Exercise-sheet 1 (October 20, 2017)

1 In-class exercises

1.1 Floquet's theorem (due to Gaston Floquet (1883))

Consider the second-order differential equation

$$\frac{d^2y}{dx^2}+\big(\epsilon+f(x)\big)y=0, \tag{1}$$

with $f(x+a)=f(x)$ and ϵ a constant.

(a) Show that one can always find a solution of the form

$$y(x+a)=k\,y(x), \tag{2}$$

where k is a complex constant.

(b) Given

$$\phi(x)=e^{-\mu x}y(x), \tag{3}$$

with $\mu=\frac{1}{a}\ln k$. Show that $\phi(x)$ is a periodic function with period a.

(c) What can you say about $y(x)$ depending on the values of μ?

1.2 Reciprocal lattice and Brillouin zone — two examples: square and honeycomb lattices

(a) Find the reciprocal vectors and construct the first Brillouin zone of both square and honeycomb lattices.

(b) What is the set of possible wavevectors $\boldsymbol{k}$ within the first Brillouin zone if one assumes periodic boundary conditions for a 16-site (32-site) square (honeycomb) lattice?

2 Homework - due date: October 27, 2017 (30 points).

2.1 Reciprocal lattice and Brillouin zone of the kagomé lattice (20 points)

(a) Find the reciprocal vectors of the lattice.

(b) Construct its first Brillouin zone.

(c) Draw the allowed wave-vectors within the first Brillouin zone for a 48-site kagomé lattice with periodic boundary conditions.

2.2 Point group symmetries of some 2D lattices (5 points)

(a) Enumerate the symmetry operations that leave the square, triangular and honeycomb lattices unchanged?

(b) Consider a square lattice (of lattice constant a) with the following two-atom basis: one atom centered at the origin $(0, 0)$, while the other is slightly off site towards the center of the square at $(a/4, a/4)$. Which symmetry operations do you find now?

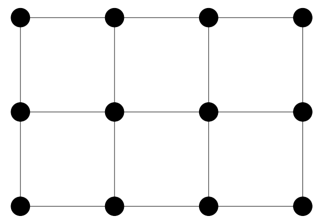
2.3 Spin-orbit coupling and time-reversal symmetry (5 points)

Consider a single electron (with charge $-e$) moving in the field of a nucleus with charge Ze. The electric field of the nucleus is $\boldsymbol{E} = -(\boldsymbol{r}/r)d\phi/dr$. As seen by the electron, the nucleus is orbiting around it with velocity $\boldsymbol{v}$, thereby generating a magnetic field $\boldsymbol{H}$ which couples to the electronic spin $\boldsymbol{S}$ through $\mu_B \boldsymbol{S} \cdot \boldsymbol{H}$, where μ_B is the Bohr magneton.

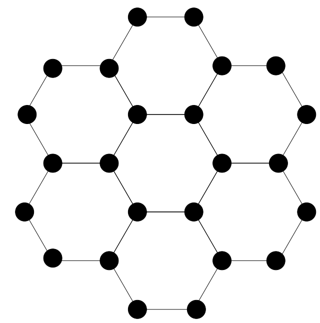
(a) Write down the explicit expression of the spin-orbit coupling term $\mu_B \boldsymbol{S} \cdot \boldsymbol{H}$

(b) Does this term break time-reversal symmetry?

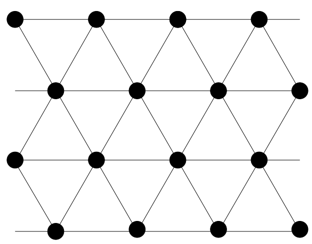
(a) Linear lattice



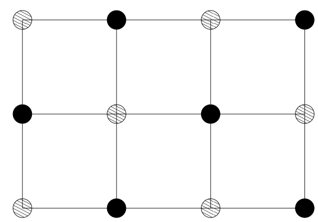
(b) Square lattice



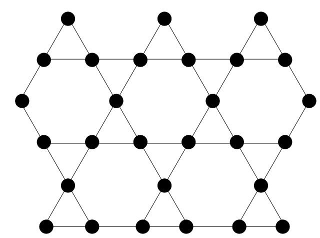
(c) Honeycomb lattice



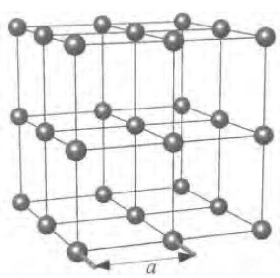
(d) Triangular lattice



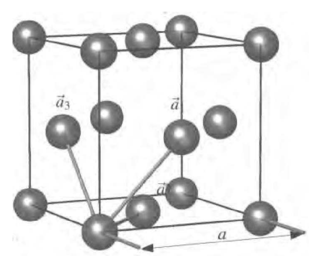
(e) Square lattice of two atoms



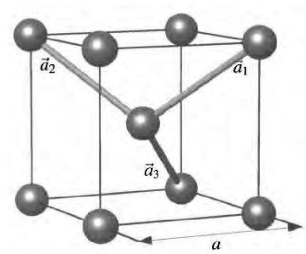
(f) Kagomé lattice



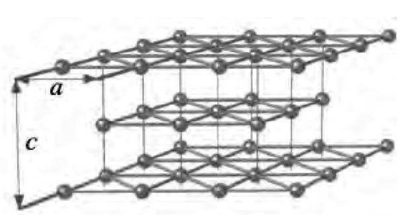
(g) Simple cubic lattice



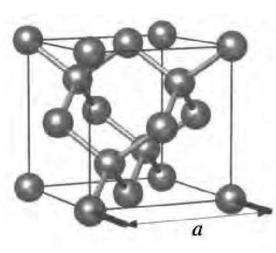
(h) Face-centered cubic lattice



(i) Body-centered cubic lattice



(j) Hexagonal closed-packed lattice



(k) Diamond lattice

Figure 1: Some lattices. Figures (g)-(k) were taken from *Condensed Matter Physics*, Marder (2010)