**Written exam of Condensed Matter Physics - February 3th 2020**
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**Exercise 1: X ray scattering.**

Germanuim (Ge) is a face-centred cubic (fcc) lattice with two-atom basis that can be regarded as two interpenetrating fcc primitive lattices displaced by $\boldsymbol{d} = \frac{a}{4}(\hat{\boldsymbol{x}} + \hat{\boldsymbol{y}} + \hat{\boldsymbol{z}})$, where $a$ is the side of the conventional unit cell (this is the diamond lattice, see the left panel of Fig. 1; the black circles indicate the second atom of the basis), and $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}, \hat{\boldsymbol{z}}$ are the Cartesian reference unit vectors. The atomic density of Ge is $\rho_{\rm at} = 4.412 \times 10^{28}\,{\rm m}^{-3}$.

1. A powder diffraction experiment is performed using an x-ray beam with wavelength $\lambda = 1.476 \times 10^{-10}\,{\rm m}$. Determine the angle $\phi$ of the 5th reflection (see the central panel of Fig. 1).

2. Suppose that the experiment described in the previous point is performed with and incident beam consisting of neutrons. What must the neutron velocity $v$ be in order to produce reflections at the same angles as those produced by x-rays?

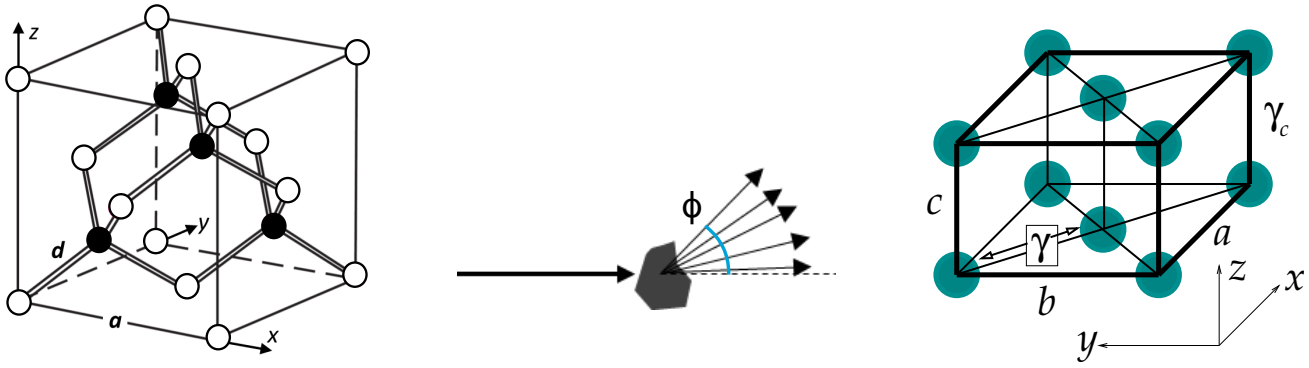


Fig. 1.

**Exercise 2: Tight binding.**

Consider a three dimensional base-centered orthorhombic Bravais lattice, whose conventional unit cell is shown in the right panel of Fig. 1. The lattice parameters are $a = 0.15\,{\rm nm}$, $b = 0.20\,{\rm nm}$, $c = 0.13\,{\rm nm}$. The sites of the lattice host $s$ orbitals. Consider the tight-binding description of the electron band structure, where only nearest-neighbors (nn) transfer integrals are considered. Let $\gamma = 0.75\,{\rm eV}$ be the value of the transfer integral along the diagonals of the conventional unit cell on the basal plane, and $\gamma_c = 0.70\,{\rm eV}$ the value for nearest neighbors along the $c$ axis. Fix the zero of the energy at the atomic level of the $s$ orbital, $E_s = 0$, and let $\beta = 2.25\,{\rm eV}$ be the parameter determining the tight-binding correction to the atomic level. Neglect all overlap integrals.

1. Determine the positions of the nearest neighbors on the basal plane, $\boldsymbol{R}$, the positions of the nearest neighbors along the $c$ axis, $\boldsymbol{R}_c$, and the tight-binding dispersion law $\varepsilon_{\boldsymbol{k}}$, with wavevector $\boldsymbol{k} = (k_x, k_y, k_z)$.

2. Determine the expression of the velocity $\boldsymbol{v}_{\boldsymbol{k}} = (v_x, v_y, v_z)$ of the electrons. What is the maximum value of the velocity at $k_x = k_y = 0$, as a function of $k_z$? Determine the values of the elements of the mass tensor $m_{ij}$ at the $\Gamma$ point of the Brillouin zone.

3. Suppose that each orbital contributes one electron to the conduction band. What is the density $n$ of conduction electrons? What is the value of the Fermi energy $\varepsilon_F$?

[Note that the neutron mass is $m_n = 1.675 \times 10^{-27}\,{\rm kg}$; $1\,{\rm eV}$ corresponds to an energy of $1.60 \times 10^{-19}\,{\rm J}$; the Planck constant is $\hbar = 1.05 \times 10^{-34}\,{\rm J{\cdot}s}$; the free electron mass is $m_0 = 9.11 \times 10^{-31}\,{\rm kg}$].

**Solution of the written exam**
**Profs. S. Caprara and A. Polimeni**

**Exercise 1**.

1. The lattice constant of Ge is $a = (8/\rho_{\rm at})^{1/3} = 0.566\,{\rm nm}$. The 5th reflection can be determined by

$$\theta = \sin^{-1}\left(\frac{\lambda}{2d}\right), \qquad \text{with } d = \frac{a}{\sqrt{h^2+k^2+l^2}},$$

and $(hkl) = (331)$, according to the diamond selection rules. One finds $\theta = 34.635°$, hence $\phi = 2\theta = 69.27°$.

2. Form the condition

$$\lambda_{\rm neutron} = \frac{h}{mv} = \lambda_{\rm x-ray}$$

one finds

$$v = \frac{h}{\lambda m} = \frac{2\pi\hbar}{\lambda m} = 2.68\times 10^3\,{\rm m/s}.$$

**Exercise 2**.

1. We have four nearest neighbors on the basal plane, at $\boldsymbol{R} = (\pm\frac{a}{2}, \pm\frac{b}{2}, 0)$, and two nearest neighbors along the $c$ axis, at $\boldsymbol{R}_c = (0, 0, \pm c)$. Then

$$\varepsilon_{\boldsymbol{k}} = E_s - \beta - \gamma\sum_{\boldsymbol{R}} {\rm e}^{{\rm i}\boldsymbol{k}\cdot\boldsymbol{R}} - \gamma_c\sum_{\boldsymbol{R}_c} {\rm e}^{{\rm i}\boldsymbol{k}\cdot\boldsymbol{R}_c} = E_s - \beta - 4\gamma\cos\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y b}{2}\right) - 2\gamma_c\cos(k_z c). \tag{1}$$

2. The velocity of Bloch electrons is

$$\boldsymbol{v}_{\boldsymbol{k}} = \frac{1}{\hbar}\frac{\partial\varepsilon_{\boldsymbol{k}}}{\partial\boldsymbol{k}} = \frac{2}{\hbar}\left(\gamma a\sin\left(\frac{k_x a}{2}\right)\cos\left(\frac{k_y b}{2}\right), \gamma b\cos\left(\frac{k_x a}{2}\right)\sin\left(\frac{k_y b}{2}\right), \gamma_c c\sin(k_z c)\right),$$

hence the maximum of the velocity at $k_x = k_y = 0$, as a function of $k_z$ is found at $k_z = \frac{\pi}{2c}$, where $v_x = v_y = 0$ and

$$v_z^{\rm max} = \frac{2\gamma_c c}{\hbar} = 2.77\times 10^5\,{\rm m/s}.$$

Expanding the band dispersion around the $\Gamma$ point, we find

$$\varepsilon_{\boldsymbol{k}} \approx E_s - \beta - 4\gamma - 2\gamma_c + \frac{1}{2}\left(\gamma a^2 k_x^2 + \gamma b^2 k_y^2 + 2\gamma_c c^2 k_z^2\right),$$

hence, the inverse mass tensor is diagonal, and so is the mass tensor. Then

$$m_{xy} = m_{yx} = m_{xz} = m_{zx} = m_{yz} = m_{zy} = 0,$$

and

$$m_{xx} = \frac{\hbar^2}{\gamma a^2} = 4.11\times 10^{-30}\,{\rm kg} = 4.52\,m_0, \qquad m_{yy} = \frac{\hbar^2}{\gamma b^2} = 2.31\times 10^{-30}\,{\rm kg} = 2.54\,m_0,$$

$$m_{zz} = \frac{\hbar^2}{2\gamma_c c^2} = 2.93\times 10^{-30}\,{\rm kg} = 3.22\,m_0.$$

3. The conventional unit cell has volume $\mathcal{V} = abc = 3.9\times 10^{-30}\,{\rm m}^3$, and hosts 2 atoms, hence

$$n = \frac{2}{\mathcal{V}} = 5.13\times 10^{29}\,{\rm m}^{-3}.$$

Since the band is half filled, when there is one electron per lattice site, and the band is symmetric around the mid point, the Fermi energy is $\varepsilon_F = E_s - \beta = -2.25\,{\rm eV}$.