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Institut für Theoretische Physik
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http://www.itp.tu-berlin.de/menue/lehre/lv/ss08/wpfv/tfkp/

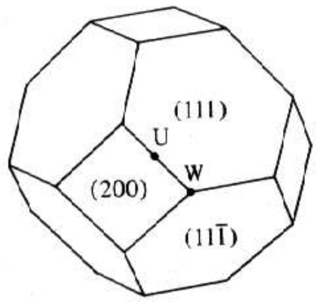
Theoretical Material Science: exercise sheet 7

Return: Monday, June 9 in the exercise

Exercise 16 (4 points): *Effect of weak periodic potential at places in k-space where Bragg planes meet*

In presence of degeneracy the first order approximation for the energy of electrons in a weak periodic potential is $(\epsilon - \epsilon^0_{\mathbf{k}-\mathbf{G}_i})c_{\mathbf{k}-\mathbf{G}_i} = \sum_{j=1}^{m} U_{\mathbf{G}_j-\mathbf{G}_i} c_{\mathbf{k}-\mathbf{G}_j}$. Consider the point W ($\mathbf{k}_W = (2\pi/2)(1, \frac{1}{2}, 0)$) in the Bruillouin zone of the fcc structure (picture). Here three Bragg planes ($(200), (111), (11\bar{1})$) meet, and accordingly the free electron energies

$$\begin{aligned}
\epsilon_1^0 &= \frac{\hbar^2}{2m}k^2, \\
\epsilon_2^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(1,1,1)\right)^2, \\
\epsilon_3^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(1,1,\bar{1})\right)^2, \\
\epsilon_4^0 &= \frac{\hbar^2}{2m}\left(\mathbf{k} - \frac{2\pi}{a}(2,0,0)\right)^2
\end{aligned}$$



are degenerate when $\mathbf{k} = \mathbf{k}_W$, and equal to $\epsilon_W = \hbar^2\mathbf{k}_W^2/2m$.

a) Show that in a region of k-space near W, the first order energies are given by solutions to

$$\begin{vmatrix}
\epsilon_1^0 - \epsilon & U_1 & U_1 & U_2 \\
U_1 & \epsilon_2^0 - \epsilon & U_2 & U_1 \\
U_1 & U_2 & \epsilon_3^0 - \epsilon & U_1 \\
U_2 & U_1 & U_1 & \epsilon_4^0 - \epsilon
\end{vmatrix} = 0$$

b) Using a similar method, show that the energies at the point U ($\mathbf{k}_U = (2\pi/a)(1, \frac{1}{4}, \frac{1}{4})$) are

$$\epsilon_W = U_2, \ \epsilon = \epsilon_U + \frac{1}{2}U_2 \pm \frac{1}{2}\sqrt{U_2^2 + 8U_1^2},$$

where $\epsilon_U = \hbar^2\mathbf{k}_U^2/2m$.

Exercise 17 (4 points): *p-band of a square lattice*

Consider a two-dimensional square lattice. Use the LCAO concept to construct a semi-quantitative description of the band formed from the three lowest atomic p-orbitals. Only nearest-neighbour interactions need to be taken into account. Plot the resulting band diagram along the $\mathbf{k}$-space path $M \to \Gamma \to X \to M$.

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. Therefore

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

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

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 anticommuts with momentum- and spin operator.

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/ss08/wpfv/tfkp/
- **Lecture:** Tue. & Fri., 10:00 a.m.-12:00 p.m. in room EW 203, TU Berlin
- **Exercise:** Mon., 14:00 a.m. in room H 1029
- **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: Festk?rpertheorie, 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
- **"Übungsschein"-criteria:**
  - Regular and active participation in the exercises
  - Presentation of homework tasks and
  - 50% of the homework points.
- **Consultation hours:**
  - Prof. Dr. Matthias Scheffler: on appointment
  - Dr. Volker Blum: on appointment
  - Philipp Zedler: Wed, 11:00 - 12:00 a.m. in room EW 711