8.511 Theory of Solids I **Problem Set 1** **Due 8:00pm**
September 22, 2015

Lecturer: Prof. Patrick A Lee, TA: Jacob Colbert

1. Constructive Interference and Bravais lattice:
In class (Mon, Sept 8), we learn that in order to get constructive interference in diffraction from a crystal lattice, we require that:

$$e^{\mathrm{i}\,\vec{Q}\cdot\vec{R}_j} = e^{\mathrm{i}\,\alpha}, \tag{1}$$

where α is a constant phase. Eq.(1) is obeyed for **all** R_j in the Bravais lattice (say in 3 spatial dimensions), i.e.

$$\vec{R_j} = n_1\vec{a_1} + n_2\vec{a_2} + n_3\vec{a_3} \tag{2}$$

   (a) Show that α in Eq. (1) must be zero in order to have a constructive interference.

   (b) Show that the solution we found for Eq. (1), i.e. $Q = \{\vec{G}\}$, where $\vec{G}$ are the reciprocal lattice vectors,

$$\vec{G_j} = m_1\vec{b_1} + m_2\vec{b_2} + m_3\vec{b_3} \tag{3}$$

   is unique.

2. (a) Prove that the product of the volume of the first Brillouin zone and the volume of the unit cell of the Bravais lattice equals $(2\pi)^3$.

   (b) The reciprocal lattice of an fcc lattice is the bcc lattice. Both lattices are conveniently represented as a cubic lattice with a basis. If the linear dimension of the cube for the fcc lattice is a, use the result of part (a) to show that the linear dimension of the bcc lattice is $\frac{4\pi}{a}$.

3. The common building blocks for most high temperature (high T_c) superconductors are copper oxide layers, as depicted in Figure I.1.6. Assume the distance between copper atoms (filled circles) is a. For simplicity let us also assume 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 first approximation the layers have a four-fold symmetry; the crystal is tetragonal.

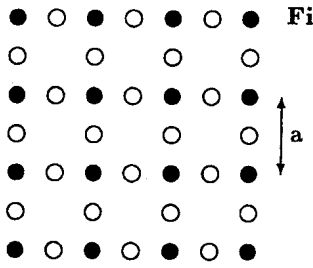

Fig. I.1.6. CuO_2 lattice

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

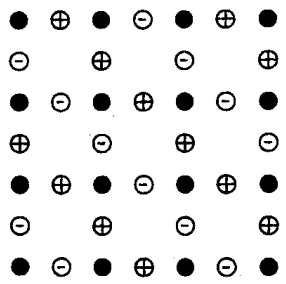

Fig. I.1.7. Distorted CuO_2 lattice

(b) In $LaCuO_4$ one discovers, at closer inspection, that the CuO_2 lattice is actually not flat, but that the oxygen atoms are moved a small amount out of the plane ("up" or "down") in an alternating fashion (in Figure I.1.7, a + means up and a - means down).[1] What is the primitive cell and lattice spacing for this crystal? What is the reciprocal lattice? Describe (qualitatively) what happens in the X-ray diffraction pattern as the distortion is decreased gradually to zero.

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[1] $LaCuO_4$ is an antiferromagnetic insulator. High temperature superconductivity was discovered in a closely related compound, $La_{1-x}Ba_xCuO_4$. See J.G. Bednorz and K.A. Müller, Z. Physik B **64**, 189 (1986).