Institute for Theoretical Physics
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Solid State Theory

Problem set 0

Winter Term 2016

Website: http://www.thp.uni-koeln.de/trebst/Lectures/2016-SolidState.shtml
Due date: Discussed in class on **Thursday, October 27th**.

1. Discovering crystal structures with VESTA

The physical properties of solids depend decisively on the chemical composition and the structure in which the respective atoms are arranged. It is often desirable to abstract these properties and build a simpler, more tractable model. An important aspect in building such a model is to capture the essential patterns of the given crystal structure. This can be done with the help of programs such as **VESTA** that allow to visualize crystal structures. In this exercise, we want to use *VESTA* to find the dominant patterns in the solid $Ba_3IrTi_2O_9$.

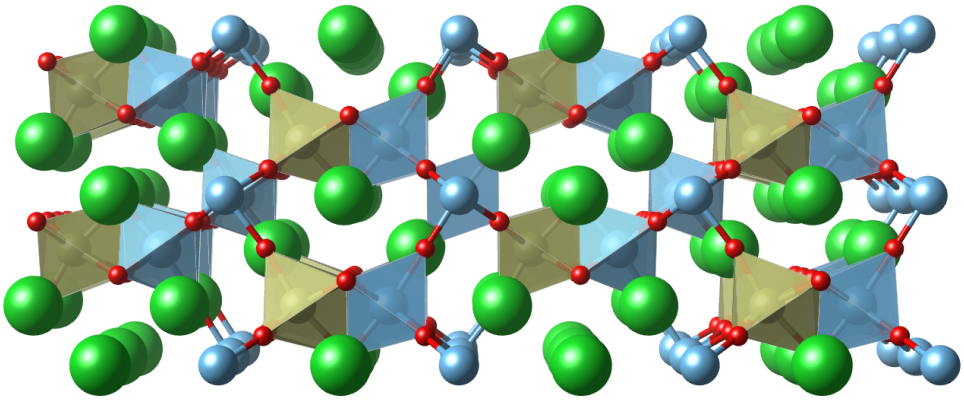

Figure 1: $Ba_3IrTi_2O_9$.

Setting up VESTA

Start by downloading *VESTA* from the official website. The crystal structure we are going to study is available for download from the course website. Upon opening, an empty frame is displayed. Go to "*File*→*Open*" and select the file you just downloaded. *VESTA* now displays a single unit cell that you can rotate it using your mouse. To replicate this cell, switch to the *Style* tab available on the left hand side and click on *Boundary...*. In the top half of the window, you can change the values for *x(max), y(max), z(max)*, which control how many unit cells are drawn in each direction. A good choice for this exercise is *x(max)* = *y(max)* = *z(max)*= 3. Also in the *Style* tab, change the display style to *Polyhedral*. This setting emphasizes the octahedral environment of oxygen atoms around the iridium and titanium atoms.

Exercises

To discover the relevant structural properties, rotate the lattice such that the $\mathbf{b}-\mathbf{c}$ plane is shown. Why can the iridium atoms be viewed as forming several individual two-dimensional layers? To find out which structure these layers possess, go to the *Objects* tab and select *Polyhedra* to deactivate the cages around the titanium atoms. Now you can observe how the iridium cages are connected. To explore the structure of the titanium layers, deactivate the iridium cages and reactivate the titanium cages. In the same fashion as before, explore the structure of the titanium atoms.

2. Wigner-Seitz cells

The **Wigner-Seitz cell** around a particular lattice point is defined as the region of space of which all constituting points are closer to the chosen lattice point than to any other lattice point. It plays its most prominent role as the **Brillouin zone**, when the input lattice is chosen to be the reciprocal lattice.

Construction in two dimensions

The construction of the Wigner-Seitz cell is straightforward, and in two dimensions can even be done by hand. In a first step, lines are drawn between the chosen point and its surrounding neighbors. In two dimensions, the next step is to draw the bisecting perpendiculars to the lines. The inner area enclosed by all of these perpendiculars constitutes the Wigner-Seitz cell, see also Fig. 2.

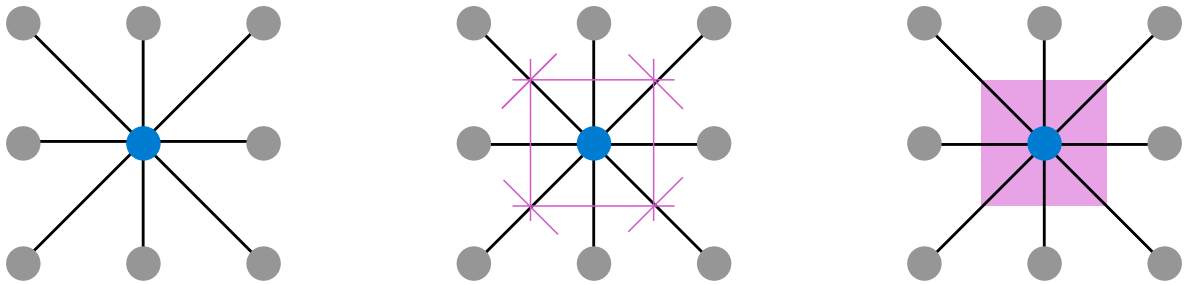

Figure 2: Construction of the Wigner Seitz cell in two dimensions.

Construction in three dimensions

In three dimensions, instead of using perpendicular lines, we now add perpendicular *planes* that will enclose a volume around the chosen lattice point, constituting the Wigner-Seitz cell. In three dimensions, we will use the fact that the Wigner-Seitz cell is a special case of the so-called **Voronoi cell**, a well-known concept in geometry. Its definition is as follows: Pick a subset of points of an n-dimensional space and call them seeds. The Voronoi cell of each of these seeds is made up of those points that are closer to the chosen seed than to any other point in space. The Wigner-Seitz cell is a special case in the sense that we are dealing with a regular arrangement of the seeds, namely the lattice vectors. The algorithm creating the partition into Voronoi cells is implemented in SciPy and we will use to construct the Wigner-Seitz cell in three dimensions. For its visualization, you will have to install the package *mayavi*, which can be done by *either* of the two commands:

```
pip install mayavi
easy_install --user "Mayavi[App]"
```

In case you are using Windows and the Anaconda python distribution, you might have to use the following lines of code:

```
conda install -c anaconda mayavi=4.4.0
```

We prepared the procedure in a well documented python script or alternatively an ipython notebook that you can use to calculate the Wigner-Seitz cell for a lattice of your choice.

Exercises

Your task is to first construct a Wigner-Seitz cell by hand for a lattice defined by the two lattice vectors

$$a = (1,0)$$
$$b = (1/2,1).$$

How does the shape of the Wigner-Seitz cell change when the vectors are not orthonormal anymore? Is there another special arrangement that yields a similarly shaped Wigner-Seitz cell as that of two orthonormal lattice vectors?

Now move on to the python code we supplied. Initially, the script will display the Wigner-Seitz cell of a simple cubic lattice. Change the lattice vectors such that they represent those of a body-centered cubic (*bcc*) and face-centered cubic (*fcc*) lattice and study their respectives Wigner-Seitz cells.

3. Reciprocal lattices and Brillouin zones

In this exercise, we will determine the reciprocal lattice vectors and the Brillouin zone for a number of important lattices. First, recall that given a lattice in real space spanned by the set of lattice vectors $\{\mathbf{a}_i\}$, its reciprocal lattice vectors $\{\mathbf{b}_j\}$ are defined by the relation

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

Start by computing the reciprocal lattice vectors for the *bcc* and the *fcc* lattice.

The lattices above are both Bravais lattices whose lattice points are generated by combinations of the elementary lattice vectors. Many materials with interesting properties have multiple atoms in a unit cell and are therefore not made up of Bravais lattices. What is, however, arranged in a Bravais lattice are the unit cells. This allows us to use the familiar notion nevertheless. One important example for such lattice is the diamond lattice. You can open the file with *VESTA* and study the crystal structure. There are two atoms in the unit cell of the diamond lattice, which is then translated along the three vectors

$$a_1 = (0,1,1)$$
$$a_2 = (1,0,1)$$
$$a_3 = (1,1,0).$$

Note that if the atoms are of different elements, the lattice is referred to as the *zinc blende* lattice, which is at the heart of many semiconductor materials mixing elements from the third and fifth group of the periodic table such as GaAs, InAs, or InP.

Another important lattice that has garnered much interest lately is the so-called hyper honeycomb lattice, which is regarded as the three-dimensional analogue of the honeycomb lattice that makes up graphene.

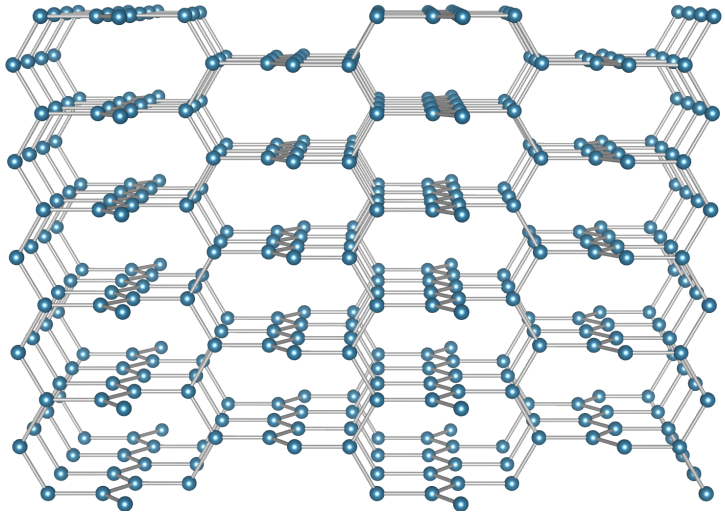

Figure 3: The hyperhoneycomb lattice.

It has four atoms in each unit cell and its lattice vectors are

$$\begin{aligned} a_1 &= (-1,1,-2) \\ a_2 &= (-1,1,2) \\ a_3 &= (2,4,0)\,. \end{aligned}$$

The reciprocal lattice vectors can be calculated in just the same fashion as above. Do so and use the python script from the previous exercise to study the Wigner-Seitz cell in reciprocal space, i.e. the Brillouin zone, of all lattices we considered in this exercise.