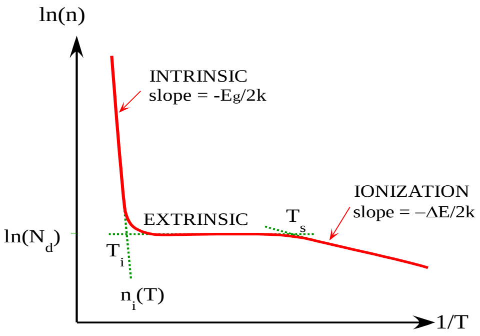
Draft of solution Exam TFY4220, Solid State Physics, 29. May 2015.

Problem 1 (15%) Introductory questions (answers can be found in the books)

1a) Small Ewald sphere, not many reflections in Bragg with a single crystal. Make powder or rotate to get more reflections .. See lab text

1b) Properties of materials were asked for – not properties of bonds!
Ionic – high melting point, solves in water, non-conductive, Ex NaCl
Metallic- medium melting points, conductors, dense, ductile, Ex Al
Covalent –brittle, directional bonds, (no/semi/ conductors, medium/high melting points, Ex Si

1c) Given in lectures (and in book)



The temperature dependence of the electron concentration in an n-type semiconductor.

1d) Free electrons - See lecture notes/Kittel

Problem 2 (15%) Multiple Choice

1 a)

2 b)

3 d)

~~4 c)~~

5 c)

6 c)

7 d)

8 b)

9 b)

10 b)

Problem 3 (25%) Structure and Diffraction

3a)

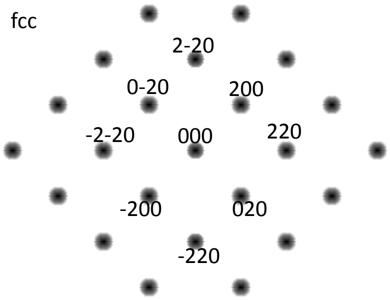
I) Ag is fcc Bravais lattice with one atom in basis. (The fcc Bravais lattice has these 4 lattice points in the unit cell –Ag in (000), (½ , 0, ½) (0, ½ , ½) and (½ , ½ , 0)).

II) Perovskite has a simple cubic Bravais lattice – 5 atoms in basis – Ca in (0,0,0), Ti in (½,½,½,) and O on the three cube faces (½,½,0,)(½,0,½,)(0,½,½,) one lattice point in unit cell

III) Titanaluminid is tetragonal, primitive, with 4 atoms in basis – Ti in 000 and ½ ½ 0, Al in ½ 0 ½ and 0 ½ ½ .. One lattice point in unit cell..

2b) fcc is extinct when mixed indices, all odd or all even gives 4f. See Kittel page 40. The three lowest are 111, 200 and 220, in this order .. (lowest h2+k2+l2 give highest intensity)

3c)



Extinct reflections between everyone 100, 110 etc …

3d) Perovskite – CaTiO3- ,one Ca, one Ti and three O in the unit cell-

Simple cubic – no extinction rules, that means all can be seen, but they will show different strengths, depending on type of atoms .. ..

Problem 4 (25%) Phonons

3a) This was given in lecture, and in the book, I just give some keywords here .. – Start out with equations of motion (M instead of m, ϒ instead of C) ,

$$M\frac{d^2u_n}{dt^2} = -\gamma(u_n - u_{n-1}) + \gamma(u_{n+1} - u_n)$$

insert suggested answer $u_n(t) = ue^{i(kan-\omega t)}$

And we get

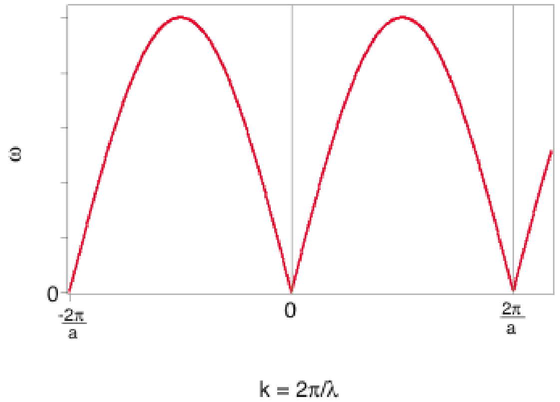
$$-M\omega^2 ue^{i(kan-\omega t)} = -\gamma[2 - e^{-ika} - e^{ika}]ue^{i(kan-\omega t)} = -2\gamma(1-\cos ka)ue^{i(kan-\omega t)}$$

solve with respect to ω and we get

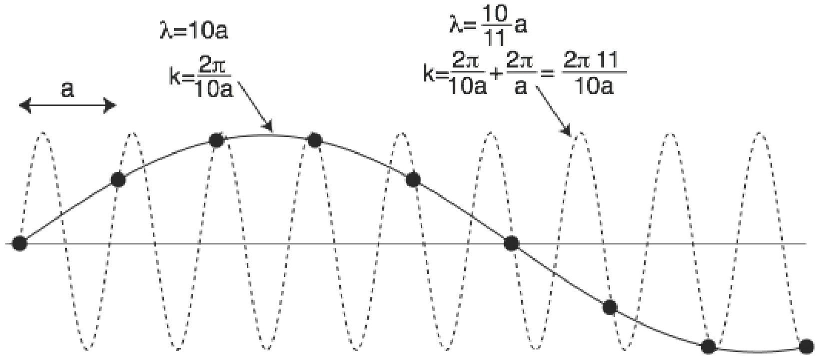
$\omega(k) = \sqrt{\frac{2\gamma(1-coska)}{M}} = 2\sqrt{\frac{\gamma}{M}}|sin\frac{ka}{2}|$ which is the dispersion relation for one dimensional chain of one type of equidistance atoms. (With values here $\omega(k) = 2\sqrt{\frac{C}{m}} \cdot \left|\sin\frac{ka}{2}\right|$)

4b)

When we plot this we get



All physics within 1BZ. Changing k by one reciprocal lattice vector gives exactly the same movement of the atoms, as shown in figure below.



Remember that the wave is defined by the lattice points!

We have one branch, acoustical modes. At zone centre acoustic down to zero… Standing waves at zone boundary, group velocity $v_g = \frac{\partial\omega}{\partial k}$ is zero.

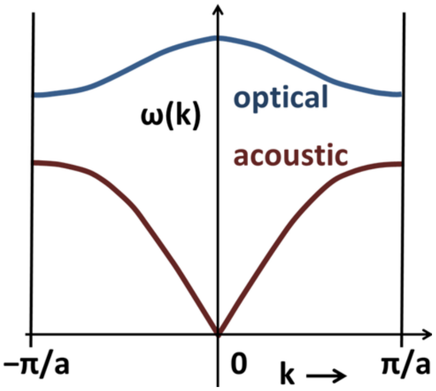
c) We have that $\omega(k) = 2\sqrt{\frac{C}{m}} \cdot \left|\sin\frac{ka}{2}\right| = \omega_{\max} \cdot \left|\sin\frac{ka}{2}\right|$. For 1D we have $N_k = \frac{L}{2\pi}$ and $N(\omega)d\omega = 2N_k dk$. This gives (solving with respect to k) $k(\omega) = \frac{2}{a}\arcsin\left(\frac{\omega}{\omega_{\max}}\right)$.The number 2 is there because we have an interval dk with frequencies between ω and dω both for positive and negative k values in the first Brillouin zone. The number of wave solutions with frequencies between ω₁ and ω₂ will then be

$$N=\int_{\omega_1}^{\omega_2} N(\omega)d\omega=\frac{L}{\pi}\int_{k_1}^{k_2} dk=\frac{L}{\pi}\left(k_2-k_1\right)=\frac{L}{\pi}\left(\frac{2}{a}\right)\left[\arcsin\left(\frac{\omega_2}{\omega_{\max}}\right)-\arcsin\left(\frac{\omega_1}{\omega_{\max}}\right)\right]$$

$$\approx\frac{2L}{\pi a}\frac{\left(\omega_2-\omega_1\right)}{\omega_{\max}}=\frac{2\cdot1\cdot10^{-2}\,\mathrm{m}}{\pi\cdot3\cdot10^{-10}\,\mathrm{m}}\cdot\frac{\left(10^{11}-10^{12}\right)}{10^{13}}=\frac{2\cdot1\cdot9\cdot10^{9}}{9{,}425\cdot10^{3}}=1{,}91\cdot10^{6}$$

We have used that $\arcsin(x)\approx x$ for small x.

4d) If we have two atoms per unit cell, we do the same – more complicated equations, twice as long unit cell in real space – half in reciprocal space.. we will get 2 solutions per k - acoustic and optical branch. See book/lecture.



4e) In the figure; dispersion relation for phonons in 3D, different directions in the reciprocal space. Two type of branches, optical and acoustical, LA and TA modes – with s atoms per primitive unit cell (in basis) we have 3s dispersion curves, 3 acoustical and 3s-3 optical – here the two transversal modes are degenerated and we have 2 atoms in the primitive unit cell (basis).. GaAs is cubic with two atoms in basis..

Problem 5 (20%) Free-electron model

5a) Assume conduction electrons are a free electron gas. No interaction with ions or lattice, or interaction between conduction electrons. Charged particles; follow the Pauli principle $E(k)=\frac{\hbar^2}{2m}k^2$. The Fermi energy is the highest occupied energy, corresponding to the Fermi energy wave vector k_F, corresponding to a sphere in 3D. The number of states inside the sphere with radius k_F is N. The volume in k-space which is occupied by one state is given so that the size of the material is $V=L^3$ in real space; which is $\left(\frac{2\pi}{L}\right)^3$. There is one allowed wave vector for each $\left(\frac{2\pi}{L}\right)^3$ this will then give:

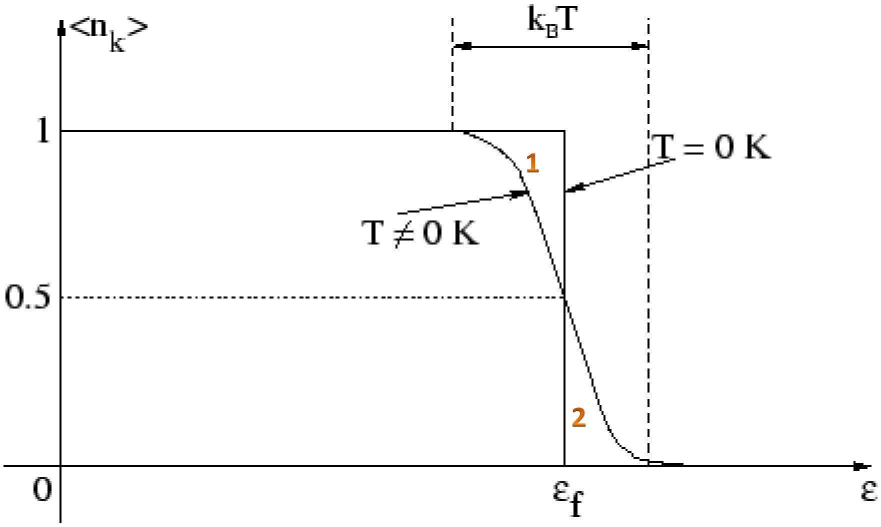
$N = 2\frac{\frac{4}{3}\pi k_F^3}{\left(\frac{2\pi}{L}\right)^3} = \frac{k_F^3 V}{3\pi^2}$ which gives $k_F = \left(\frac{3\pi^2 N}{V}\right)^{1/3}$ as should be shown. This gives the Fermi energy

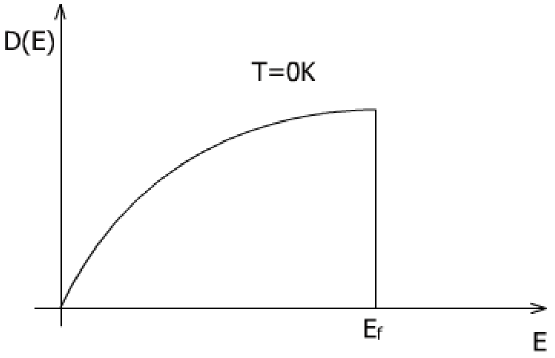
$E_F = \frac{\hbar^2}{2m}\left(\frac{3N\pi^2}{V}\right)^{2/3}$. From this expression we can now find the number of states less than E, given by N(E): $E_F = \frac{\hbar^2}{2m}\left(\frac{3N(E)\pi^2}{V}\right)^{2/3}$

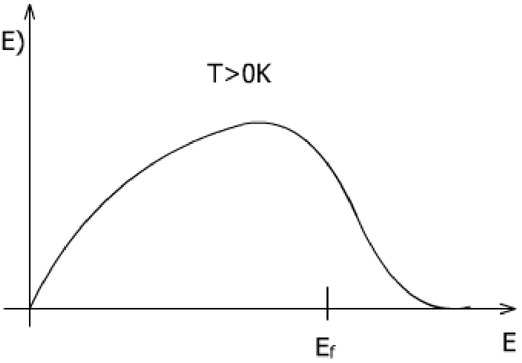
gives $N(E) = \frac{V}{3\pi^2}\left(\frac{E2m}{\hbar^2}\right)^{3/2}$ Then we can find

$$D(E) = \frac{dN}{dE} = \frac{V}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \cdot \frac{3}{2}E^{\frac{1}{2}} = \frac{V}{2\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} E^{\frac{1}{2}}$$

5b) Number of occupied states is given by $D(E)$ multiplied with the probability that the state is occupied, which is given by the Fermi-Dirac distribution $f(E) = \frac{1}{e^{(E-\mu)/k_B T} + 1}$. When T>0 we get excitation from area 1 in the figure to area 2, the extension of this areas is typically $k_B T$ as shown in the figure.







At zero temperature, the energy = divides the occupied levels from the empty ones. Therefore, (T =0) is Fermi energy. (see also fig 5 chapter 6 in Kittel or Figure 57 in Hemmer). According to these figures, only those electrons in orbitals within an energy roughly $k_B T$ are excited thermally. The energy gain for such an excited electron is of magnitude $k_B T$. The number of electrons that would be excited is estimated by $D(E_F)\cdot \Delta E \approx \frac{3N}{2E_F}\cdot k_B T$

5c) Si and GaAs are quite similar – we see inside each part a curve looking similar to parabolas.. Both have bandgap around the Fermi energy (E=0 in the curves), between 1-2 eV; both are semiconductors. We see that Si is an indirect bandgap semiconductor and that GaAs is a direct bandgap semiconductor.