \cdot \mathbf{g}_j = 2\pi\delta_{ij}$$

real lattice reciprocal lattice

Unit vectors of the reciprocal lattice

$$\mathbf{g}_1 = \frac{2\pi}{\Omega}\mathbf{t}_2 \times \mathbf{t}_3, \quad \mathbf{g}_2 = \frac{2\pi}{\Omega}\mathbf{t}_3 \times \mathbf{t}_1, \quad \mathbf{g}_3 = \frac{2\pi}{\Omega}\mathbf{t}_1 \times \mathbf{t}_2, \quad \text{and} \quad \Omega = \mathbf{t}_1 \cdot (\mathbf{t}_2 \times \mathbf{t}_3).$$

General reciprocal lattice vector

$$\mathbf{g}_m = m_1\mathbf{g}_1 + m_2\mathbf{g}_2 + m_3\mathbf{g}_3$$

Useful relationships between lattice vectors

$$\Omega_k = \mathbf{g}_1 \cdot (\mathbf{g}_2 \times \mathbf{g}_3) = \frac{(2\pi)^3}{\Omega^3}(\mathbf{t}_2 \times \mathbf{t}_3) \cdot [(\mathbf{t}_3 \times \mathbf{t}_1) \times (\mathbf{t}_1 \times \mathbf{t}_2)] = \frac{(2\pi)^3}{\Omega}.$$

$$\mathbf{g}_m \cdot \mathbf{t}_n = \text{integer} \cdot 2\pi \; = 0, \pm 2\pi, \pm 4\pi, \pm 6\pi, \ldots,$$

➔ This implies that the distance between successive lattice planes is given by

$$d = \frac{2\pi}{|\mathbf{g}_m|}.$$

Note that: $\mathbf{v}_1 \times (\mathbf{v}_2 \times \mathbf{v}_3) \equiv \mathbf{v}_2(\mathbf{v}_1 \cdot \mathbf{v}_3) - \mathbf{v}_3(\mathbf{v}_1 \cdot \mathbf{v}_2).$

$$d = \frac{2\pi}{|\mathbf{g}_m|}.$$

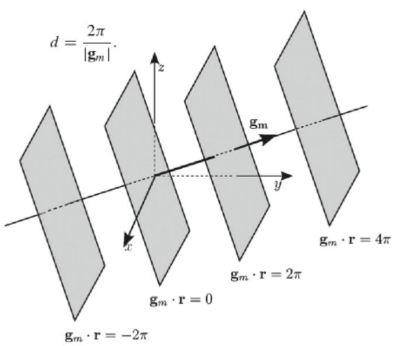


Figure 2.15 Family of planes in direct space defined by the equations $\mathbf{g}_m \cdot \mathbf{r} = 0, \pm 2\pi, \pm 4\pi, \ldots$; all the translation vectors of the Bravais lattice belong to the family of planes.

Unit cells of reciprocal space – Brillouin zones

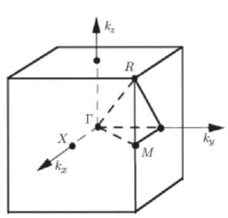


Figure 2.17 Brillouin zone for the simple cubic lattice. Some high symmetry points are indicated: $\Gamma = 0$; $X = (2\pi/a)(1/2, 0, 0)$; $M = (2\pi/a)(1/2, 1/2, 0)$; $R = (2\pi/a)(1/2, 1/2, 1/2)$.

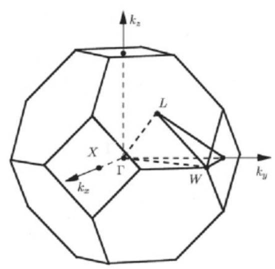


Figure 2.18 Brillouin zone for the face-centered cubic lattice (truncated octahedron). Some high symmetry points are: $\Gamma = 0$; $X = (2\pi/a)(1,0,0)$; $L = (2\pi/a)(1/2, 1/2, 1/2)$; $W = (2\pi/a)(1/2, 1, 0)$.

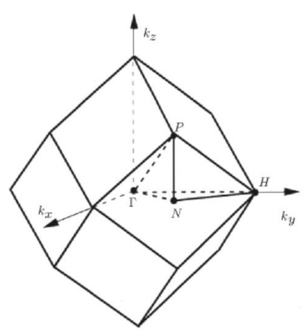


Figure 2.19 Brillouin zone for the body-centered cubic lattice (rhombic dodecahedron). Some high symmetry points are also indicated: $\Gamma = 0$; $N = (2\pi/a)(1/2, 1/2, 0)$; $P = (2\pi/a)(1/2, 1/2, 1/2)$; $H = (2\pi/a)(0, 1, 0)$.

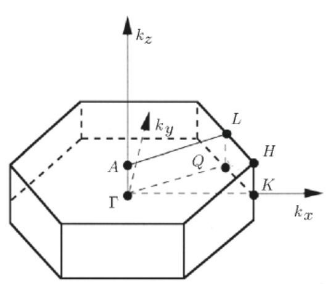


Figure 2.20 Brillouin zone for the hexagonal Bravais lattice. Some high symmetry points are also indicated: $\Gamma = 0$; $K = (2\pi/a)(2/3, 0, 0)$; $Q = (\pi/a)(1, 1/\sqrt{3}, 0)$; $A = (\pi/c)(0, 0, 1)$.

Properties of the wave vector

Consider the Schroedinger equation for an electron in a periodic solid

$$\left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right]\psi(\mathbf{r}) = E\psi(\mathbf{r}) \quad \text{with} \quad V(\mathbf{r}) = V(\mathbf{r}+\mathbf{t}_n)$$

$$V(\mathbf{r}) = \sum_{\mathbf{g}_m} V(\mathbf{g}_m)e^{i\mathbf{g}_m\cdot\mathbf{r}}.$$

Wavefunctions with Bloch symmetry

$$\boxed{\psi(\mathbf{k},\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u(\mathbf{k},\mathbf{r})},$$

$$\psi(\mathbf{k},\mathbf{r}+\mathbf{t}_n) = e^{i\mathbf{k}\cdot(\mathbf{r}+\mathbf{t}_n)}u(\mathbf{k},\mathbf{r}+\mathbf{t}_n) = e^{i\mathbf{k}\cdot\mathbf{t}_n}\psi(\mathbf{k},\mathbf{r});$$

Analysis of the significance of the Bloch wavevector; Schoedinger equation in terms of periodic part of wavefunction:

$$\left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})\right]e^{i\mathbf{k}\cdot\mathbf{r}}u_n(\mathbf{k},\mathbf{r}) = E_n(\mathbf{k})e^{i\mathbf{k}\cdot\mathbf{r}}u_n(\mathbf{k},\mathbf{r});$$

$$\left[\frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V(\mathbf{r})\right]u_n(\mathbf{k},\mathbf{r}) = E_n(\mathbf{k})u_n(\mathbf{k},\mathbf{r}).$$

$$H(\mathbf{k})u_n(\mathbf{k},\mathbf{r}) = E_n(\mathbf{k})u_n(\mathbf{k},\mathbf{r}),$$

$$H(\mathbf{k}) = \frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V(\mathbf{r}) = \frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar^2k^2}{2m}.$$

Taking the **k** derivative of the equation:

$$\left[\frac{1}{2m}(\mathbf{p}+\hbar\mathbf{k})^2 + V(\mathbf{r})\right]u_n(\mathbf{k},\mathbf{r}) = E_n(\mathbf{k})u_n(\mathbf{k},\mathbf{r}).$$

$$\frac{\hbar}{m}(\mathbf{p}+\hbar\mathbf{k})u_n(\mathbf{k},\mathbf{r}) + H(\mathbf{k})\frac{\partial u_n(\mathbf{k},\mathbf{r})}{\partial\mathbf{k}} = \frac{\partial E_n(\mathbf{k})}{\partial\mathbf{k}}u_n(\mathbf{k},\mathbf{r}) + E_n(\mathbf{k})\frac{\partial u_n(\mathbf{k},\mathbf{r})}{\partial\mathbf{k}}.$$

Diagonal matrix element

$$\langle u_n(\mathbf{k},\mathbf{r})|\frac{\hbar}{m}(\mathbf{p}+\hbar\mathbf{k})|u_n(\mathbf{k},\mathbf{r})\rangle = \frac{\partial E_n(\mathbf{k})}{\partial\mathbf{k}};$$

$$\boxed{\langle\psi_n(\mathbf{k},\mathbf{r})|\frac{\mathbf{p}}{m}|\psi_n(\mathbf{k},\mathbf{r})\rangle = \frac{1}{\hbar}\frac{\partial E_n(\mathbf{k})}{\partial\mathbf{k}}}.$$

Another useful identity

$$[H, \mathbf{r}] = \left[\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}), \mathbf{r}\right] = -i\,\frac{\hbar}{m}\,\mathbf{p}.$$

$$\langle \psi_m(\mathbf{k},\mathbf{r})| - i\frac{\hbar}{m}\mathbf{p}|\psi_n(\mathbf{k},\mathbf{r})\rangle = \langle \psi_m(\mathbf{k},\mathbf{r})|[H,\mathbf{r}]|\psi_n(\mathbf{k},\mathbf{r})\rangle$$
$$= [E_m(\mathbf{k}) - E_n(\mathbf{k})]\langle \psi_m(\mathbf{k},\mathbf{r})|\mathbf{r}|\psi_n(\mathbf{k},\mathbf{r})\rangle.$$

$$\boxed{\langle u_m(\mathbf{k},\mathbf{r})|\mathbf{r}|u_n(\mathbf{k},\mathbf{r})\rangle = i\langle u_m(\mathbf{k},\mathbf{r})|\frac{\partial}{\partial \mathbf{k}}u_n(\mathbf{k},\mathbf{r})\rangle \quad \text{for } m \neq n}\,.$$

k·p perturbation theory

$$\psi(\mathbf{k},\mathbf{r}) = \sum c_n(\mathbf{k}) e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{n0}(\mathbf{r})$$

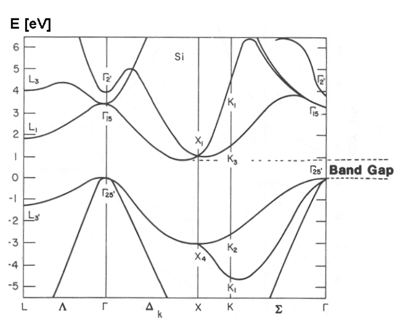
$$M_{nn'}(\mathbf{k}) = \langle e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{n0}(\mathbf{r})|\frac{\mathbf{p}^2}{2m} + V(\mathbf{r})|e^{i\mathbf{k}\cdot\mathbf{r}}\psi_{n'0}(\mathbf{r})\rangle$$
$$= \langle \psi_{n0}(\mathbf{r})|\frac{\mathbf{p}^2}{2m} + V(\mathbf{r}) + \frac{\hbar}{m}\mathbf{k}\cdot\mathbf{p} + \frac{\hbar^2 k^2}{2m}|\psi_{n'0}(\mathbf{r})\rangle$$
$$= \left[E_{n0} + \frac{\hbar^2 k^2}{2m}\right]\delta_{nn'} + \frac{\hbar}{m}\langle \psi_{n0}(\mathbf{r})|\mathbf{k}\cdot\mathbf{p}|\psi_{n'0}(\mathbf{r})\rangle.$$

$$\boxed{\left\|\left(E_{n0} + \frac{\hbar^2 k^2}{2m} - E\right)\delta_{nn'} + \frac{\hbar}{m}\mathbf{k}\cdot\langle \psi_{n0}|\mathbf{p}|\psi_{n'0}\rangle\right\| = 0}\,.$$

Second order expansion

$$E_n(\mathbf{k}) = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n'(\neq n)}\frac{|\langle \psi_{n'0}|\mathbf{k}\cdot\mathbf{p}|\psi_{n0}\rangle|^2}{E_{n0} - E_{n'0}} = E_{n0} + \sum_{\alpha\beta}\frac{\hbar^2}{2m}\left(\frac{m}{m^*}\right)_{\alpha\beta}k_\alpha k_\beta,$$

From: http://www.yambo-code.org/tutorials/GW/



Effective mass tensor

$$\left(\frac{m}{m^*}\right)_{\alpha\beta} = \delta_{\alpha\beta} + \frac{2}{m}\sum_{n'(\neq n)} \frac{\langle\psi_{n0}|\mathbf{p}_\alpha|\psi_{n'0}\rangle\langle\psi_{n'0}|\mathbf{p}_\beta|\psi_{n0}\rangle}{E_{n0} - E_{n'0}}$$

Results from http://ecee.colorado.edu/~bart/book/effmass.htm

Effective mass and energy bandgap of Ge, Si and GaAs

Name	Symbol	Germanium	Silicon	Gallium Arsenide
Smallest energy bandgap at 300 K	E_g (eV)	0.66	1.12	1.424
Effective mass for density of states calculations				
Electrons	$m_{e}^{*}{}_{,dos}/m_0$	0.56	1.08	0.067
Holes	$m_{h}^{*}{}_{,dos}/m_0$	0.29	0.57/0.81[1]	0.47
Effective mass for conductivity calculations				
Electrons	$m_{e}^{*}{}_{,cond}/m_0$	0.12	0.26	0.067
Holes	$m_{h}^{*}{}_{,cond}/m_0$	0.21	0.36/0.386[1]	0.34

$m_0 = 9.11 \times 10^{-31}$ kg is the free electron rest mass.

Averaging over states; integrating over the Brillouin Zone

$$\boxed{\sum_{\mathbf{k}} f(\mathbf{k}) \Longrightarrow \frac{V}{(2\pi)^3}\int f(\mathbf{k})d\mathbf{k}} \; ,$$

Note that in general each band is doubly occupied due to electron spin

Densities of states

For electron spin

$$D(E) = 2\sum_{\mathbf{k}} \delta(E(\mathbf{k}) - E) = 2\int_{\mathrm{B.Z.}} \frac{V}{(2\pi)^3}\,\delta(E(\mathbf{k}) - E)\,d\mathbf{k},$$

$$D(E) = 2\int_{E(\mathbf{k})\equiv E} \frac{V}{(2\pi)^3}\frac{dS}{|\nabla_{\mathbf{k}}E(\mathbf{k})|}.$$

Density of states analysis -- continued

$$D(E) = 2\int_{E(\mathbf{k})\equiv E} \frac{V}{(2\pi)^3}\frac{dS}{|\nabla_{\mathbf{k}}E(\mathbf{k})|}. \qquad ($$

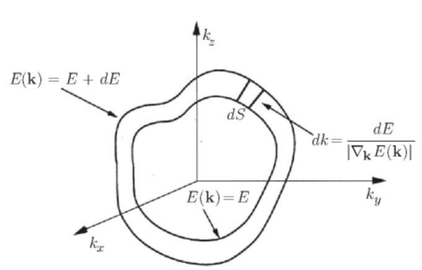


Figure 2.21 Schematic representation of two isoenergetic surfaces in the **k** space.

Properties of delta functions

following property of the delta function:

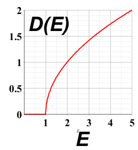
$$\delta[f(x)] = \sum_n \frac{\delta(x - x_n)}{|f'(x_n)|},$$

where x_n are the simple zeroes of the function $f(x)$.

Example in one dimension

$$D(E) = \frac{2L_x}{2\pi} \int \delta\left(E_0 + \frac{\hbar^2 k_x^2}{2m_x} - E\right) dk_x = L_x \frac{\sqrt{2m_x}}{\pi\hbar} \int \delta(E_0 + q_x^2 - E)\, dq_x,$$

$$D(E) = L_x \frac{\sqrt{2m_x}}{\pi\hbar} \frac{1}{\sqrt{E - E_0}}, \quad E > E_0.$$



9/14/2015 PHY 752 Fall 2015 -- Lecture 9 19