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Theoretical Condensed Matter Physics
Exercise 1

(Submission: 26.10.18, discussion: 29./31.10.18)
(Note: The points on this problem sheet will not count for the admission to the final exam.)

1.1 Crystal symmetries **6 Points**

a) Recall and write down the definitions of (i) the *Bravais lattice*, (ii) the *space group* $\mathcal{S}$ and (iii) the *point group* $\mathcal{P}$ of a Bravais lattice.

b) Show that $\mathcal{P}$ can only contain rotations with 1-, 2-, 3-, 4- or 6-fold symmetries.

Hint: Rotate a lattice point $\mathbf{R}$ by $\pm\varphi$ and consider the sum of the two new vectors. Then which condition must φ fulfil?

1.2 Bravais lattice **4 Points**

a) Prove that the two-dimensional honeycomb crystal (Fig. 1) is not a Bravais lattice.

b) Find an example of how the honeycomb crystal can be described as a Bravais lattice with a basis. Give the set of basis vectors for that Bravais lattice as well as the crystal basis. What is the (maximal) point group $\mathcal{P}$ of that Bravais lattice?

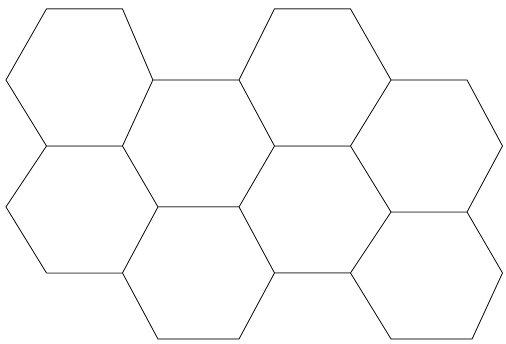

Figure 1: The honeycomb crystal is the crystal structure of graphene (a two-dimensional structure formed by carbon atoms). This lattice is especially interesting, because electrons moving on that lattice behave like relativistic Dirac particles (here without proof) carrying a pseudospin degree of freedom which is related to the two inequivalent sites of the crystal basis.

1.3 Primitive unit cell **4 points**

The primitive unit cell of a Bravais lattice is defined as a body in (continuous) space which, when translated by all vectors of the Bravais lattice, covers the *entire* space *without overlap*. Note that, according to this definition, the choice of primitive cell is not unique.

a) Show that all primitive unit cells have the same volume.

   Hint: Consider first a finite-size lattice of total volume V. What is the volume v of a primitive unit cell according to the definition? Then generalize to the infinite lattice.

b) Why does a primitive unit cell always contain exactly one lattice point?

1.4 Reciprocal lattice and symmetries **6 points**

Consider a Bravais lattice $\mathcal{B}$ spanned by the basis vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$. The *reciprocal lattice* $\mathcal{R}$ is the Bravais lattice spanned by $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$, which fulfil $\mathbf{k}_i \cdot \mathbf{a}_j = 2\pi\delta_{ij}$ $(i, j = 1, 2, 3)$.

a) Give one possible realization of $\mathbf{k}_1$, $\mathbf{k}_2$, $\mathbf{k}_3$ (see lecture). What is the reciprocal lattice of the reciprocal lattice $\mathcal{R}$?

b) Consider a (scalar) function $f(\mathbf{r})$, $\mathbf{r} \in \mathbb{R}^3$, which has the same symmetry $\mathcal{S}$ as the Bravais lattice, that is,

$$\text{in position space:} \quad \mathcal{S}:\ \mathbf{R} \mapsto \mathcal{S}(\mathbf{R}) = \mathbf{S}, \quad \text{with } \mathbf{S} \in \mathcal{B}\ \forall\ \mathbf{R} \in \mathcal{B}$$

$$\text{in function space:} \quad \mathcal{S}:\ f(\mathbf{r}) \mapsto \mathcal{S}(f(\mathbf{r})) = f(\mathcal{S}(\mathbf{r})), \quad \text{with } f(\mathcal{S}(\mathbf{r})) = f(\mathbf{r})\ \forall\ \mathbf{r} \in \mathbb{R}^3.$$

   Show that f can be represented as

$$f(\mathbf{r}) = \sum_{\mathbf{K}\in\mathcal{R}} f(\mathbf{K}) e^{\mathrm{i}\mathbf{K}\cdot\mathbf{r}}.$$

   In this sense, $\mathcal{R}$ is the "Fourier transform" of $\mathcal{B}$.

c) Prove: $\mathcal{P}$ is the point group of $\mathcal{B}$ $\iff$ $\mathcal{P}$ is the point group of $\mathcal{R}$.