Technische Universität Berlin
Institut für Theoretische Physik
Lecture Course: Prof. Dr. Matthias Scheffler, Dr. Patrick Rinke, Dr. Alex Tkatchenko
Exercises: Dr. Volker Blum

May 23, 2012

http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/

Theoretical Material Science: Exercise Sheet 7

Please hand in solutions by: Wednesday, May 30, start of the exercise class

Exercise 17 (8 points): *Tight binding approximation: s-levels in an fcc crystal*
In the tight-binding approximation, one expands the crystal (Bloch) eigenfunctions $\varphi_{n,\mathbf{k}}(\mathbf{r})$ into localized atomic eigenfunctions $\hat{\varphi}_\alpha(\mathbf{r}-\mathbf{R}_I)$, with $\hat{h}^{\mathrm{at}}\hat{\varphi}_\alpha = \epsilon_\alpha^{\mathsf{at}}\hat{\varphi}_\alpha$ ($\hat{h}^{\mathrm{at}}$ is the atomic Hamiltonian). We consider the case of only a single atomic s orbital $\hat{\varphi}_s$ at each lattice site $\mathbf{R}_I$.

a) Show that the expression for the band energy $\epsilon(\mathbf{k})$ (only one band) can be written as:

$$[\epsilon^{\mathsf{at}} - \epsilon(\mathbf{k})]S(\mathbf{k}) + A(\mathbf{k}) = 0\,, \tag{1}$$

where S is called the overlap and A the potential matrix element:

$$S(\mathbf{k}) = \sum_I e^{i\mathbf{k}\mathbf{R}_I} \int d^3r \hat{\varphi}_s^*(\mathbf{r})\hat{\varphi}_s(\mathbf{r}-\mathbf{R}_I) \tag{2}$$

$$A(\mathbf{k}) = \sum_I e^{i\mathbf{k}\mathbf{R}_I} \int d^3r \hat{\varphi}_s^*(\mathbf{r})\Delta v(\mathbf{r})\hat{\varphi}_s(\mathbf{r}-\mathbf{R}_I)$$

$$\text{with} \quad \Delta v(\mathbf{r}) = v(\mathbf{r}) - v^{\mathsf{at}}(\mathbf{r})\,.$$

$\Delta v(\mathbf{r})$ is the difference between the atomic potential in $\hat{h}^{\mathsf{at}}$ and the full crystal potential $v(\mathbf{r})$. Rewrite Eq. (1) for the band energy by explicitly separating out the "on-site terms" ($\mathbf{R}_I$=0).

b) Express the band energy $\epsilon(\mathbf{k})$ for an fcc crystal explicitly for the following approximations:

i) All terms except $\mathbf{R}_I$=0 in $S(\mathbf{k})$ vanish (and $\hat{\varphi}_s$ is normalized to 1).

ii) All potential terms in $A(\mathbf{k})$ beyond nearest neighbours vanish.

Hint: Use the notation $\int d^3r\hat{\varphi}_s^*(\mathbf{r})\Delta v(\mathbf{r})\hat{\varphi}_s(\mathbf{r})$=$-\beta$, $\int d^3r\hat{\varphi}_s^*(\mathbf{r})\Delta v(\mathbf{r})\hat{\varphi}_s(\mathbf{r}-\mathbf{R}_{NN})$=$-\gamma(\mathbf{R}_{NN})$, and use the symmetry of the lattice and of the s wave function explicitly to relate $-\gamma(\mathbf{R}_{NN})$ to one another for different nearest neighbours.

c) Show that the explicit form of the s bands along the following lines in reciprocal space is:

i) Along ΓX (k_y=k_z=0, k_x=$\frac{2\pi}{a}\zeta$, 0< ζ <1): $\epsilon = \epsilon^{\mathsf{at}} - \beta - 4\gamma[1 + 2\cos(\pi\zeta)]$

ii) Along ΓL (k_y=k_z=k_x=$\frac{2\pi}{a}\zeta$, 0< ζ <1/2): $\epsilon = \epsilon^{\mathsf{at}} - \beta - 12\gamma\cos^2(\pi\zeta)$

iii) Along ΓK (k_z=0, k_x=k_y=$\frac{2\pi}{a}\zeta$, 0< ζ <3/4): $\epsilon = \epsilon^{\mathsf{at}} - \beta - 4\gamma[\cos^2(\pi\zeta) + 2\cos(\pi\zeta)]$

iv) Along ΓW (k_z=0, k_x=$\frac{2\pi}{a}\zeta$, k_y=$\frac{\pi}{a}\zeta$, 0< ζ <1):
$\epsilon = \epsilon^{\mathsf{at}} - \beta - 4\gamma[\cos(\pi\zeta) + \cos(\frac{\pi\zeta}{2}) + \cos(\pi\zeta)\cos(\frac{\pi\zeta}{2})]$

d) Show that the normal derivative of ϵ vanishes on the square faces of the Brillouin zone (the BZ face normal to the ΓX direction).

e) Compute the ratio of "band widths" Θ of the bands along ΓX and ΓL:

$$\Theta = \frac{\epsilon(X) - \epsilon(\Gamma)}{\epsilon(L) - \epsilon(\Gamma)}\,. \tag{3}$$

Compare the s-wave tight binding result to the result that one would obtain for the lowest-energy bands in the free-electron case.

Please turn over!⟶

Exercise 18 (4 points): *Time reversal symmetry*
Prove that the spin-orbit coupling breaks the time reversal symmetry of a wave function in a crystal lattice. Steps:

a) First, show that time reversal symmetry exists in the absence of spin-orbit coupling. Prove and use that $\varphi_n(-\mathbf{k},\mathbf{r}) = \varphi_n^*(\mathbf{k},\mathbf{r})$ and $\epsilon_n(\mathbf{k}) = \epsilon_n(-\mathbf{k})$.

b) Introduce the spin-orbit coupling via a spin operator in the hamiltonian

$$h = \left[-\frac{\hbar^2}{2m}\nabla^2 + v^{eff}(\mathbf{r})\right]\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \frac{\hbar^2}{4m^2c^2}\boldsymbol{\sigma}\cdot\left(\boldsymbol{\nabla}v^{eff}(\mathbf{r})\times\frac{\hbar}{i}\boldsymbol{\nabla}\right),$$

where the vector $\boldsymbol{\sigma}$ is composed of the three Pauli matrices. Introduce the time reversal operator T_t and find that it commutes with the position operator, while it anticommutes with momentum and spin operators.

c) Show that $T_t\psi(\mathbf{r},\sigma) = -\psi(\mathbf{r},\sigma)$.

- **Webpage of the lecture:**
  http://www.itp.tu-berlin.de/menue/lehre/lv/ss12/
  wahlpflichtveranstaltungen/theoretische_festkoerperphysik_i_ii_theoretical_material_science/
  http://th.fhi-berlin.mpg.de/sitesub/lectures/spring_2012/
- **Lecture:** Tue. & Wed., 10:00 h -12:00 h (sharp!) in room EW 203, TU Berlin
- **Exercise:** Wed., 14:00 h in room EW 229
- **Literature:**
  - Ashcroft, Mermin, David: Solid state physics, Saunders College, Philadelphia, 1981
  - Kittel: Quantum theory of solids, Wiley, New York, 1963
  - Ziman: Principles of the theory of solids, Cambridge University Press, Cambridge, 1964
  - Ibach, Lueth: Solid-state physics: an introduction to principles of materials science, Springer, Berlin, 1995
  - Madelung: Festkörpertheorie, Springer, Berlin, 1972
  - Scherz: Quantenmechanik, Teubner, Stuttgart, 1999
  - Dreizler, Gross: Density functional theory: an approach to the quantum many-body problem, Springer, Berlin, 1990
  - Parr, Yang: Density-functional theory of atoms and molecules, Oxford University Press, Oxford, 1994
  - Anderson: Basic notations of condensed matter physics, Benjamin/Cummings, London, 1984
  - Marder: Condensed matter physics, Wiley, New York, 2000
  - Martin: Electronic Structure, Cambridge University Press, Cambridge, 2004
  - Kohanoff: Electronic Structure Calculations for Solids and Molecules: Theory and Computational Methods, Cambridge University Press, Cambridge, 2006
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
  - Active participation in computational exercises
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler, Dr. Alex Tkatchenko, Dr. Patrick Rinke: by appointment
  - Dr. Volker Blum: Available Wed. 16:00 (after the exercise class) or by appointment