FYS3410 - Vår 2016 (Kondenserte fasers fysikk)

http://www.uio.no/studier/emner/matnat/fys/FYS3410/v16/index.html

Pensum: Introduction to Solid State Physics
by Charles Kittel (Chapters 1-9 and 17, 18, 20)

Andrej Kuznetsov

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2016 FYS3410 Lectures (based on C.Kittel's Introduction to SSP, Chapters 1-9, 17,18,20)

Module I – Periodic Structures and Defects (Chapters 1-3, 20)

M18/1: 9-12 am	**Introduction. Crystal bonding. Periodicity and lattices, Brag diffraction and Laue condition, reciprocal space**	**3h**
W20/1 cancelled		
M25/1: 9-12 am	**Ewald construction, interpretation of a diffraction experiment , Brag planes, and Brillouin zones**	**3h**
W27/1 cancelled		
M01/2: 10-12 am	**Elastic strain and structural defects in crystals**	**2h**
W03/2: 9-10 am	**Atomic diffusion in solids**	**1h**
M08/2: 10-12 am	**Summary of Module I**	**2h**

Module II – Phonons (Chapters 4 and 5)

W10/2: 9-10 am	**Vibrations in monoatomic and diatomic chains of atoms**	**1h**
M15/2: 10-12am	**Periodic boundary conditions, phonons and density of states (DOS)**	**2h**
W17/2: 9-10 am	**Planck distribution**	**1h**
M22/2 : 10-12am	**Lattice heat capacity: Dulong-Petit, Einstein, and Debye models**	**2h**
W24/2 cancelled		
M29/2: 9-12am	**Comparison of different models for lattice heat capacity, thermal conductivity with phonons**	**3h**
W02/3: 9-10 am	**Thermal expansion**	**1h**
M07/3: 10-12am	**Summary of Module II.**	**2h**

Module III – Electrons (Chapters 6, 7, 18 - pp.528-530, and Appendix D)

W09/3: 9-10 am	**Free electron gas (FEG) versus free electron Fermi gas (FEFG)**	**1h**
M14/3: 10-12am	**DOS of FEFG in 3D. Effect of temperature – Fermi-Dirac distribution**	**2h**
W16/3: 9-10 am	**Heat capacity of FEFG in 3D**	**1h**
W30/3: 9-10 am	**DOS in 2D - quantum wells**	**1h**
M04/4: 10-12am	**DOS in 1D and 0D, i.e. quantum wires and quantum dots; transport properties of electrons**	**2h**
W06/4: 9-10 am	**Origin of the energy band gap**	
M11/4: 10-12am	**Nearly free electron model. Kronig-Penney model. Empty lattice approximation.**	**2h**
W13/4: 9-10 am	**Number of orbitals in a band**	**1h**
M18/4: 10-12am	**Summary of Module III.**	**2h**

Module IV – Semiconductors and interfaces (Chapters 8, 9-pp 223-231, 17)

W20/4: 9-10 am	**Metals versus semiconductors. Surfaces and interfaces.**	**1h**
M25/4: 9-12 am	**Effective mass method.**	**3h**
W27/4: 9-10 am	**Intrinsic carrier generation – elctrons and holes.**	**1h**
M02/5: 9-12 am	**Localized levels for hydrogen-like impurities – donors and acceptors. Doping.**	**3h**
W04/5: 9-10 am	**Carrier statistics in semiconductors**	**1h**
M09/5: 9-12 am	**p-n junctions**	**3h**
W11/5: 9-10 am	**Optoelectronic semiconductor properties and devices**	**1h**
M18/5: 9-12 am	**Device demonstrations. Summary of Module IV**	**3h**

Repetition

M23/5 9-12 am	**The course in a nutshell**	**2h**
W25/5, M30/5 and W1/6 cancelled		

Exam during week 22 (tentatively 30-31/5)

Lecture 9: Thermal conductivity

- **We understood phonon DOS and occupancy as a function of temperature, but what about transport properties?**

- **Phenomenological description of thermal conductivity**

- **Temperature dependence of thermal conductivity in terms of phonon properties**

- **Phonon collisions: N and U processes**

- **Comparison of temperature dependence of κ in crystalline and amorphous solids**

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Understanding phonons as «harmonic waves» can not explain thermal restance since harmonic wafes perfectly move one through another

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Phenomenological description of thermal conductivity

When thermal energy propagates through a solid, it is carried by lattice waves or phonons. If the atomic potential energy function is harmonic, lattice waves obey the superposition principle; that is, they can pass through each other without affecting each other. In such a case, propagating lattice waves would never decay, and thermal energy would be carried with no resistance (infinite conductivity!). So…thermal resistance has its origins in an anharmonic potential energy.

low T  high T

Classical definition of thermal conductivity

$$\kappa = \frac{1}{3} C_V v \Lambda$$

Thermal energy flux (J/m^{2}s)

$$J = -\kappa \frac{dT}{dx}$$

C_V heat capacity per unit volume

v wave velocity

Λ mean free path of scattering (would be ∞ if no anharmonicity)

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Temperature dependence of thermal conductivity in terms of phonon prperties

Mechanisms to affect the mean free pass (Λ) of phonons in periodic crystals:

1. Interaction with impurities, defects, and/or isotopes
2. Collision with sample boundaries (surfaces)

} deviation from translation symmetry

3. Collision with other phonons

} deviation from harmonic behavior

To understand the experimental dependence $\kappa(T)$, consider limiting values of C_V and Λ (since v does not vary much with T).

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$$C_V \begin{cases} \propto T^3 & low\,T \\ 3R & high\,T \end{cases}$$

$$\Lambda \propto \frac{1}{n_{ph}} = e^{\hbar\omega/kT} - 1 \begin{cases} \rightarrow \infty & low\,T \\ \dfrac{\hbar\omega}{kT} & high\,T \end{cases}$$

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[1)] **Please note, that the temperature dependence of T^{-1} for Λ at the high temperature limit results from considering n_{ph} , which is the total phonon occupancy, from 0 to ω_D. However, already intuitively, we may anticipate that low energy phonons, i.e. those with low *k*-numbers in the vicinity of the center of the 1st BZ may have quite different appearence conparing with those having bigger *k*-numbers close to the edges of the 1st BZ.**

Temperature dependence of thermal conductivity in terms of phonon properties

Thus, considering defect free, isotopically clean sample having limited size D

	C_V	Λ	κ
low T	$\propto T^3$	$n_{ph} \rightarrow 0$, so $\Lambda \rightarrow \infty$, but then $\Lambda \rightarrow D$ (size)	$\propto T^3$
high T	3R	$\propto 1/T$	$\propto 1/T$

How well does this match experimental results?

Temperature dependence of thermal conductivity in terms of phonon prperties

Experimental κ(T)

T^3 estimation for κ the low temperature limit is fine!

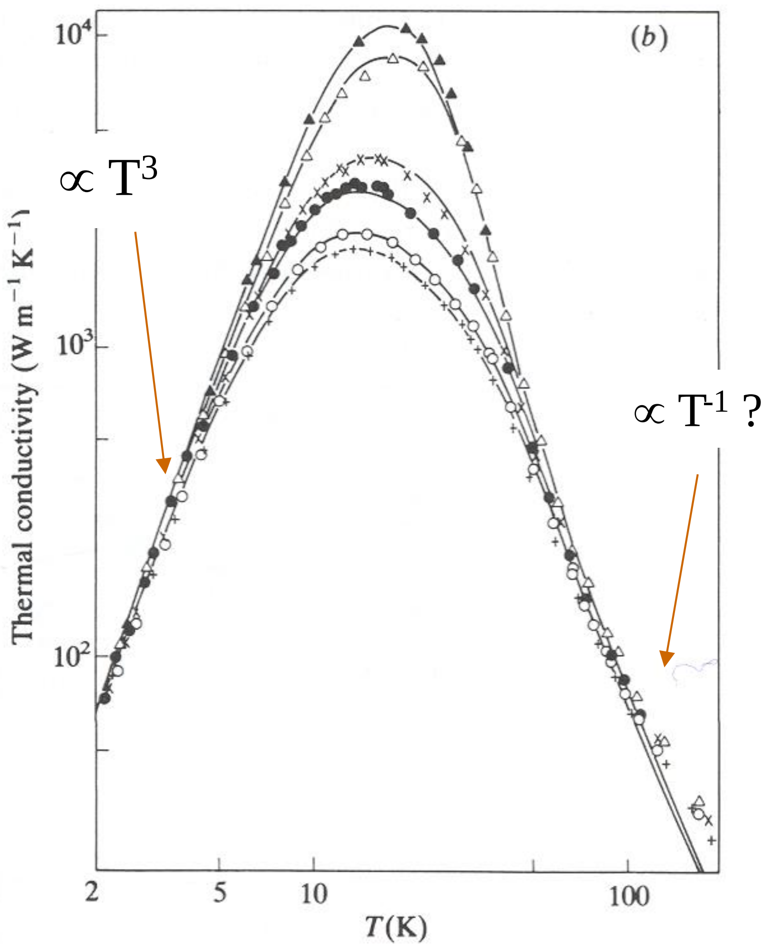
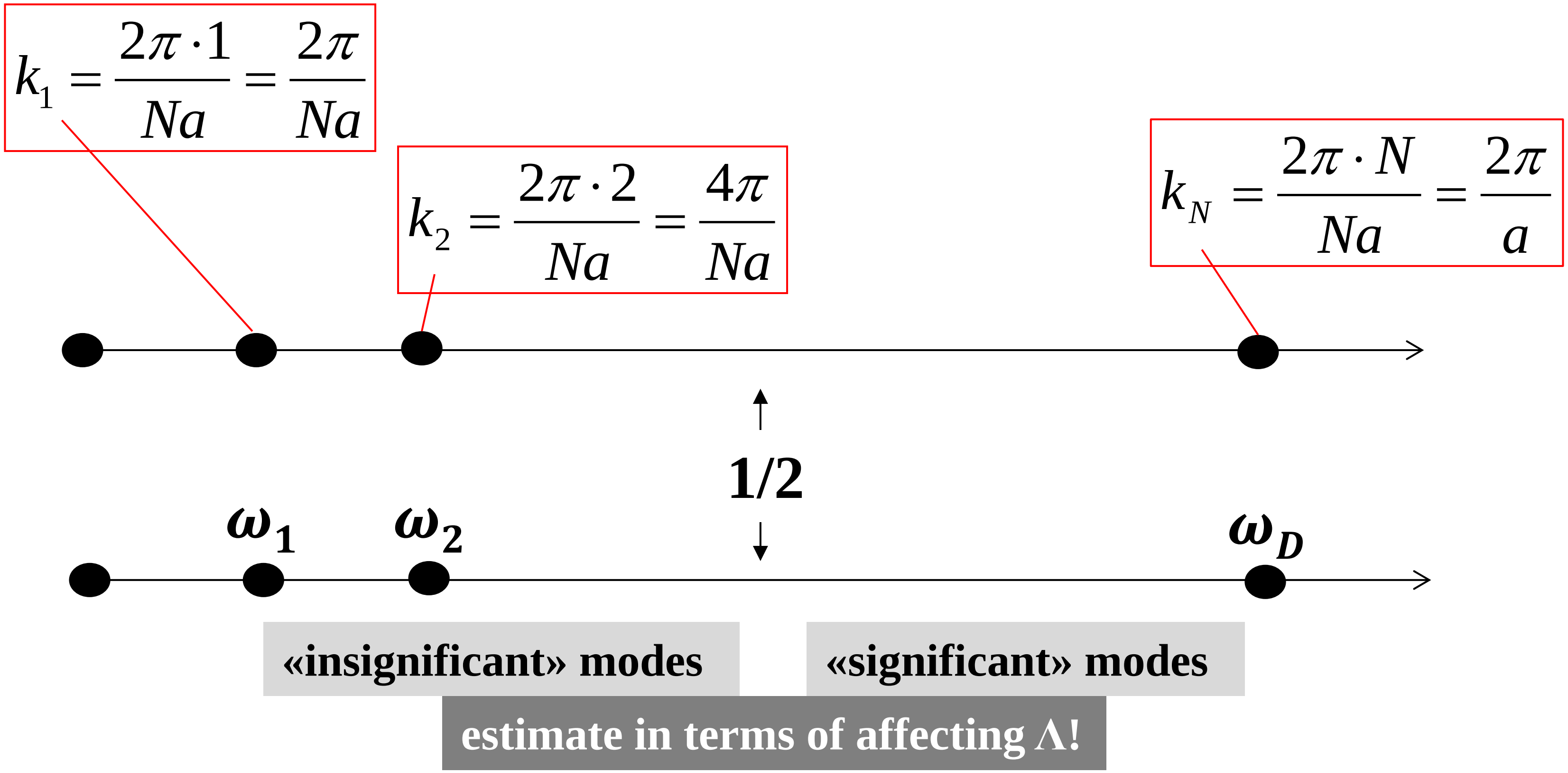


Figure 5.27 (a) The principal form for the variation of thermal conductivity. (b) Experimental data for LiF crystals containing different amounts of the isotope ^{6}Li: ▲, 0.02% ^{6}Li; △, 0.01%; ×, 4.6%; ●, 9.4%; ○, 25.4%; +, 50.1%. (After Berman and Brock 1965.)

However, T^{-1} estimation for κ in the high temperature limit has a problem. Indeed, κ drops much faster – see the data – and the origin of this disagreement is because – when estimating Λ – we accounted for all excited phonons, while a more correct approximation would be to consider "high" energetic phonons only. But what is "high" in this context?

Better estimation for Λ in high temperature limit



The fact that «low energetic phonons» having *k*-values << π/a do not participate in the energy transfer, can be understood by considering so called N- and U-phonon collisions readily visualized in the reciprocal space. Anyhow, we account for modes having energy $E_{1/2} = (1/2)\hbar\omega_D$ or higher. Using the definition of $\theta_D = \hbar\omega_D/k_B$, $E_{1/2}$ can be rewritten as $k_B\theta_D/2$. Ignoring more complex statistics, but using Boltzman factor only, the propability of $E_{1/2}$ would of the order of $\exp(- k_B\,\theta_D/2\,k_B\,T)$ or $\exp(-\theta_D/2T)$, resulting in $\Lambda \propto \exp(\theta_D/2T)$.

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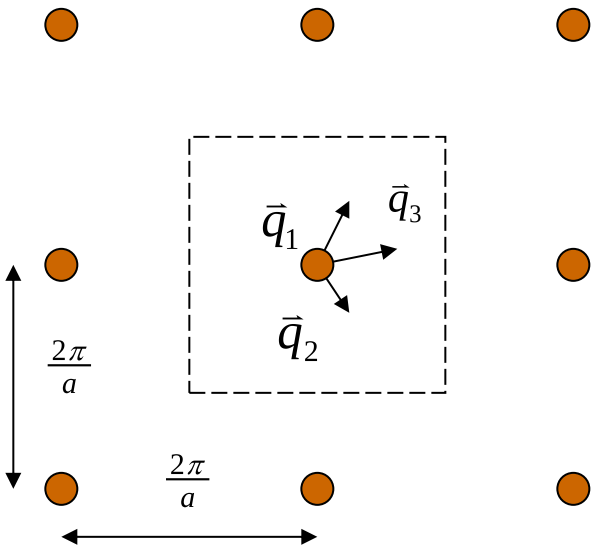
Phonon collisions: N and U processes

How exactly do phonon collisions limit the flow of heat?

2-D lattice → 1st BZ in k-space:



$$\hbar\vec{q}_1 + \hbar\vec{q}_2 = \hbar\vec{q}_3$$

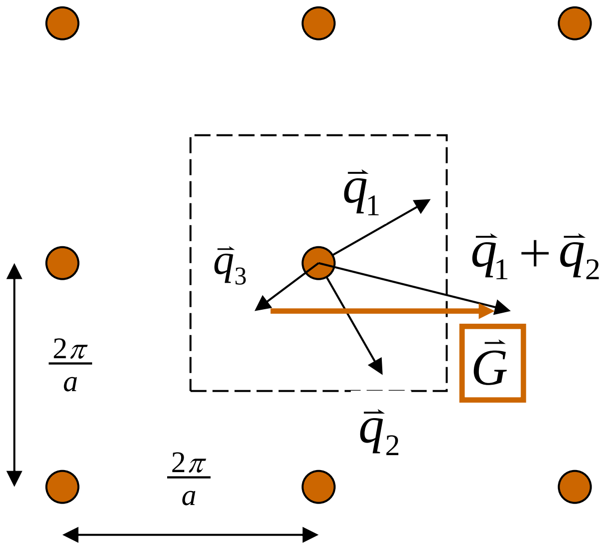
No resistance to heat flow
(N process; phonon momentum conserved)

→ Predominates at low T << θ_D since ω and q will be small

Phonon collisions: N and U processes

What if the phonon wavevectors are a bit larger?

2-D lattice → 1st BZ in k-space:



$$\hbar\vec{q}_1 + \hbar\vec{q}_2 = \hbar\vec{q}_3 + \hbar\vec{G}$$

Two phonons combine to give a net phonon with an opposite momentum! This causes resistance to heat flow.
(U process; phonon momentum "lost" in units of ħG.)

→ More likely at high T >> θ_D since ω and q will be larger

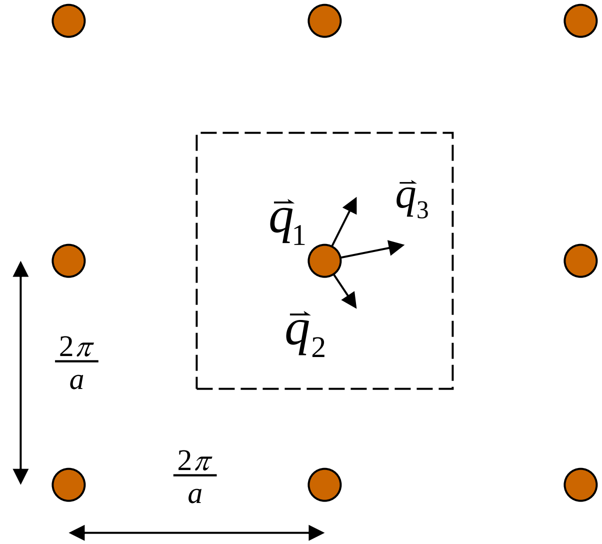
Umklapp = "flipping over" of wavevector!

Explanation for κ ∝ exp(θ_D/2T) at high temperature limit

The temperature dependence of *T^{-1}* for *Λ* results from considering the total phonon occupancy, from *0* to *ω_D*. However, interactions of low energy phonons, i.e. those with low *k*-numbers in the vicinity of the center the 1st BZ, are not changing energy. These are so called N-processes having little impact on Λ.

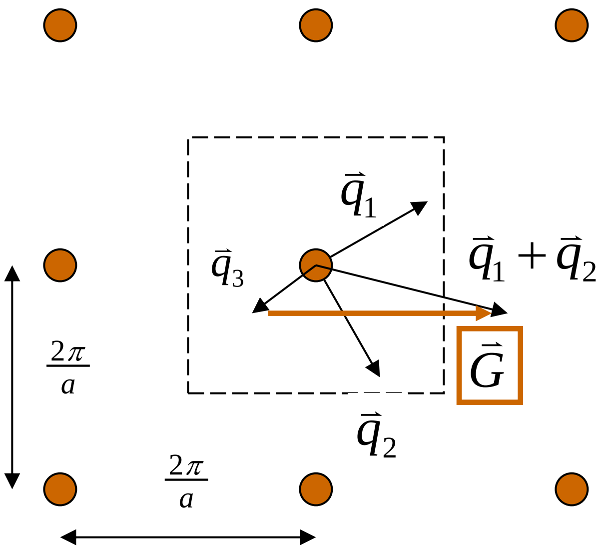
$$\kappa = \frac{1}{3} C_V v \Lambda$$

$$\Lambda \propto \frac{1}{n_{ph}} = e^{\hbar\omega/kT} - 1 \quad \begin{cases} \to \infty & low\, T \\ T^{-1} & high\, T \end{cases}$$



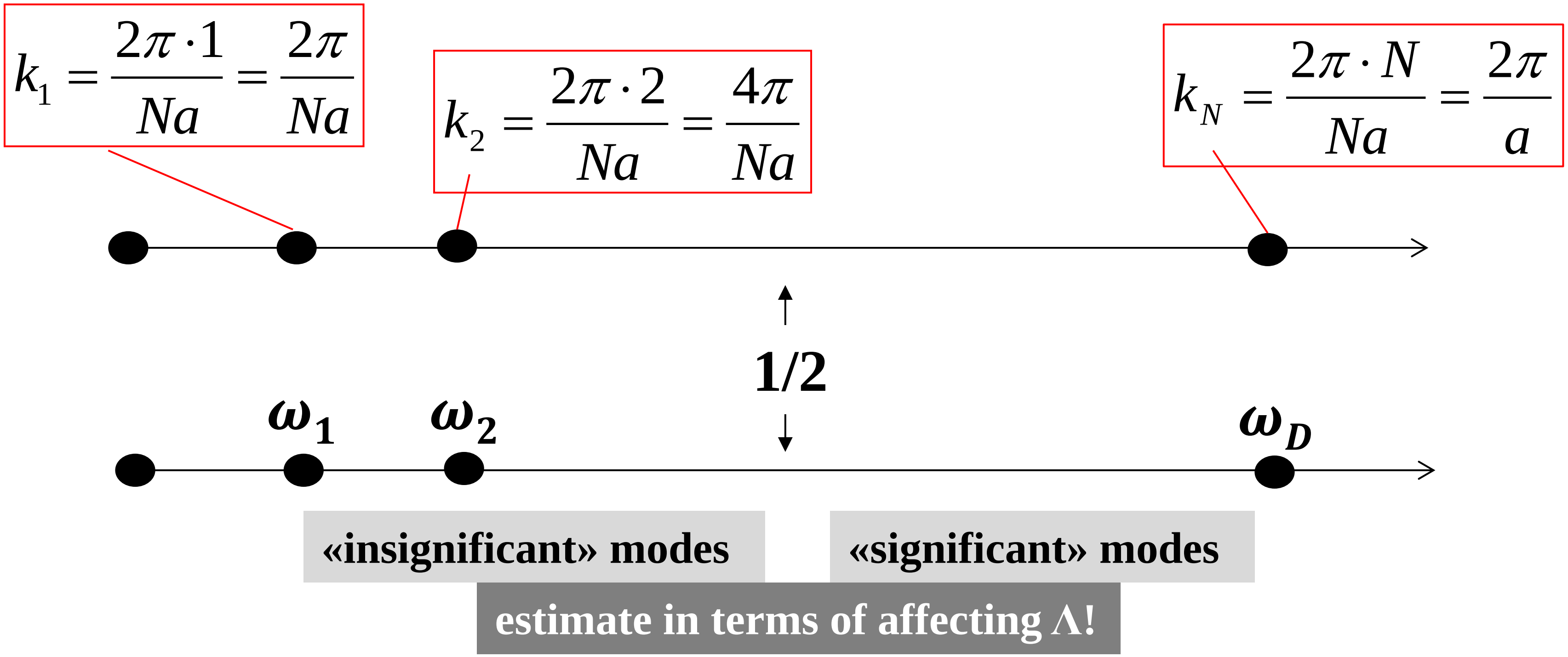
Explanation for $\kappa \propto \exp(\theta_D/2T)$ at high temperature limit

A more correct approximation for Λ (in high temperature limit) would be to consider "high" energetic phonons only, i.e those participating in U- processes.



U-process , i.e. to turn over the wavevector by $\vec{G}$, from the German word *umklappen*.

Explanation for $\kappa \propto \exp(\theta_D/2T)$ at high temperature limit



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Comparison of temperature dependence of κ in crystalline and amorphous solids

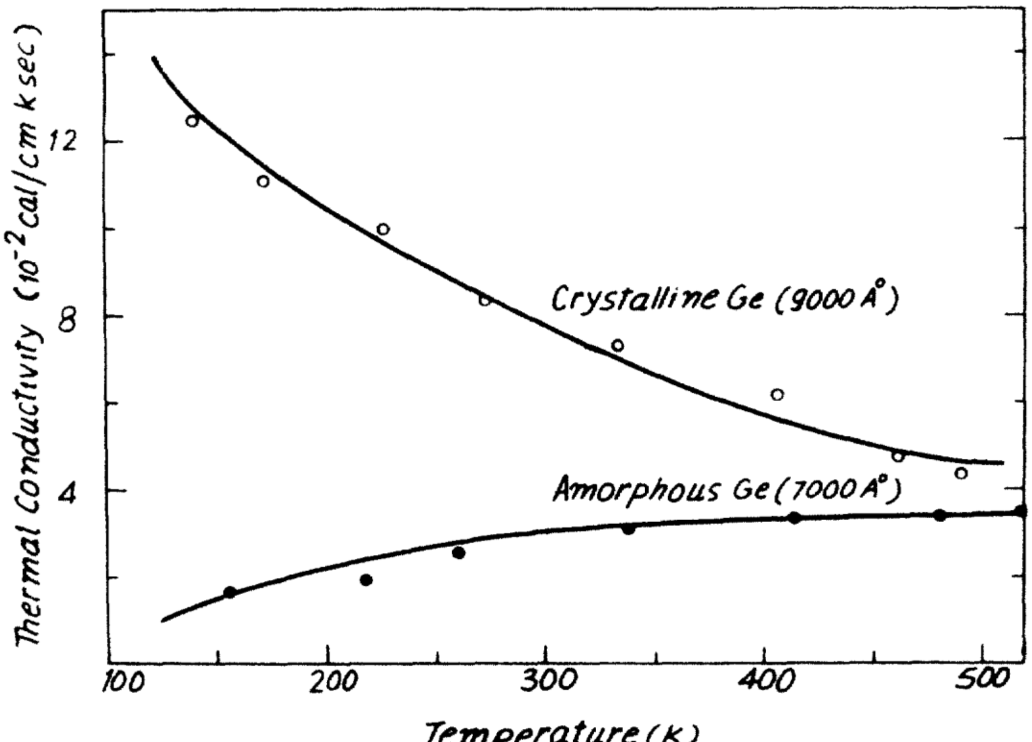

FIG. 2. Thermal conductivity vs temperature for amorphous and crystalline Ge films.