LMU München
WS 2016/2017
Lehrstuhl für Theoretische Nanophysik
PD Dr. F. Heidrich-Meisner
Jan Stolpp, *Questions: jan.stolpp@physik.uni-muenchen.de*

3. Exercise Sheet TA1: Theoretical Solid State Physics

To be discussed on Friday, November 11, 2016.

Exercise 1: Tight-Binding p-bands in Cubic Crystals

In dealing with cubic crystals the most convenient linear combinations of the three degenerate atomic p-levels have the form $x\phi(r)$, $y\phi(r)$ and $z\phi(r)$, where the function ϕ depends only on the magnitude of the vector $\boldsymbol{r}$. The energy of the three corresponding p-bands are found from the tight-binding theory setting to zero the determinant,

$$\left| \; (\epsilon(\boldsymbol{k}) - E_p)\delta_{ij} + \beta_{ij} + \tilde{\gamma}_{ij}(\boldsymbol{k}) \; \right| = 0 \tag{1}$$

where

$$\begin{aligned} \tilde{\gamma}_{ij}(\boldsymbol{k}) &= \sum_{\boldsymbol{R}} \mathrm{e}^{i\boldsymbol{k}\cdot\boldsymbol{R}} \; \gamma_{ij}(\boldsymbol{R}), & (2)\\ \beta_{ij} &= \gamma_{ij}(\boldsymbol{R}=0), & (3)\\ \gamma_{ij}(\boldsymbol{R}) &= -\int \mathrm{d}\boldsymbol{r} \; \Psi_{\mathrm{i}}^{*}(\boldsymbol{r}) \; \Psi_{\mathrm{j}}(\boldsymbol{r}-\boldsymbol{R}) \; \Delta\mathrm{U}(\boldsymbol{r}). & (4) \end{aligned}$$

a. As a consequence of the cubic symmetry, show that,

$$\beta_{xx} = \beta_{yy} = \beta_{zz} = \beta \tag{5}$$

and

$$\beta_{xy} = 0 \tag{6}$$

b. For the face centered cubic lattice with only nearest-neighbor $\gamma_{ij}(\boldsymbol{R})$ different from zero, using Eq. 1, show that the energy bands are given by the roots of,

$$\left| \begin{array}{ccc} \left(\begin{array}{c} \varepsilon(\boldsymbol{k}) - \varepsilon^0(\boldsymbol{k}) + \\ 4\gamma_0 \cos\frac{1}{2}k_y a \;\; \cos\frac{1}{2}k_z a \end{array} \right) & -4\gamma_1 \sin\frac{1}{2}k_x a \;\; \sin\frac{1}{2}k_y a & -4\gamma_1 \sin\frac{1}{2}k_x a \;\; \sin\frac{1}{2}k_z a \\ -4\gamma_1 \sin\frac{1}{2}k_y a \;\; \sin\frac{1}{2}k_x a & \left(\begin{array}{c} \varepsilon(\boldsymbol{k}) - \varepsilon^0(\boldsymbol{k}) + \\ 4\gamma_0 \cos\frac{1}{2}k_z a \;\; \cos\frac{1}{2}k_x a \end{array} \right) & -4\gamma_1 \sin\frac{1}{2}k_y a \;\; \sin\frac{1}{2}k_z a \\ -4\gamma_1 \sin\frac{1}{2}k_z a \;\; \sin\frac{1}{2}k_x a & -4\gamma_1 \sin\frac{1}{2}k_z a \;\; \sin\frac{1}{2}k_y a & \left(\begin{array}{c} \varepsilon(\boldsymbol{k}) - \varepsilon^0(\boldsymbol{k}) + \\ 4\gamma_0 \cos\frac{1}{2}k_x a \;\; \cos\frac{1}{2}k_y a \end{array} \right) \end{array} \right| = 0$$

where,

$$\begin{aligned} \varepsilon^0(\boldsymbol{k}) &= E_p - \beta \\ &\quad -4\gamma_2 \left(\cos\frac{1}{2}k_x a \;\; \cos\frac{1}{2}k_z a + \cos\frac{1}{2}k_x a \;\; \cos\frac{1}{2}k_y a + \cos\frac{1}{2}k_y a \;\; \cos\frac{1}{2}k_z a \right) \end{aligned} \tag{7}$$

and,

$$\gamma_0 = -\int \mathrm{d}\boldsymbol{r}[x^2 - y(y-\frac{1}{2}a)]\ \phi^*(r)\ \phi([x^2+(y-\frac{1}{2}a)^2+(z-\frac{1}{2}a)^2]^{1/2})\ \Delta U(\boldsymbol{r}) \quad (8)$$

$$\gamma_1 = -\int \mathrm{d}\boldsymbol{r}[x(y-\frac{1}{2}a)]\ \phi^*(r)\ \phi([(x-\frac{1}{2}a)^2+(y-\frac{1}{2}a)^2+z^2]^{1/2})\ \Delta U(\boldsymbol{r}) \quad (9)$$

$$\gamma_2 = -\int \mathrm{d}\boldsymbol{r}[x(x-\frac{1}{2}a)]\ \phi^*(r)\ \phi([(x-\frac{1}{2}a)^2+(y-\frac{1}{2}a)^2+z^2]^{1/2})\ \Delta U(\boldsymbol{r}) \quad (10)$$

c. Show that all three bands are degenerate at $\boldsymbol{k}=0$. Show also that when $\boldsymbol{k}$ is directed along either cube axis ΓX or cube diagonal ΓL there is a double degeneracy. Sketch the energies along these directions. We give:

$$\boldsymbol{k}_X = \frac{2\pi}{a}\hat{x} \qquad \text{and} \qquad \boldsymbol{k}_{\mathrm{L}} = \frac{2\pi}{\mathrm{a}}\left(\hat{\mathrm{x}}+\hat{\mathrm{y}}+\hat{\mathrm{z}}\right)$$

Exercise 2: $\boldsymbol{k}\cdot\boldsymbol{p}$ -theory

We consider a model material with just three bands. We assume that for $\boldsymbol{k}=0$, the energy levels are known: The lowest state is $|xy\rangle$, with two other degenerate states $|x\rangle$ and $|y\rangle$, such that $E_{xy}=0$, $E_x=E_y=\Delta E$. The states transform under symmetry transformations like the functions xy, x and y, respectively. Assume that the crystal has inversion symmetry.

The goal is the calculation of the band structure close to $\boldsymbol{k}=0$ using perturbation theory in

$$H_{kp} = \frac{1}{m}\boldsymbol{k}\cdot\boldsymbol{p}\,.$$

a. Argue that because of symmetry, there are no first order correction in H_{kp}.

b. For the second order correction, you'll need six matrix elements which are of the form

$$\langle\psi|H_{pert}|\psi'\rangle = \sum_m \frac{\langle\psi|H_{kp}|m\rangle\langle m|H_{kp}|\psi'\rangle}{E^0-E_m}.$$

Show that they are given by

$$\langle xy|H_{pert}|xy\rangle = -\frac{A^2}{m^2\Delta E}\ (k_x^2+k_y^2), \quad (11)$$

$$\langle xy|H_{pert}|x\rangle = 0, \quad (12)$$

$$\langle xy|H_{pert}|y\rangle = 0, \quad (13)$$

$$\langle x|H_{pert}|x\rangle = \frac{A^2}{m^2\Delta E}\ k_y^2, \quad (14)$$

$$\langle y|H_{pert}|y\rangle = \frac{A^2}{m^2\Delta E}\ k_x^2, \quad (15)$$

$$\langle x|H_{pert}|y\rangle = \frac{A^2}{m^2\Delta E}\ k_x k_y. \quad (16)$$

with

$$A = \left|\ \langle x|p_y|xy\rangle\ \right| = \left|\ \langle y|p_x|xy\rangle\ \right|$$

c. Compute the second order corrections to the energy. What are the energies of the three bands?

d. Compute the effective mass-tensors of the three bands.