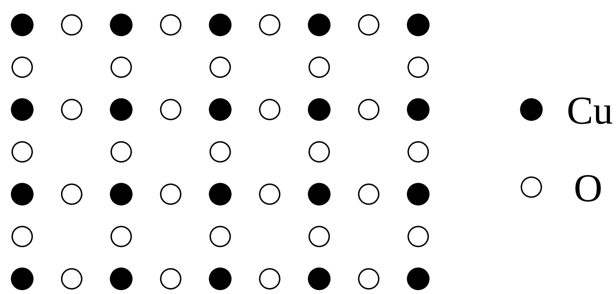
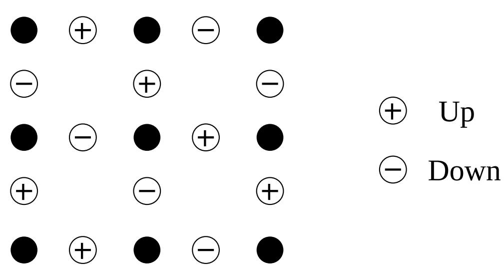
Problem 1. The common building blocks for most high T_c superconductors are copper oxide layers. Assume that the distance between Copper atoms is a, and that in the third dimension these CuO_2 layers are simply stacked with spacing c, and there are no other atoms in the crystal. In the first approximation the layers have a four-fold symmetry, the crystal is tetragonal.



(a) Sketch the Bravais lattice and indicate a possible set of primitive vectors. What is the unit cell, and what is the basis?

(b) In $LaCuO_4$ one discovers that the CuO_2 lattice is not flat, but that the oxygen atoms are moved a small amount out of the plane ("up" or "down") in an alternating fashion. What is the primitive cell and lattice spacing for this crystal? What is the reciprocal lattice?



Problem 2. Consider four lattice structures:

1. Face centered cubic (FCC)
2. Body centered cubic (BCC)
3. Simple cubic (SC)
4. Diamond (D)

Suppose identical solid spheres are distributed through space in such a way that their centers lie on the points of each of these four structures, and spheres on neighboring points just touch, without overlapping. Assuming that the spheres have unit density, show that the density of a set of close-packed spheres on each of the four structures is:

$$\text{FCC}: \quad \frac{\sqrt{2}\pi}{6} = 0.74$$

$$\text{BCC}: \quad \frac{\sqrt{3}\pi}{8} = 0.68$$

$$\text{SC}: \quad \frac{\pi}{6} = 0.52$$

$$\text{D}: \quad \frac{\sqrt{3}\pi}{16} = 0.34$$

Problem 3. Let $\vec{a}_1, \vec{a}_2, \vec{a}_3$ be a set of primitive vectors for the direct lattice. Define the reciprocal lattice primitive vectors as

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

$$\vec{b}_3 = 2\pi \frac{\vec{a}_1 \times \vec{a}_2}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

(a) Prove that

$$\vec{b}_1 \cdot (\vec{b}_2 \times \vec{b}_3) = \frac{(2\pi)^3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)}$$

(b) Suppose primitive vectors are constructed from $\vec{b}_i$ in the same manner as the $\vec{b}_i$ are constructed from $\vec{a}_i$. Prove that these vectors are just the $\vec{a}_i$ themselves.

(c) Prove that the volume of a Bravais lattice primitive cell is $\nu = |\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)|$. Explain how this helps to establish that the volume of the reciprocal lattice primitive cell is $\frac{(2\pi)^3}{\nu}$.

Problem 4. Atoms are arranged in a 1-d chain with a lattice spacing of a. Each atom is represented by the potential $V(x) = aV_0\,\delta(x)$.

(a) Show that the electron energy E and wavenumber K satisfy the relationship

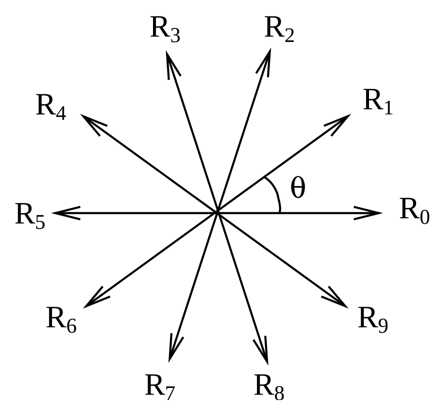
$$\cos ka = \frac{\mathcal{H}}{K}\sin(Ka) + \cos(Ka),$$

where $K^2 = \frac{2mE}{\hbar^2}$ and $\mathcal{H} = \alpha V_0$. Determine the coefficient α.

(b) Calculate the energy gaps between the bands for weak potential $V_0 \ll \frac{\hbar}{ma^2}$.

(c) Calculate the bandwidth of the lowest energy band for strong potential $V_0 \gg \frac{\hbar}{ma^2}$.

Problem 5. Suppose a $2d$ Bravais lattice has *tenfold* rotational symmetry. Then, for any given lattice vector $\vec{R}_0 = n_1\vec{a}_1 + n_2\vec{a}_2$ joining two points on the lattice, we must have 9 other lattice vectors $\vec{R}_1, \ldots, \vec{R}_9$ that are related to $\vec{R}_0$ through rotations by multiples of $\theta = \frac{2\pi}{10}$. Show that this construction is mathematically inconsistent, and therefore a Bravais lattice with tenfold symmetry does not exist. What other rotational symmetries in two dimensions can you rule out by your argument?



Problem 6. Show that a band overlap is not allowed in one dimension, assuming that the Schroedinger equation is strictly one-dimensional.