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

May 16, 2012

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

Theoretical Material Science: Exercise Sheet 6

Please hand in solutions by: Wednesday, May 23, start of the exercise class

Exercise 15 (8 points): *Kronig-Penney model.*
The Kronig-Penney model (the Dirac comb) is a simple one-dimensional model to understand the electron band structure of a crystalline solid. Consider the periodic potential (lattice parameter a):

$$V(x) = V_0 \sum_{n=-\infty}^{+\infty} \delta(x - na) \quad , \quad V_0 > 0\,. \tag{1}$$

According to the Bloch theorem, for the eigenstates we must have

$$\varphi_q(x + a) = \exp(iqa) \cdot \varphi_q(x)\,. \tag{2}$$

where q takes the role of the crystal momentum. Our eventual goal is to understand some properties of the band structure $E(q)$.

a) In each interval $na < x < (n + 1)a$ (n integer), the solutions have the form

$$\varphi_q(x) = A_n \exp(ikx) + B_n \exp(-ikx) \quad \text{with} \quad k^2 = \frac{2mE(q)}{\hbar^2}\,, \tag{3}$$

($k > 0$). Using $\varphi_q'(\epsilon) - \varphi_q'(-\epsilon) = \int_{-\epsilon}^{\epsilon} dx\, \varphi_q''(x)$, show that $\varphi_q'(x)$ is discontinuous at each $x{=}na$, and calculate the magnitude of the "jump" of $\varphi_q'(x)$.

b) Show that the solutions φ_q satisfy the following equation (Kronig-Penney equation):

$$\cos(qa) = \cos(ka) + k_0 a \cdot \frac{\sin(ka)}{ka}\,, \tag{4}$$

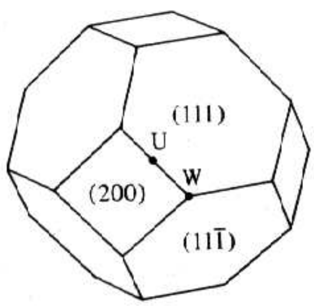
with $k_0 = \frac{mV_0}{\hbar^2}$.
Hint: Use the Ansatz made in a), the Bloch theorem, the continuity of $\varphi_q(x)$ and the discontinuity of $\varphi_q'(x)$ to determine the coefficients A_n and B_n.

c) Plot $f(ka) = \cos(ak) + k_0 a \frac{\sin(ka)}{ka}$ as a function of ka. Show that for $V_0 \neq 0$, the Kronig-Penney equation leads to "forbidden" energy regions (energy gaps).

d) In a periodic structure, we are interested in the band structure $E(q)$ as a function of the crystal momentum q, not of the free-electron momentum k defined above. Show that there must be an "energy gap" (forbidden value of $E(q)$, i.e., ka) located at $qa{=}\pi$, 3π, 5π, ... (the Brillouin zone boundary). (Hint: Show that qa is an odd-integer multiple of π for each odd-integer multiple of ka. Then, inspect the derivative $\frac{d}{d(ka)} f(ka)$ to demonstrate that a "forbidden k region" starts here.)

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 ($\mathbf{k}_W = (2\pi/a)(1, \frac{1}{2}, 0)$) in the Brillouin zone of the fcc structure (picture). Here three Bragg planes ($(200), (111), (11\bar{1})$) meet, and accordingly the free electron energies

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



Please turn over!⟶

are degenerate when $\mathbf{k} = \mathbf{k}_W$, and equal to $\epsilon_W = \hbar^2 \mathbf{k}_W^2 / 2m$.
Show that in a region of k-space near W, the first order energies are given by solutions to

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

- **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