

# Condensed Matter Physics, 2013

## Solutions to Exercise 6

handed out: 29. Oct. 2013

### Solution 23

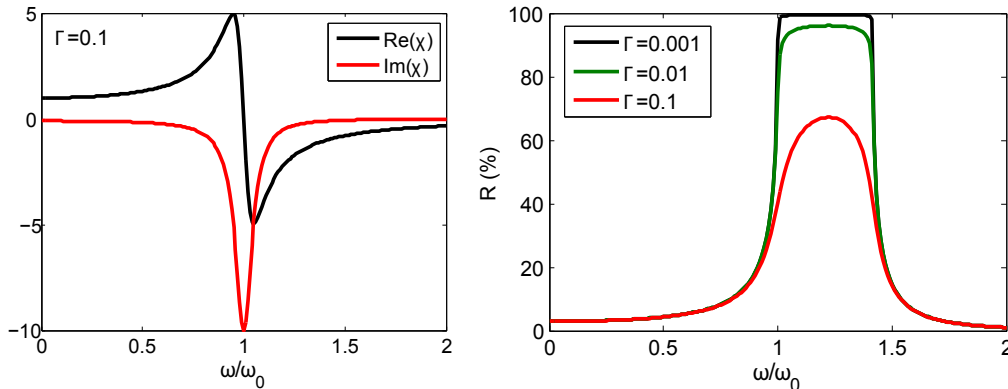
We find the expression for the susceptibility in the limit of  $k \rightarrow 0$  in the script on page 3.19:

$$\chi = \frac{\frac{2q^2N}{m\epsilon_0}}{\omega_0^2 - \omega^2 + i\Gamma}. \quad (1)$$

We calculate the reflection coefficient  $R(\omega) = \left| \frac{n_2 - n_1}{n_2 + n_1} \right|^2$ , which is Fresnel's equation for TE (transverse electric polarized) light and perpendicular incidence. We assume a crystal in vacuum or air, so that  $n_1 = 1$  and  $n_2 \equiv n$ , which simplifies the reflection coefficient to  $R(\omega) = \left| \frac{n-1}{n+1} \right|^2$ . The relation between susceptibility and the refractive index is  $n = \sqrt{1 + \chi}$ .

An analytic solution is given below, but we first plot the solution using MATLAB (any other mathematics software does the job almost as well). Here is the most rudimentary code:

```
i = sqrt(-1);
w = 0:0.01:2;
Gamma= 0.1;
chi = 1./(1-w.^2+i*Gamma);
n = sqrt(1+chi);
R = abs((n-1)/(n+1))^2;
plot(w,R*100,'r')
```



In the plots above we find the resonances in  $\chi$  for  $\Gamma = 0.1$ , similar as in the script, and the reflection coefficient  $R$  for different values of  $\Gamma$ , as indicated. For not too lossy materials (small  $\Gamma$ ) we obtain an extended frequency range in which all the radiation is reflected, i.e. for frequencies slightly larger than the resonance frequency of the phonons (oscillator). The physical meaning of this curve shape is that below the resonance ( $\omega < \omega_0$ ) the photon energy is too small to excite the phonons, and at large frequencies there is too much energy. Only slightly above  $\omega_0$  the optical phonons can be excited with large amplitudes and the oscillating dipole re-emits photons in the reflection process.

Now we also develop an analytical solution. We start with Eq. (1) and separate this expression in real and imaginary part:

$$\begin{aligned}\chi &= \frac{\frac{2q^2N}{m\epsilon_0}}{\omega_0^2 - \omega^2 + i\Gamma} \cdot \frac{(\omega_0^2 - \omega^2) - i\Gamma}{(\omega_0^2 - \omega^2) - i\Gamma} \\ &= \frac{\frac{2q^2N}{m\epsilon_0}(\omega_0^2 - \omega^2) - i\frac{2q^2N\Gamma}{m\epsilon_0}}{(\omega_0^2 - \omega^2)^2 + \Gamma^2} \\ &= \underbrace{\frac{\frac{2q^2N}{m\epsilon_0}(\omega_0^2 - \omega^2)}{(\omega_0^2 - \omega^2)^2 + \Gamma^2}}_{=\chi_1} + i \underbrace{\frac{-\frac{2q^2N\Gamma}{m\epsilon_0}}{(\omega_0^2 - \omega^2)^2 + \Gamma^2}}_{=\chi_2} := \chi_1 + i\chi_2\end{aligned}$$

to get  $n$  we need :  $n = \sqrt{1 + \chi} = \sqrt{\underbrace{1 + \chi_1}_{=x} + i \underbrace{\chi_2}_{=y}}$  and  $z = x + iy = r^{i\varphi}$

we get  $r$  from  $r = |z| = \sqrt{x^2 + y^2}$  and  $\varphi$  from  $\varphi = \arg z$

$\Rightarrow$  here  $r$  is :  $r = \sqrt{(1 + \chi_1)^2 + \chi_2^2}$  and  $\varphi = \arctan \frac{y}{x} = \arctan \frac{\chi_2}{1 + \chi_1}$

$$\begin{aligned}\Rightarrow n &= \sqrt{\sqrt{(1 + \chi_1)^2 + \chi_2^2} \cdot \exp[i \arctan(\frac{\chi_2}{1 + \chi_1})]} \\ &= \underbrace{[(1 + \chi_1)^2 + \chi_2^2]^{\frac{1}{4}}}_{=A} \cdot \underbrace{\exp[i \frac{\arctan(\frac{\chi_2}{1 + \chi_1})}{2}]}_{=B} \\ &= A \cdot \exp(iB) \\ \Rightarrow \frac{n - 1}{n + 1} &= \frac{Ae^{(iB)} - 1}{Ae^{(iB)} + 1}\end{aligned}$$

And again we have to separate this expression in real and imaginary part:

$$\begin{aligned}\frac{n - 1}{n + 1} &= \frac{(Ae^{(iB)} - 1)(Ae^{(-iB)} + 1)}{(Ae^{(iB)} + 1)(Ae^{(-iB)} + 1)} = \frac{A^2 + Ae^{iB} - Ae^{-iB} - 1}{A^2 + Ae^{iB} + Ae^{-iB} + 1} \\ &= \frac{A^2 + A(e^{iB} - e^{-iB}) - 1}{A^2 + A(e^{iB} + e^{-iB}) + 1}\end{aligned}$$

with  $e^{iB} = \cos B + i \sin B$  and  $e^{-iB} = \cos B - i \sin B$

$$\Rightarrow \frac{n - 1}{n + 1} = \frac{A^2 + i 2A \sin B - 1}{A^2 + 2A \cos B + 1} = \frac{A^2 - 1}{A^2 + 2A \cos B + 1} + i \frac{2A \sin B}{A^2 + 2A \cos B + 1}$$

$$\Rightarrow R = \left| \frac{n - 1}{n + 1} \right|^2 = \frac{(A^2 - 1)^2}{(A^2 + 2A \cos B + 1)^2} + \frac{(2A \sin B)^2}{(A^2 + 2A \cos B + 1)^2}$$

$$\Rightarrow R = \frac{(A^2 - 1)^2 + 4A^2 \sin^2 B}{(A^2 + 2A \cos B + 1)^2}$$

## Solution 24

The Eigenvalues of a 1 dimensional harmonic oscillator are (see skript):

$$E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

$$\Rightarrow \text{ for the 2 dimensional case: } E_n = E_{n_x} + E_{n_y} = (n_x + n_y + 1)\hbar\omega$$

This means, the spectra of a 2 dimensional oscillator contains discrete energy levels separated by  $\hbar\omega$ !

The quantum numbers for the first 5 eigenstates and their degeneracy are:

- $n = 0 \rightarrow n_x = 0, n_y = 0 \rightarrow (0, 0)$  no degeneracy
- $n = 1 (0,1) (1,0)$  2-fold degenerate
- $n = 2 (2,0) (0,2) (1,1)$  3-fold degenerate
- $n = 3 (3,0) (0,3) (1,2) (2,1)$  4-fold degenerate
- $n = 4 (0,4) (4,0) (2,2) (1,3) (3,1)$  5-fold degenerate
- $n = 5 (0,5) (5,0) (3,2) (2,3) (4,1) (1,4)$  6-fold degenerate

## Solution 25

We look at  $N$  atoms on a chain (or  $N$  unit cells in 1D) at a nearest neighbor distance  $a$  (lattice constant). In 1D each atom has only one spatial degree of freedom, so that we expect  $N$  eigenmodes and thus  $N$  different  $k$ -values that can be folded back into the first Brillouin zone. Since the chain length is  $L = Na$ , the spacing in  $k$ -space is  $\Delta k = \frac{2\pi}{L}$ . Intuitively, by the definition of the Debye wave vector  $k_D$  (or the Debye frequency  $\omega_D$ ), all states from  $-k_D$  to  $+k_D$  are occupied, so that

$$N = \frac{2k_D}{\Delta k} = \frac{k_D L}{\pi}$$

and

$$k_D = \frac{N\pi}{L}$$

This can also be obtained more formally by noting that the density of states in the  $k$ -space is one state per  $\frac{2\pi}{L}$ , i.e.  $\rho_k = \frac{L}{2\pi}$ , and

$$N = \int_{-k_D}^{k_D} \rho_k dk = 2 \int_0^{k_D} \rho_k dk = 2 \int_0^{k_D} \frac{L}{2\pi} dk = k_D \cdot \frac{L}{\pi}.$$

We obtain the Debye frequency  $\omega_D$  from the dispersion relation  $\omega = ck$ :

$$\omega_D = ck_D = \frac{\pi c N}{L}$$

The density of states in energy is then given by

$$DoS = \frac{1}{L} \frac{dN}{d\omega_D} = \frac{1}{\pi c}.$$

## Solution 26

A single harmonic oscillator in three dimensions consists of three independent one-dimensional harmonic oscillators with the energy eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right), \quad n \in \mathbb{N}_0$$

The specific heat is defined as:

$$c_V = \left(\frac{\partial U}{\partial T}\right)_{V=\text{const.}}$$

with  $U$  the internal energy of the system.

To calculate  $U$  we need the relative occupation probabilities of an energy level  $n$  and the ground state 0 is given by the Boltzmann distribution,  $\frac{p_n}{p_0} = e^{-\frac{E_n - E_0}{k_B T}}$ . First, we look at the internal energy of a single one-dimensional oscillator,  $U_{1D}$ , which is given by the expectation value of the energy, measured with respect to the ground state energy  $E_0$  (see also statistical mechanics, the denominator essentially normalizes the probabilities):

$$U_{1D} = \frac{\sum_{n=0}^{\infty} p_n \cdot (E_n - E_0)}{\sum_{n=0}^{\infty} p_n} = \frac{\sum_{n=0}^{\infty} p_0 e^{-\frac{n \cdot \hbar\omega}{k_B T}} n \cdot \hbar\omega}{\sum_{n=0}^{\infty} p_0 e^{-\frac{n \cdot \hbar\omega}{k_B T}}} = \frac{\hbar\omega \sum_{n=0}^{\infty} n \left[ e^{-\frac{\hbar\omega}{k_B T}} \right]^n}{\sum_{n=0}^{\infty} \left[ e^{-\frac{\hbar\omega}{k_B T}} \right]^n}$$

The numerator and denominator can be evaluated using (e.g. from Wikipedia):

$$\sum_{n=0}^{\infty} k z^k = \frac{z}{(1-z)^2} \quad \text{and} \quad \sum_{n=0}^{\infty} z^n = \frac{1}{1-z} \quad (\text{geometrical series})$$

Inserting  $z = e^{-\frac{\hbar\omega}{k_B T}}$  we find

$$U_{1D} = \hbar\omega \frac{z}{1-z} = \hbar\omega \frac{1}{z^{-1} - 1} = \hbar\omega \frac{1}{e^{\frac{\hbar\omega}{k_B T}} - 1}$$

The total internal energy of a three-dimensional oscillator is the sum of three identical individual oscillators:  $U_{3D} = 3U_{1D} = \frac{3\hbar\omega}{e^{\frac{\hbar\omega}{k_B T}} - 1}$ . From this expression follows the specific heat at constant volume (this means that the geometric boundary conditions of the states and thus the states do not change):

$$c_V = \left(\frac{\partial U_{3D}}{\partial T}\right)_V = \frac{3(\hbar\omega)^2}{k_B T^2} \frac{e^{\frac{\hbar\omega}{k_B T}}}{\left[ e^{\frac{\hbar\omega}{k_B T}} - 1 \right]^2}$$

For  $k_B T \gg \hbar\omega$ , i.e. in the high-temperature limit, the exponential function can be developed into a Taylor series:  $e^{\frac{\hbar\omega}{k_B T}} \approx 1 + \frac{\hbar\omega}{k_B T}$  (the numerator goes to 1) and one recovers the classical result

$$\lim_{T \rightarrow \infty} c_V = 3k_B$$

For  $k_B T \ll \hbar\omega$  the exponential function grows much larger than 1, which then can be neglected in the denominator:

$$\lim_{T \rightarrow 0} c_V = \lim_{T \rightarrow 0} \frac{3\hbar\omega}{k_B T^2} \frac{1}{e^{\frac{\hbar\omega}{k_B T}}} = 0$$

The last step follows from the fact that the exponential function diverges faster than any polynomial.