Mid-term assessment test of Condensed Matter Physics - November 19th 2018
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Exercise 1. Consider a lattice with cubic symmetry and chemical formula AB. When measuring the X-ray diffraction pattern of the sample using the powder (or Debye-Scherrer) method by a radiation with $\lambda = 0.1542\,\mathrm{nm}$, ten diffraction peaks are obtained with the scattering angle $\phi = 2\theta$, as shown below.

2θ (degrees): 36.95, 42.91, 62.30, 74.64, 78.64, 94.06, 105.75, 109.78, 127.29, and 143.77.

1. After demonstrating that the given lattice is a Bravais face-centered cubic, label each diffraction peak using the Miller indexing of the simple cubic lattice (h, k, l). Then, compute the lattice parameter a of the conventional cubic cell as the mean of the 10 values deduced by each peak.

2. Indicate which of the above peaks would disappear if the A and B atoms were the same and: a) atom B were displaced by $a(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$ with respect to A; b) atom B were displaced by $a(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ with respect to A.

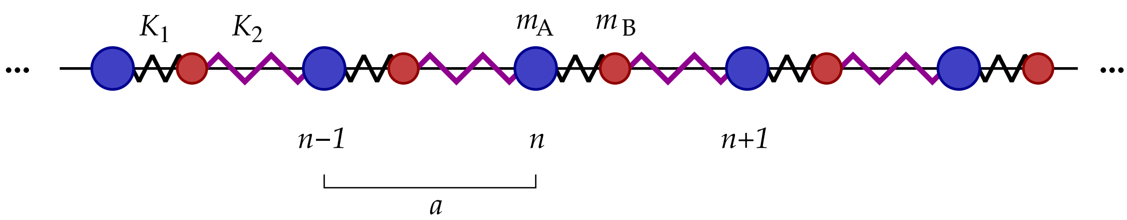

Fig. 1.

Exercise 2. Consider a linear chain representing a Bravais lattice composed of N units cells of size a, with a two-atom basis. All atoms are constrained to move only along the chain. The two inequivalent atoms, A and B, have masses $m_{\mathrm{A}} = 2m$ and $m_{\mathrm{B}} = m$, respectively. B atoms are connected to nearest-neighbors A atoms by inequivalent springs, whose elastic constant are $K_1 = 2K$ and $K_2 = K$, respectively (see Fig. 1). Indicate with u_n^{A} and u_n^{B} the displacement of A and B atoms in the n-th unit cell, with respect to their equilibrium positions. Adopt Born-von Karman periodic boundary conditions. To assign numerical values, consider $m = 92 \times 10^{-27}\,\mathrm{kg}$, $a = 0.5\,\mathrm{nm}$, $K = 4.5\,\mathrm{kg/s^2}$.

1. Assuming traveling-wave solutions $u_n^{\mathrm{A}} = A\mathrm{e}^{i(qna-\omega t)}$ and $u_n^{\mathrm{B}} = B\mathrm{e}^{i(qna-\omega t)}$, where q is the wave vector, determine the dispersion of the acoustic and optical phonon branches, $\omega_a(q)$ and $\omega_o(q)$.

2. Verify that, for small q, $\omega_a(q) \approx c_s|q|$, and determine the numerical value of the velocity of sound c_s.

3. Adopting a Debye model for the acoustic branch, $\omega_a(q) = c_s|q|$, and an Einstein model for the optical branch, with $\omega_E = \omega_o(q = 0)$, determine the low-temperature and high-temperature asymptotic expressions for the specific heat c_V of the lattice. Provide the value of c_V at $T = 1\,\mathrm{K}$. Consider that $\int_0^\infty \frac{x}{\mathrm{e}^x - 1}\,\mathrm{d}x = \frac{\pi^2}{6}$.

Solution of the mid-term assessment test
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Exercise 1.

1. With the help of the Debye-Scherrer relation $K = 2\kappa \sin\theta$, with $\kappa = 2\pi/\lambda$, we obtain the following table

	θ (deg)	$\sin\theta$	K (nm^{-1})	K/K_1
1	18.475	0.3169	25.825	1.000
2	21.455	0.3658	29.808	1.154
3	31.150	0.5173	42.155	1.632
4	37.320	0.6063	49.407	1.954

The ratios being $K_2/K_1 \approx 2/\sqrt{3}$, $K_3/K_1 \approx 2\sqrt{2}/\sqrt{3}$, $K_4/K_1 \approx \sqrt{11/3}$, the reciprocal lattice of the given Bravais lattice is a BCC, hence the given Bravais lattice is FCC.

The reciprocal lattice vectors of an FCC can be written as $\mathbf{K} = \frac{2\pi}{a}(h,k,l)$ with h,k,l all even or all odd, a being the size of the conventional FCC unit cell. By means of the Bragg relation $d = \lambda/(2\sin\theta) = a/\sqrt{h^2+k^2+l^2}$, we find

	θ (deg)	$\sin\theta$	d (nm)	hkl	$h^2+k^2+l^2$	$\sqrt{h^2+k^2+l^2}$	a (nm)
1	18.475	0.3169	0.2433	111	3	1.732	0.4214
2	21.455	0.3658	0.2108	200	4	2.000	0.4215
3	31.150	0.5173	0.1490	220	8	2.828	0.4216
4	37.320	0.6063	0.1272	311	11	3.317	0.4217
5	39.320	0.6337	0.1217	222	12	3.464	0.4215
6	47.030	0.7317	0.1054	400	16	4.000	0.4215
7	52.875	0.7973	0.0967	331	19	4.359	0.4215
8	54.890	0.8180	0.0942	420	20	4.472	0.4215
9	63.645	0.8961	0.0860	422	24	4.899	0.4215
10	71.885	0.9504	0.0811	333, 511	27	5.196	0.4215

The last peak takes contribution from two different families of lattice planes. The average lattice parameter is $a = 0.4215\,\mathrm{nm}$.

2. If the atoms in the basis are the same, some peaks disappear because of destructive interference upon scattering on the lattice basis.
a) Taking the basis $\mathbf{d}_1 = (0,0,0)$ and $\mathbf{d}_2 = a(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, and $\mathbf{K} = \frac{2\pi}{a}(h,k,l)$ with h,k,l all even or all odd, we find the structure factor

$$S_{\mathbf{K}} = \sum_{\ell=1,2} \mathrm{e}^{i\mathbf{d}_\ell\cdot\mathbf{K}} = 1 + \mathrm{e}^{i\pi(h+k+l)/2},$$

which gives destructive interference whenever $h+k+l = 2(2m+1)$, with integer $m = 0, \pm1, \pm2, \ldots$. Of the ten measured peaks, those that would be missing are the 2nd ($hkl = 200$), 5th ($hkl = 222$), and 8th ($hkl = 420$).
b) Takig now $\mathbf{d}_1 = (0,0,0)$ and $\mathbf{d}_2 = a(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, we find

$$S_{\mathbf{K}} = \sum_{\ell=1,2} \mathrm{e}^{i\mathbf{d}_\ell\cdot\mathbf{K}} = 1 + \mathrm{e}^{i\pi(h+k+l)},$$

which gives destructive interference whenever $h+k+l = 2m+1$, with integer $m = 0, \pm1, \pm2, \ldots$. Of the ten measured peaks, those that would be missing are the 1st ($hkl = 111$), 4th ($hkl = 311$), 7th ($hkl = 331$), and 10th ($hkl = 333, 511$).

Exercise 2.

1. The equations of motion are

$$\begin{cases} m_A \ddot{u}_n^A = -K_1\left(u_n^A - u_n^B\right) - K_2\left(u_n^A - u_{n-1}^B\right) \\ m_B \ddot{u}_n^B = -K_1\left(u_n^B - u_n^A\right) - K_2\left(u_n^B - u_{n+1}^A\right) \end{cases} \quad\Rightarrow\quad \begin{cases} 2m\ddot{u}_n^A = -2K\left(u_n^A - u_n^B\right) - K\left(u_n^A - u_{n-1}^B\right) \\ m\ddot{u}_n^B = -2K\left(u_n^B - u_n^A\right) - K\left(u_n^B - u_{n+1}^A\right). \end{cases}$$

Substituting the traveling-wave solutions we find

$$\begin{cases} \left(2m\omega^2 - 3K\right)A + K\left(2 + \mathrm{e}^{-iqa}\right)B = 0 \\ K\left(2 + \mathrm{e}^{iqa}\right)A + \left(m\omega^2 - 3K\right)B = 0, \end{cases}$$

which admits nontrivial solutions for A, B if and only if the determinant of the matrix associated to the system of linear equations vanishes. Letting in the following $\overline{\Omega} \equiv \sqrt{K/m}$, which is the relevant frequency scale in our problem, the equation that determines the phonon frequencies is

$$\omega^4 - \frac{9}{2}\overline{\Omega}^2\omega^2 + 4\overline{\Omega}^4\sin^2\frac{qa}{2} = 0,$$

whose solutions are

$$\omega_\pm^2(q) = \frac{9}{4}\overline{\Omega}^2\left(1 \pm \sqrt{1 - \frac{64}{81}\sin^2\frac{qa}{2}}\right),$$

with $\omega_a(q) = \omega_-(q)$ and $\omega_o(q) = \omega_+(q)$ describing the acoustic and optical phonon branch, respectively.

2. For the acoustic branch, since for $|q|a \ll 1$ we have $\sin^2\frac{qa}{2} \approx \left(\frac{qa}{2}\right)^2$ and $\sqrt{1 - \frac{16}{81}(qa)^2} \approx 1 - \frac{8}{81}(qa)^2$, we find

$$\omega_a(q) \approx c_s|q|, \qquad \text{with } c_s = \frac{\sqrt{2}}{3}\overline{\Omega}a.$$

Inserting the values given in the text, $c_s = 1648.5\,\mathrm{m/s}$.

3. We set $\omega_E \approx \omega_o(q=0) = \frac{3}{\sqrt{2}}\overline{\Omega}$. Then, the internal energy per unit volume is

$$u = \sum_{s=a,o}\int_{-\pi/a}^{\pi/a}\frac{\mathrm{d}q}{2\pi}\frac{\hbar\omega_s(q)}{\mathrm{e}^{\beta\hbar\omega_s(q)} - 1} \approx \int_0^{q_D}\frac{\mathrm{d}q}{\pi}\frac{\hbar c_s q}{\mathrm{e}^{\beta\hbar c_s q} - 1} + \frac{1}{a}\frac{\hbar\omega_E}{\mathrm{e}^{\beta\hbar\omega_E} - 1},$$

with $\beta = 1/(k_BT)$, and $q_D = \pi/a$, because in one dimension the Debye sphere coincides with the first Brillouin zone.

At high temperature, $k_BT \gg \hbar\omega_D, \hbar\omega_E$, with $\omega_D \equiv c_s q_D$, the exponentials in the denominators can be expanded to first order, the two phonon modes give the same contribution (equipartition), and

$$u \approx \frac{2k_BT}{a} \quad\Rightarrow\quad c_V = \frac{2k_B}{a} \equiv c_V^{DP},$$

i.e., we recover the Dulong-Petit (DP) value for a one-dimensional crystal with two atoms per unit cell. For the given set of parameters $c_V \approx 5.523 \times 10^{-14}\,\mathrm{J/(K\cdot m)}$.

At low temperature, $k_BT \ll \hbar\omega_D, \hbar\omega_E$,

$$u \approx \frac{\hbar c_s}{\pi}\left(\frac{k_BT}{\hbar c_s}\right)^2\int_0^\infty\frac{x}{\mathrm{e}^x - 1}\,\mathrm{d}x + \frac{\hbar\omega_E}{a}\mathrm{e}^{-\beta\hbar\omega_E} \approx \frac{\pi^2\hbar\omega_D}{6a}\left(\frac{k_BT}{\hbar\omega_D}\right)^2 \quad\Rightarrow\quad c_V = \frac{\pi^2 k_B}{3a}\left(\frac{k_BT}{\hbar\omega_D}\right),$$

where we adopted the change of variable $x = \beta\hbar c_s q$ in the integral over q, and extended the integration limit to infinity, to extract the leading behavior at small T. In the final expression for u, we neglected the exponentially small contribution of the optical branch, since the numerical estimate gives $\Theta_E \equiv \hbar\omega_E/k_B = 113.32\,\mathrm{K}$, i.e., at $T = 1\,\mathrm{K}$, $\mathrm{e}^{-\beta\hbar\omega_E} \approx \mathrm{e}^{-113} \approx 8.4 \times 10^{-50}$. Thus, at $T = 1\,\mathrm{K}$, $c_V \approx 0.04159\,k_B/a \approx 0.02079\,c_V^{DP} = 1.148 \times 10^{-15}\,\mathrm{J/(K\cdot m)}$, where we used the numerical value of the Debye temperature $\Theta_D \equiv \hbar\omega_D/k_B = 79.115\,\mathrm{K}$.