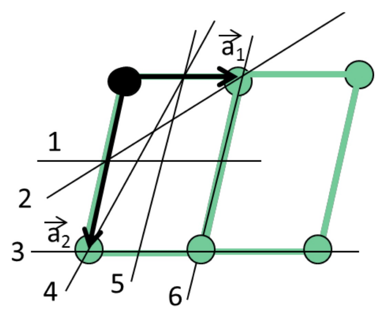
Condensed Matter Physics I
final written test
academic year 2016/2017
January 16, 2017

(*Time: 3 hours*)

Exercise 1: *Miller indices*

Consider a triclinic crystal whose unit vectors $\mathbf{a_1}$ and a_2 together with some specific planes are shown in the figure below. Vector $\mathbf{a_3}$ is orthogonal to the sheet. Two unit cells are also sketched.

1. What are the Miller indices of the planes 1-6?
2. Draw the reciprocal lattice and indicate those points corresponding to the planes in the figure.



Exercise 2: *Sommerfeld model in crystalline solids*

In a first, approximate classification of materials, metals are characterized by a partially filled band. Insulators has an empty conduction band and a completely filled valence band.

1. Consider 1D crystals having a lattice constant a and composed of either mono- or divalent atoms. Classify these crystals as metals or insulators, justifying your answer.
2. Consider 3D crystals (e.g. in form of a simple cubic lattice) composed of either mono- or divalent atoms. Would the classification made in 1D always hold for 3D crystals? Justify your answer.
3. Assume monovalent atoms crystallizing in a simple cubic (SC) lattice with a lattice parameter a. Considering the Sommerfeld model for electrons, calculate the magnitude of the Fermi wavevector $\mathbf{k_F}$ and compare it with the shortest possible distance from the origin of the k-space ($\mathbf{\Gamma}$ point) to the Bragg plane in SC lattice. Indicate with $\mathbf{X}$ that point.
4. If $\mathbf{k_F} < \mathbf{\Gamma X}$, what does it mean?
5. Compute how much of divalent atoms should be added to such SC lattice to make the Fermi sphere touching the Bragg planes in the alloy. Would such alloying result in an improvement or degradation of electrical conductivity?

Exercise 3: *Tight-binding model and Semiclassical model of Electron Dynamics*

1. Calculate the expression for the energy band of a BCC crystal with lattice parameter a, using the tight-binding model assuming one s orbital per atom and nearest neighbor interaction of strength γ, neglecting overlaps and higher order hopping contributions.

2. Using the band calculated above and the semiclassical model of electron dynamics, write the explicit expression for the velocity of an electron of this band, $\mathbf{v}(\mathbf{k}(t))$ (i.e., v_x, v_y, v_z as a function of $\mathbf{k}$(t)).

3. Consider an electron in a uniform electric field E constant in time. Calculate explicitly $\mathbf{k}$(t)) considering that $\mathbf{k}$(0)=0.

4. Consider the electron initially at rest and at the origin. Derive the explicit expression of $\mathbf{r}$(t), i.e. of $x(t)$, $y(t)$ and $z(t)$, using the expression of $\mathbf{k}$(t)) previously derived.

5. Specify the results for $x(t)$, $y(t)$ and $z(t)$ in the case of $\mathbf{E}$ in [110] direction.

6. You should find an oscillatory motion. Sketch the trajectory in the real space. Estimate Δr, the amplitude of oscillation, for a realistic electric field and bandwidth.

NOTE:

- Give all the steps necessary to understand in detail the solution procedure. Answers with the final result only or with insufficient details will not be considered valid.

- When required, numerical evaluations should be given exactly with 3 significant figures, if not otherwise indicated.