

Modul 2

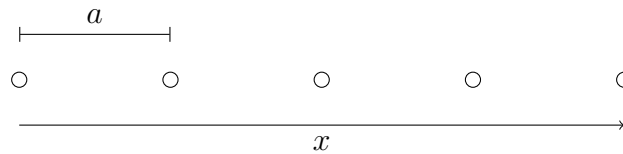
Kandidatnummer: 27

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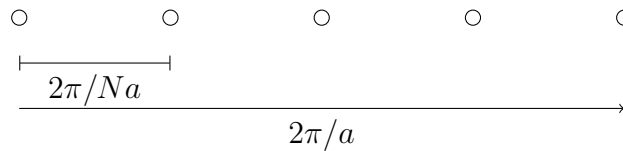
a

Assuming i have a one dimentional lattice with atoms in the real space:



Figur 1: Basis to a one dimentional lattice in the real space.

This in the reciprocal space becomes:



Figur 2: Basis to a one dimentional lattice in reciprocal space.

Any given wave propagating in a solid will have a motion formed by the boundary conditions. In the case of a one dimensional chain of N atoms the wave will have the same boundary condition for both ends of the chain. Thus the chain can be viewed as connected in both ends creating a looped chain. By doing this particles s and $s + N$ has the same displacement, $u_s = u_{s+N}$.

$$ue^{i(ksa-\omega t)} = ue^{i(k(s+N)a-\omega t)} \implies 1 = e^{ikNa}$$
$$1 = \cos(kNa) + i \sin(kNa)$$

Since sinus and cosine are functions with repeating values every 2π one can derive the conditions for the allowed k values:

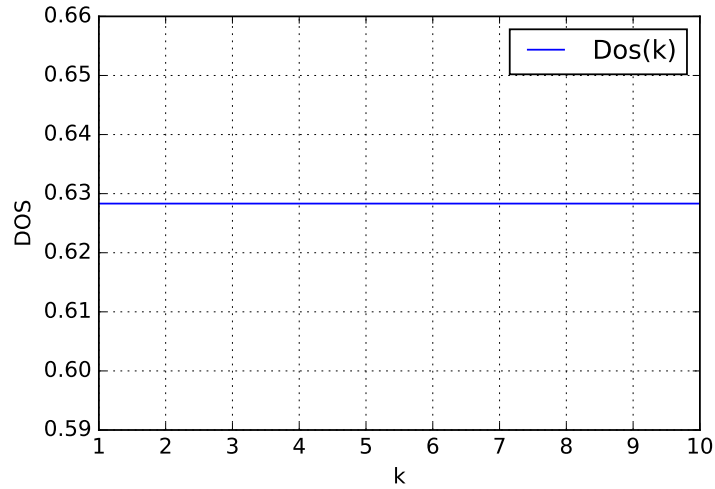
$$kNa = 2\pi n \implies k = \frac{2\pi n}{Na}$$

Here n is an integer number.

The distance between allowed k values is then $\frac{2\pi}{Na}$. Note that the density of k is independent on k itself. So it has a uniform density in k -space. From this DOS becomes:

$$\frac{\text{nr modes}}{\text{interval}} = \frac{1}{\Delta k} = 2 \cdot \frac{\overbrace{Na}^{=L}}{2\pi} = \frac{L}{\pi}$$

Here the DOS in k -space is multiplied by two because of the symmetry around 0 for the first 1brillouin zone. This is the same assumption that the book does on page 110 to calculate DOS in one dimension. Note that this is not an assumption made when deriving this in class.



Figur 3: Figure showing the density of states in k -space. See appendix for code.

b

$$\begin{aligned}
D(k) dk &= D(\omega) d\omega \\
D(\omega) d\omega &= D(k) \frac{dk}{d\omega} d\omega \\
\text{group velocity: } v_g &= \frac{d\omega}{dk} \implies \frac{1}{v_g} = \frac{dk}{d\omega} \\
D(\omega) d\omega &= D(k) \frac{1}{v_g} d\omega \\
D(\omega) d\omega &= \frac{L}{2\pi} \frac{1}{v_g} d\omega
\end{aligned}$$

Inserting for values found in a and in task 1:

$$\begin{aligned}
\omega &= \omega_0 \sin\left(\frac{ka}{2}\right) \\
v_g &= \frac{d}{dk} \omega_0 \sin\left(\frac{ka}{2}\right) = \omega_0 \frac{a}{2} \cos\left(\frac{ka}{2}\right)
\end{aligned}$$

Before inserting this into the expression all dependency of k must be removed. An expression of k only dependent on ω can be obtained:

$$\begin{aligned}
\omega &= \omega_0 \sin\left(\frac{ka}{2}\right) \\
\sin\left(\frac{ka}{2}\right) &= \frac{\omega}{\omega_0} \\
k &= \frac{2}{a} \sin^{-1}\left(\frac{\omega}{\omega_0}\right) \\
v_g &= \omega_0 \frac{a}{2} \cos\left(\frac{ka}{2}\right) = \omega_0 \frac{a}{2} \cos\left(\frac{2}{a} \sin^{-1}\left(\frac{\omega}{\omega_0}\right) \cdot \frac{a}{2}\right)
\end{aligned}$$

Using geometrical identities this can also be represented as:

$$v_g = \frac{\omega_0 a}{2} \sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2}$$

This gives the density of states:

$$D(\omega) d\omega = \frac{L}{a\omega_0\pi\sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2}} d\omega$$

$$D(\omega) d\omega = \frac{N}{\omega_0\pi\sqrt{1 - \left(\frac{\omega}{\omega_0}\right)^2}} d\omega$$

$$D(\omega) d\omega = \frac{N}{\pi\sqrt{\omega_0^2 - \omega^2}} d\omega$$

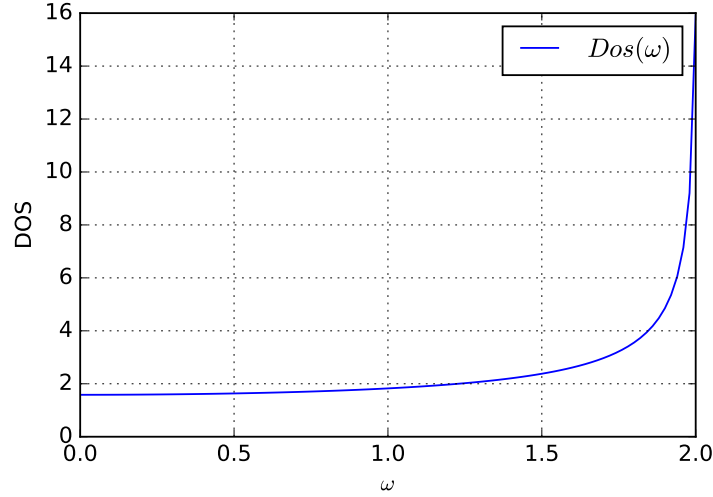


Figure 4: $D(\omega)$ plotted from 0 to 2. Arbitrary values for ω_0 . See appendix for code.

In the end point of the plot the function goes to infinity fast. This is expected from the dispersion relation because at the end point of this plot the group velocity goes to zero.

C

From plot 3 there is a constant value for all k 's. Comparing this to plot 4 where a significantly more complicated trend is shown. An obvious reason to use the reciprocal space is because it is easier to work with. It may be harder to visualize the reciprocal space, but when one is trying to work with density

of states the added complexity becomes greater in the real space than in the reciprocal space. In addition to this is the tight relation of the reciprocal space to light waves and other waves. When working with multiple waves it is easier to work with them in the reciprocal space.

3

Debye model

The Debye model assumes that the speed of sound is constant for each polarization type, as it is for a classical elastic continuum $\omega = vk$. It treats the waves traveling in the crystal as phonons in a box. The phonon in a box approximation is a good approximation for low temperature phonons but it is not a good model for mid range temperature phonons. This is one of the limitations of this model. The Debye model will at higher temperatures follow the Dulong-Petit model but is not a sufficient model in midrange due to the simplification of the phonon nature. For low temperatures the derivative $\frac{d\omega}{dk}$ of the dispersion relation can be approximated to a constant value for v . If this is taken over a longer range of k this is not the case.

For low temperatures is Debye model a good approximation and will give the T^3 law by letting ω_D go to infinity.

Einstein model

The Einstein model assumes two things. That each atom moves as an independent three dimensional harmonic oscillator, and that all atoms oscillates with the same frequency. This contrasts the Debye model whereas this is not the case, thus the dispersion relation will be more correct for mid range temperatures. In the Einstein model will at low temperatures approach zero exponentially ($e^{-\hbar\omega/\tau}$). This is not the case, here the T^3 model better predicts the actual dependency as accounted for by Debye.

As the Debye model, the Einstein model correctly predicts the high temperature trend.

Dulong-Petit model

The Dulong-Petit model assumes that the atoms has classical oscillators with continuous energy. This model, as stated above correctly predicts the heat capacity at high temperatures. This model is a good approximation at higher

temperatures because higher temperatures have enough energy to assume classical oscillators with continuous energy . At lower temperatures, where this assumption does not hold and one has to take into account the quantized energy states this is not a good approximation.

6

The thermal conductivity coefficient κ is given by $\kappa = \frac{1}{3}C_V\Lambda v$ (v is approximately constant). Here the C_V is the heat capacity. From earlier tasks the heat capacity at low temperatures are given by the Debye model giving it a T^3 dependency. At high temperatures the heat capacity is given by the Dulong-Petit model which has is independent on the temperature giving it a constant dependency, $3R$. Due to $U = 3k_bT \rightarrow C_v = \frac{d}{dT}3k_bT = 3k_b$. Λ is the mean free path proportional to $\Lambda \propto \frac{1}{n_{ph}} = e^{\hbar\omega/kT} - 1$ which at low temperatures equals the length of the crystal. This is due to that $n_{ph} \rightarrow 0$ so $\Lambda \rightarrow \infty$ but since we are looking at a finite crystal goes to D . A more intuitive way of explaining this result is to think of the interactions the phonone has with other phonons at low temperature. At low temperature there are very few phonons thus resulting in a small probability of interaction. If there is a small probability of interaction the mean free path become very large, only limited by the size of the crystal. At high temperatures the exponent of $e^{\hbar\omega/kT} - 1$ becomes small due to large T . The expression can now be transformed into an infinite series, $e^x = 1 + x + x^2\dots$, all factors larger than x becomes very small(assuming zero). Replacing the series gives $\Lambda \simeq 1 + x - 1 = x = \hbar\omega/kT \propto 1/T$.

	C_v	Λ	κ
low T	$\propto T^3$	$\Lambda \rightarrow D$	$\propto T^3$
high T	$3k_b$	$\propto 1/T$	$\propto 1/T$

This table is accurate for low temperatures, but not for high temperatures. This is because at high temperatures the umklapp process must be taken into account. The old model accounted for exited phonons only, a more correct model takes into account high energy phonons. For high temperature dependency one can ignore the low energy phonon effects due to their much longer mean free path. Further i only take into account the phonons that takes part in the umklapp process.

When two phonons collide they can combine and create a phonon with energy equal to the sum of the colliding phonons due to a elastic collision. If the resulting phonon is within the first brillouin zone all is good. If on the other hand it results in a vector going out of the first brillouin zone the resulting vector is translated back into the first brillouin zone. This results in a vector pointing in the other direction of the colliding phonon sum. This is the process that must be taken into account when looking at high temperature trends. For the following trend only the umklapp effect is taken into consideration. The umklapp effect has incoming phonons of energy $\vec{K}_1 + \vec{K}_2 > \frac{1}{2}k_b\theta_D$. This is due to the assumption made that the resulting vector has to be outside the first brillouin zone. Further by ignoring more complex statistics and only viewing the boltzman factor the probability of the phonons having enough energy is in the order of $e^{\theta_D/2T}$

	C_v	Λ	κ
low T	$\propto T^3$	$\Lambda \rightarrow D$	$\propto T^3$
high T	$3k_b$	$\propto e^{\theta_D/2T}$	$\propto e^{\theta_D/2T}$

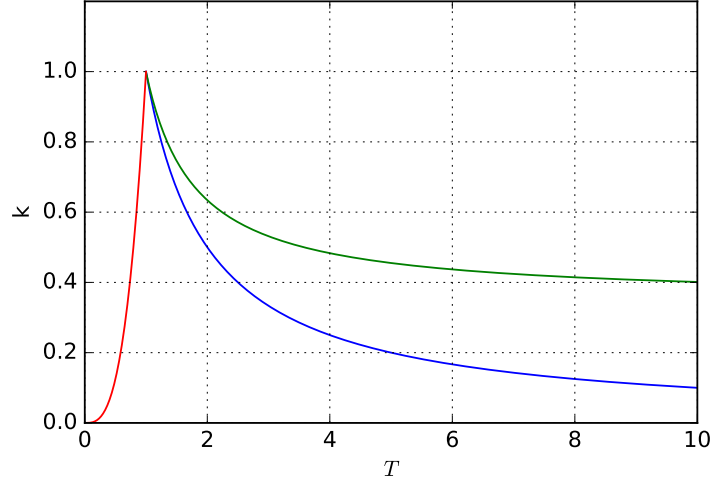


Figure 5: The temperature dependence of κ . Plot shows low temperature proportionality and the two different models for high temperature proportionality. See appendix for code.

7

a

The formula for finding the heat capacity is given by:

$$C_v = \frac{\partial U}{\partial T} = \frac{\partial}{\partial T} \int \underbrace{D(\omega)}_{\text{Density of states}} \underbrace{\langle n(\omega) \rangle}_{\text{Planck distribution}} \hbar \omega \, d\omega$$

For the density of states in one dimension the results from **2a** can be used.

$$D_{os}(k) = \frac{L}{\pi}$$

Following the same procedure as the calculations in **2b** this can be rewritten as:

$$D(\omega) \, d\omega = \frac{L}{\pi} \frac{d\omega}{\frac{d\omega}{dk}}$$

From this the Debye assumption explained in **3** can be used. Debye assumed in his model that $\omega = vk$. This gives:

$$D(\omega) \, d\omega = \frac{L}{\pi} \frac{d\omega}{v}$$

This result differs somewhat from what was done in class. In the derivation in class v was not included. If this isn't included the unit of heat capacity is wrong. Inserting this into the expression:

$$\begin{aligned} C_v &= \frac{\partial}{\partial T} \int_0^{\omega_D} \langle n(\omega) \rangle \hbar \omega \frac{L}{\pi} \frac{d\omega}{v} \\ C_v &= \frac{\partial}{\partial T} \frac{L}{v\pi} \underbrace{\int_0^{\omega_D} \langle n(\omega) \rangle \hbar \omega \, d\omega}_{\text{intra}} \\ &\quad \int_0^{\omega_D} \frac{1}{e^{\hbar\omega/k_b T} - 1} \hbar \omega \, d\omega \end{aligned}$$

Substituting $x = \hbar\omega/k_b T$ so $\omega = xk_b T/\hbar$. The upper limit can now also be changed. In the Debye model T is assumed to be small. Plugging this in

the expression for x this becomes a limit becomes a large number. To make the integral easier to work with this is approximated to ∞ :

$$\frac{dx}{d\omega} = \frac{\hbar}{k_b T} \implies dx \frac{k_b T}{\hbar} = d\omega$$

$$\frac{(k_b T)^2}{\hbar} \int_0^\infty \frac{x}{e^x - 1} dx$$

The fraction inside the integral is not easy to solve as it is, but it can be rewritten as a series:

$$\frac{(k_b T)^2}{\hbar} \int_0^\infty \frac{x e^{-x}}{1 - e^{-x}} dx \stackrel{m=e^{-x}}{=} \frac{(k_b T)^2}{\hbar} \int_0^\infty x \sum_{n=1}^\infty m^n dx$$

The sum can go from zero but this will only be zero because of the x in front of the sum. Therefore i start the series at $n = 1$.

$$\frac{(k_b T)^2}{\hbar} \sum_{n=1}^\infty \frac{d}{dn} \int_0^\infty e^{-nx} dx = \frac{(k_b T)^2}{\hbar} \sum_{n=1}^\infty \frac{d}{dn} \frac{1}{n}$$

$$\frac{(k_b T)^2}{\hbar} \sum_{n=1}^\infty \frac{1}{n^2} = \frac{(k_b T)^2}{\hbar} \frac{\pi^2}{6}$$

This can now be inserted into the original expression:

$$C_v = \frac{\partial}{\partial T} \frac{L}{v\pi} \frac{(k_b T)^2}{\hbar} \frac{\pi^2}{6}$$

$$C_v = \frac{\pi L k_b^2 T}{3\hbar v}$$

Note that in the lecture the speed of sound was not included. This gives the wrong unit.

b

For a nanowire the calculations made above can be applied. For a nanowire the heat capacity is proportional to both the length L and the temperature T . So an increase in temperature will result in a equally large increase in heat capacity. This is also the case for the length of the nanowire. A longer nanowire will result in a equally large increase in heat capacity. The heat conductivity is closely related tot he heat capacity. If the amount of energy a nanowire can hold per increase in temperature is low the overall heat conductivity when the wire interacts with the surroundings is small.

Appendix

2a

```
from numpy import *
from matplotlib.pyplot import *

k= linspace(1,10)
a=1
N=10
dos_ = ones(len(k))*2*pi/(N*a)

def dos(k):
    return 2*pi/(N*a)

figure(figsize=(6,4))
plot(k,dos_)
legend(["Dos(k)"])
xlabel ("k")
ylabel ("DOS")
grid("on")
savefig("1a.pdf",bbox_inches="tight")
```

2b

```
from numpy import *
from matplotlib.pyplot import *

omega = linspace(0,2,101)
a=1
N=10
omega0=2
print omega

def dos(omega):
    return (N/(pi*omega0))*(1/(sqrt(1.01-(omega/
        omega0)**2)))

figure(figsize=(6,4))
plot(omega,dos(omega))
```

```

legend(["$Dos(\omega)$"])
xlabel ("$\omega$")
ylabel ("DOS")
grid("on")
savefig("1b.pdf",bbox_inches="tight")

```

6

```

from numpy import *
from matplotlib.pyplot import *

T_low = linspace(0.0001,1,1000)
T_high = linspace(1,10,1000)
T = linspace(0.5,10,2000)
theta = 1

def kappa_low(T_low):
    return T_low**3

def kappa_umklapp(T):
    return e**(theta/(2*T))-0.65

def kappa(T):
    return 1/T

figure(figsize=(6,4))
plot(T_high,kappa(T_high),T_high,kappa_umklapp(
    T_high),T_low,kappa_low(T_low))
#legend(["$\kappa$ low T", " "," "])
xlabel ("$T$")
ylabel ("k")
ylim([0,1.2])
grid("on")
savefig("6a.pdf",bbox_inches="tight")

```