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Condensed Matter Theory 1 — Exercise 0

Winter term 2023/24

https://ilias.studium.kit.edu/goto.php?target=crs_2219528
To be discussed on: *Thursday 2023/10/25 (live in class)*

1. Density of close-packed spheres

Consider a body-centered cubic (bcc) and a face-centered cubic lattice (fcc) of close-packed, uniformly filled spheres, see Figure 1. Show that the ratio of densities between the lattices is $\rho_{\text{bcc}}/\rho_{\text{fcc}} = 3\sqrt{6}/8$.

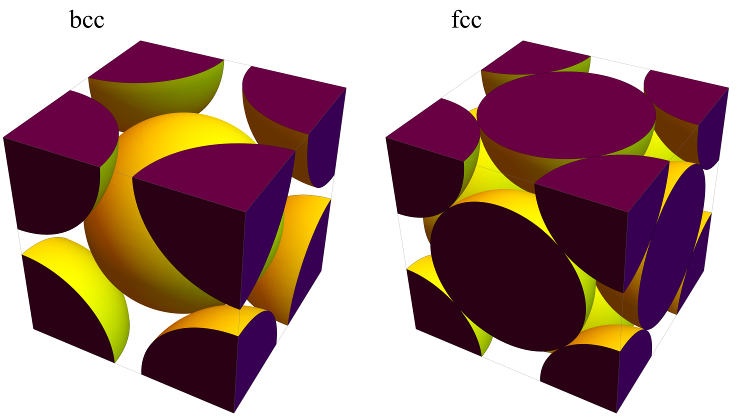

Figure 1: Body-centered cubic (bcc) and face-centered cubic (fcc) unit cells.

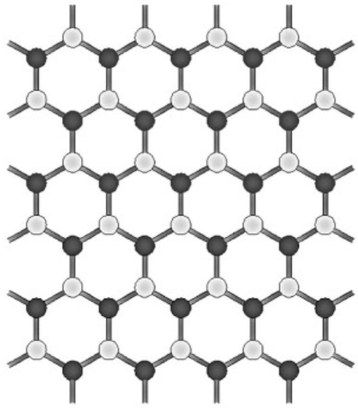

Figure 2: A sheet of graphene.

2. Honeycomb-lattice of Graphene

Graphene is a two-dimensional monatomic crystal of carbon atoms where each atom occupies a site of a honeycomb lattice, see figure 2. The honeycomb lattice is not a Bravais lattice but it can be viewed as two interpenetrating triangular or hexagonal lattices each containing one set of equivalent carbon atoms — the A and B carbon sites. In the following, we take the honeycomb lattice to be aligned in the xy-plane with the y-axis parallel to one of the nearest-neighbor atomic spacings, and let a be the distance between nearest neighbors.

a) Find a unit cell for the honeycomb lattice and determine its primitive as well as its basis vectors. Sketch the Wigner-Seitz cell of the Bravais lattice defined, e.g., by the A carbon sites, and determine its area.
Hint: $\cos\frac{\pi}{6} = \sqrt{3}/2$ and $\sin\frac{\pi}{6} = 1/2$.

b) Find the translation, rotation and mirror symmetries of the honeycomb lattice.

3. Filling the plane

Prove that the infinite two-dimensional plane can be completely filled with identical n-sided regular polygons only if $n = 3, 4, 6$.
Hint: Consider a vertex where q polygons meet and relate the integer numbers q and n.

4. Madelung constant

An infinite simple cubic lattice with a lattice constant a consists of two kinds of ions with opposite electrical charges $+q$ and $-q$. The ions occupy the lattice sites in an alternating manner similar to the NaCl structure, see Figure 3. The Coulomb energy of a single ion in the electric field of all other ions can be expressed as $U = -C_{\mathrm{M}} q^2/a$ (Gaußian units) where C_{M} is Madelung constant.

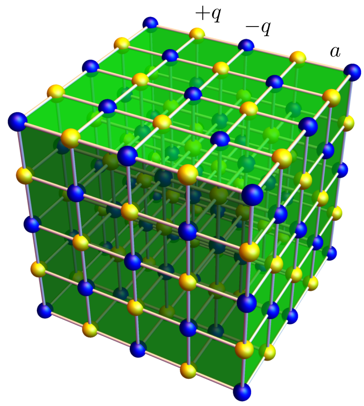

Figure 3: Simple cubic lattice occupied by oppositely charged ions.

a) Derive an analytic formula for C_{M}.

b) Compute C_{M} numerically.
Hint: Firstly, consider the single ion in the center of a finite cubic lattice consisting of $N \times N \times N$ ions where N is an odd number. Calculate the corresponding approximate value for the Madelung constant $\tilde{C}_{\mathrm{M}}^{N}$. Secondly, plot its dependence as a function of $1/N$ and consider the limit $N \to \infty$.

c) Follow the two previous steps for the two-dimensional lattice.

d) Show that for a one-dimensional chain $C_{\mathrm{M}} = 2\ln 2$.

5. Rotations and reflections

Consider the linear operators

$$R_{\varphi}^{\mathrm{2D}} = \begin{pmatrix} \cos\varphi & -\sin\varphi \\ \sin\varphi & \cos\varphi \end{pmatrix}, \quad M_{\varphi}^{\mathrm{2D}} = \begin{pmatrix} \cos\varphi & \sin\varphi \\ \sin\varphi & -\cos\varphi \end{pmatrix} \tag{1a}$$

acting on two-dimensional vectors $\boldsymbol{\rho} = \hat{\boldsymbol{x}}\rho_x + \hat{\boldsymbol{y}}\rho_y$, and linear operators

$$R_{\varphi}^{\mathrm{3D}} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad S_{\varphi}^{\mathrm{3D}} = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & -1 \end{pmatrix} \tag{1b}$$

acting on three-dimensional vectors $\boldsymbol{r} = \hat{\boldsymbol{x}}r_x + \hat{\boldsymbol{y}}r_y + \hat{\boldsymbol{z}}r_z$.

a) Convince yourself that the operators (1) do not change lengths of the vectors. Prove that if an operator A does not change the length of the vector, then $\det A = \pm 1$.

b) Discuss the geometric meaning of the operators and show that (i) $R_{\varphi}^{\mathrm{2D}}$ and $R_{\varphi}^{\mathrm{3D}}$ correspond to a rotation around the $\hat{\boldsymbol{z}}$-axis by an angle φ; (ii) $M_{\varphi}^{\mathrm{2D}}$ realizes a mirror reflection with respect to the line $y = \tan(\varphi/2)x$; (iii) $S_{\varphi}^{\mathrm{3D}}$ realizes a rotation around the $\hat{\boldsymbol{z}}$-axis by an angle φ and the subsequent mirror reflection with respect to the xy-plane.

c) Show that $M_{\varphi}^{\mathrm{2D}} M_{\psi}^{\mathrm{2D}}$ corresponds to rotation and find the rotation angle.

d) Show that $M_{\varphi}^{\mathrm{2D}} R_{\psi}^{\mathrm{2D}} M_{\varphi}^{\mathrm{2D}} = R_{-\psi}^{\mathrm{2D}}$.