Karlsruhe Institute of Technology

Institute for Theoretical
Condensed Matter physics

Condensed Matter Theory I WS 2022/2023

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Sheet 1
Tutorial: 03.11.2020

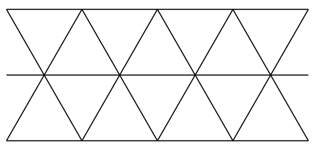
Category A

1. Reciprocal lattice

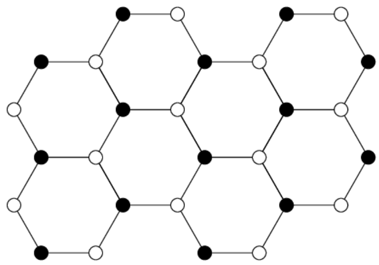
($3 + 5 + 5 + 5 = 2 = 20$ points)

(a) Let L be a D-dimensional Bravais lattice and L' its reciprocal lattice. Show that $(L')'$ is identical to L.

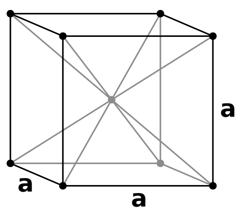
(b) Construct explicitly the reciprocal lattice of the displayed hexagonal (also called triangular) Bravais lattice. Each vertex represents an atom.



(c) Construct the reciprocal lattice of the honeycomb lattice



(d) Now we turn to three dimensions: Construct the reciprocal lattice of the body-centered cubic (bcc) Bravais lattice.



(e) Deduce, without any calculations, the reciprocal lattice of the face-centered cubic (fcc) lattice.

Category B

2. Born-Oppenheimer approximation (5 + 10 + 15 = 30 points)

(a) Explain in words what the Born-Oppenheimer approximation is and why it is important when dealing with the full solid-state Hamiltonian (cf. first lecture two days ago).

(b) Consider the quantized version of the following one-dimensional system: a mass M is attached to the point $x = 0$ by a spring of constant k_1. A second mass m is attached to the first mass by a spring of constant k_2. The Hamiltonian of this system is

$$H = \frac{p_1^2}{2M} + \frac{p_2^2}{2m} + \frac{1}{2}k_1 x_1^2 + \frac{1}{2}k_2 \left(x_1 - x_2\right)^2 ,$$

with quantum operators $p_{1,2}, x_{1,2}$. Calculate the eigenenergies using the Born-Oppenheimer approximation, assuming that $m \ll M$ (you may think of an electron bound to an ion which oscillates around its crystal position).

(c) Now calculate the eigenenergies exactly, which is still possible in this simple case. Verify that you get the same result as in (b) if you take the limit $m \ll M$.
Hint: You may follow the steps below.

1. *Substitute* $\tilde{x}_1 = (m_1/m_2)^{1/4} x_1$ *and* $\tilde{x}_2 = (m_2/m_1)^{1/4} x_2$.
2. *Transform to* $(X_1, X_2)^T = R_\alpha(\tilde{x}_1, \tilde{x}_2)^T$, *where* R_α *is a* 2×2 *rotation matrix with angle* α
3. *Determine* α *such that* X_1 *and* X_2 *decouple.*
4. $\cos(\arctan x) = 1/\sqrt{1+x^2}$, $\sin(\arctan x) = x/\sqrt{1+x^2}$.