Thermal conductivity in insulator

Masatsugu Sei Suzuki
Department of Physics, SUNY at Binghamton
(Date: March 11, 2018)

1. Definition of thermal conductivity

The thermal conductivity κ of a solid is defined with respect to the steady-state flow of heat down a long rod with a temperature gradient ∇T,

$$\mathbf{J} = -\kappa \nabla T ,$$

where ***J*** is the flux of thermal energy, energy transmitted across a unit area per unit area. The unit of J is erg/(cm^2 sec). This form implies that the process of thermal energy transfer is a random process. The random nature of the thermal conductivity process brings the temperature gradient and a mean free path into the expression for the thermal flux.

The thermal conductivity gives the ease with which energy in the form of heat can pass through a system. In the harmonic approximation, a heat source will create lattice vibrations in the form of phonons. The phonons will move through the system, and will deposit their energy at the other end of the system.

2. Derivation of the kinetic formula of κ (Ashcroft and Mermin)

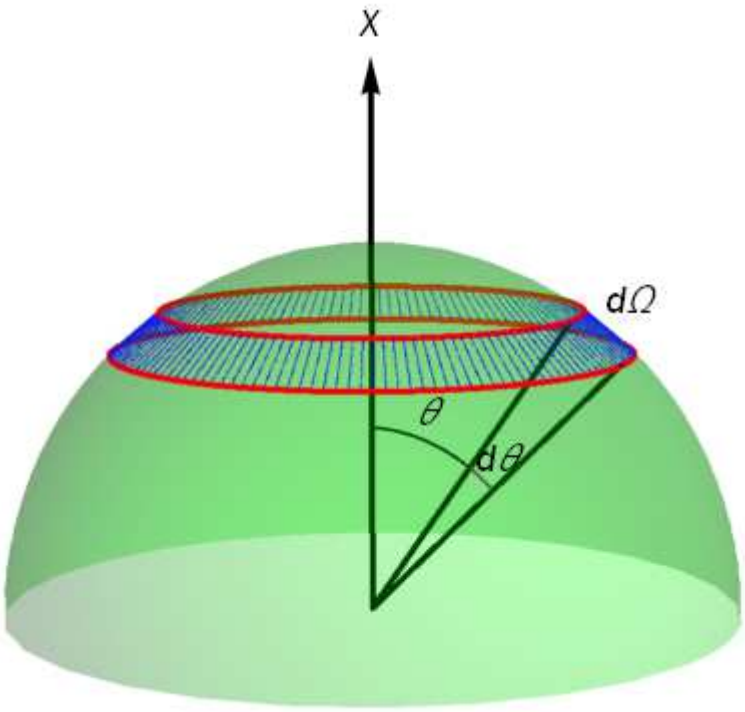


Fig.1(a) The solid angle. $d\Omega = 2\pi \sin\theta \, d\theta$. The radius of sphere is 1.

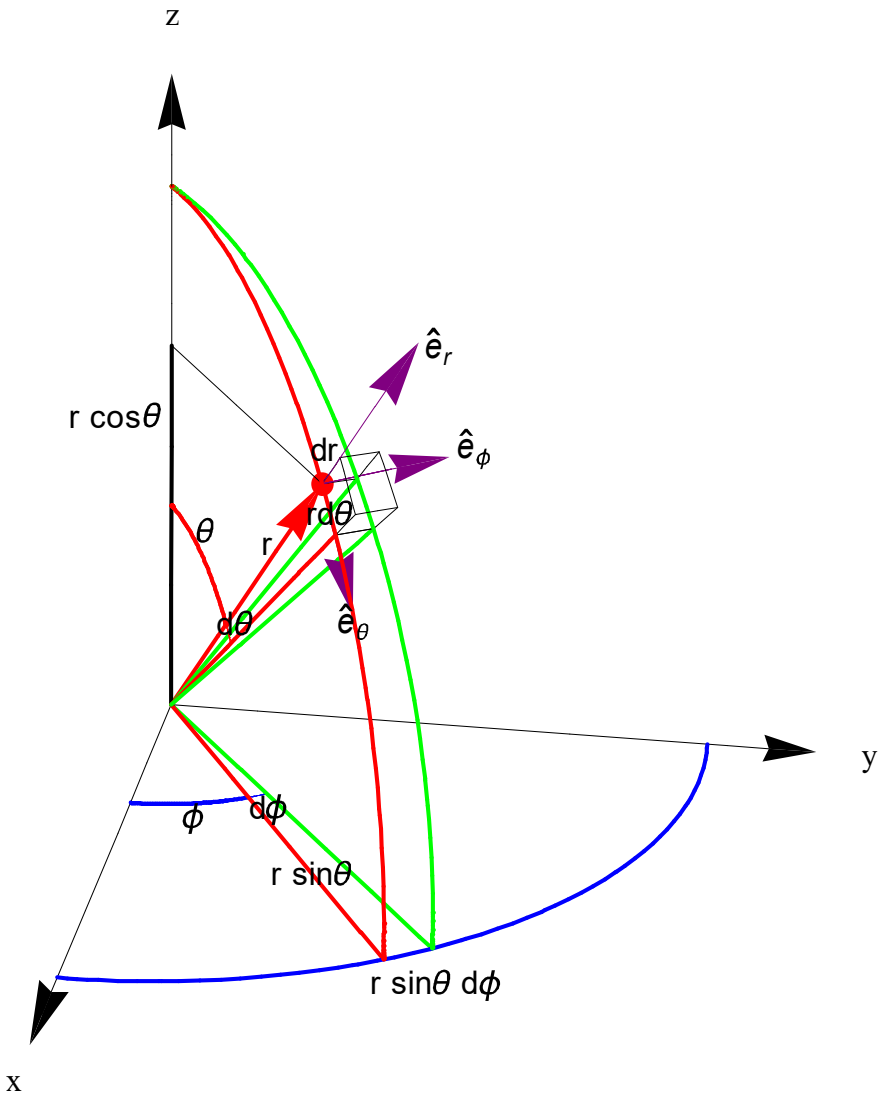


Fig.1 (b): Spherical co-ordinate system. The volume element is given by $dV = dr(\,r\,\sin\theta d\phi)(rd\theta) = r^2 dr\sin\theta d\theta d\phi$. In the present model, $dr = vdt = v$ for $dt = 1$ (unit time). $r = l$. $d\phi = 2\pi$. So we have $dV = 2\pi l^2 v\sin\theta d\theta$.

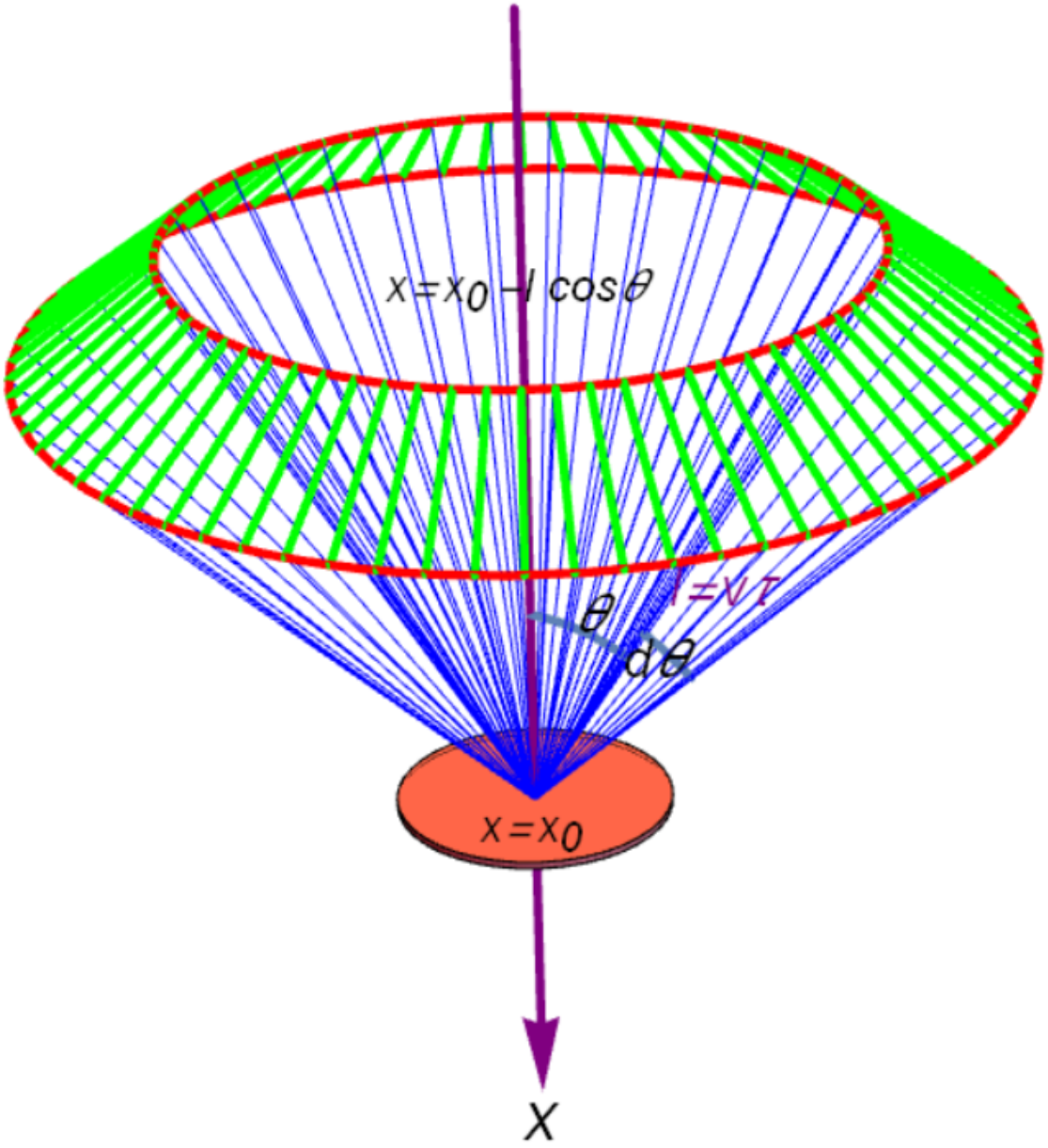


Fig.2 Propagation by phonons in the presence of a uniform temperature gradient along the x axis. Point P ($x = x_0 - l\cos\theta$). Point O ($x = x_0$). The radius of the sphere is l (= $v\tau$), where l is the mean free path, v is the velocity of phonon, and τ is the relaxation time. The total surface of the sphere with a radius l is $4\pi l^2$. The fraction of phonons with angles between θ and $\theta + \mathrm{d}\theta$ is $2\pi l^2 \sin\theta d\theta/(4\pi l^2) = \sin\theta d\theta/2$. $u(x_0)$ for the energy density at $x = x_0$ (the origin O). $u(x_0 - l\cos\theta)$ for the energy density at the point P (x =

x_0 - $l\cos\theta$). l is the mean free path for phonons entering into the sphere with the angle θ from the (-x) axis. The temperature gradient is given by $-\frac{\partial T(x)}{\partial x} > 0$.

We consider the heat propagation in the presence of a uniform temperature gradient along the x axis. The thermal current at x_0 is carried by phonons whose last collision was, on the average, a distance $l = v\tau$ away from x_0, where τ is a time. Phonons with velocities making angle θ with the x axis at x_0 collided last at a point P, a distance $l\cos\theta$ up the temperature gradient, and therefore carry an energy density $u(x_0 - l\cos\theta)$ with x-velocity $v\cos\theta$, where the energy density is a function of x; $u = u(x)$. The flux of thermal energy (energy per unit time per unit area) along the x axis is given by

$$\begin{aligned}\Delta J &= \frac{2\pi l^2 \sin\theta d\theta}{4\pi l^2}[v\cos\theta\,]u(x_0 - l\cos\theta) \\ &= \frac{\sin\theta d\theta}{2} v\cos\theta\, u(x_0 - l\cos\theta)\end{aligned}$$

or

$$J = \frac{1}{2}v\int_0^{\pi} \sin\theta d\theta \cos\theta[u(x_0 - l\cos\theta)] = \frac{1}{2}v\int_{-1}^{1} \mu d\mu[u(x_0 - l\mu)],$$

where $\mu = \cos\theta$, the unit of u is erg/cm^3 and the unit of the thermal flux J is erg/(cm^2 s). We use the Taylor expansion and take a linear order in the temperature gradient.

$$\begin{aligned}J &= \frac{1}{2}v\int_{-1}^{1} \mu d\mu\left[u(x_0) - \frac{\partial u}{\partial x}(l\mu)\right] \\ &= -vl\frac{\partial u}{\partial x}\frac{1}{2}\int_{-1}^{1}\mu^2 d\mu \\ &= -\frac{1}{3}vl\frac{\partial u}{\partial x} \\ &= \frac{1}{3}vl\frac{\partial u}{\partial T}(-\frac{\partial T}{\partial x})\end{aligned}$$

Then we have the expression of the thermal conductivity as

$$J = -\kappa \frac{\partial T}{\partial x}$$

with

$$\kappa = \frac{1}{3} v \ell \frac{\partial u}{\partial T},.$$

and

$$c = \frac{\partial u}{\partial T} = \frac{1}{V}\frac{\partial U}{\partial T} = \frac{1}{V} C$$

c is the heat capacity per unit volume. Then the thermal conductivity can be expressed as

$$\kappa = \frac{1}{3} cvl$$

where v is the velocity and $l = v\tau$ is the mean free path. Since the specific heat c is [erg/(cm^3 K)], the unit of the thermal conductivity is

$$[\kappa] = \frac{erg}{cm^3 \cdot K}\frac{cm^2}{s} = \frac{erg}{cm \cdot K \cdot \sec} \text{ (cgs units),} \qquad \text{(or } \frac{W}{K \cdot cm}\text{).}$$

The specific heat capacity of phonon c at low temperatures is given by

$$c = \frac{1}{V} C = \frac{12\pi^4}{5}\frac{N}{V} k_B \left(\frac{T}{\Theta}\right)^3 = \frac{12\pi^4}{5} n k_B \left(\frac{T}{\Theta}\right)^3$$

with the number density as

$$n = \frac{N}{V}$$

3. Derivation of the formula of thermal conductivity (by C. Kittel)

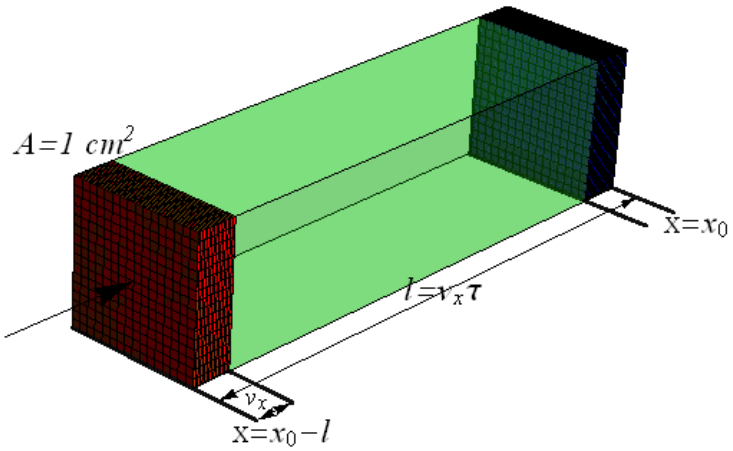


Fig.3 $u(x_0 - l)$: the energy density at $x = x_0 - l$. $l = v\tau$. The temperature gradient, $-dT/dx > 0$.

The net flux of energy (energy per unit time per unit area) is

$$\begin{aligned} J_U &= v_x u(x_0 - l_x) = v_x[u(x_0) - \frac{\partial u}{\partial x} l_x] \\ &= v_x u(x_0) - v_x \frac{\partial u}{\partial x} l_x \\ &= v_x u(x_0) - v_x^{\,2} \tau \frac{\partial u}{\partial T} \frac{\partial T}{\partial x} \\ &= v_x u(x_0) - v_x^{\,2} \tau c \frac{\partial T}{\partial x} \end{aligned}$$

Note that

$$\frac{\partial u}{\partial x} = \frac{\partial u}{\partial T} \frac{\partial T}{\partial x} .$$

and

$$c = \frac{\partial u}{\partial T} = \frac{1}{V} \frac{\partial U}{\partial T} = \frac{1}{V} C$$

$$J_U = \langle v_x \rangle u(x_0) - \langle v_x^{\,2} \rangle c\tau \frac{\partial T}{\partial x} = -\frac{1}{3}\langle v^2 \rangle c\tau \frac{\partial T}{\partial x}$$

where $\langle v_x^{\,2} \rangle = \frac{v^2}{3}$ and $\langle v_x \rangle = 0$. Then we have

$$J_U = -\frac{1}{3}cv^2\tau \frac{\partial T}{\partial x} = -\frac{1}{3}cvl\frac{\partial T}{\partial x}$$

leading to the thermal conductivity

$$\kappa = \frac{1}{3}cvl$$

where c is the specific heat per unit volume and l is the mean free path.

(a) Expression of κ at high temperatures ($T >> \Theta$)

$$< n(\omega) >= \frac{1}{\exp(\beta\hbar\omega) - 1} = \frac{k_B T}{\hbar\omega}$$

The relaxation time is inversely proportional to $1/ < n(\omega) > \propto 1/T$

$$l \propto \frac{1}{T}, \qquad c = \text{const.}$$

$$\kappa \propto \frac{1}{T}$$

(b) Expression of κ at the intermediate temperature:

The umklapp process (as shown in this Fig.) is significant, where

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{G}$$

and

$$\omega_1 + \omega_2 = \omega_3$$

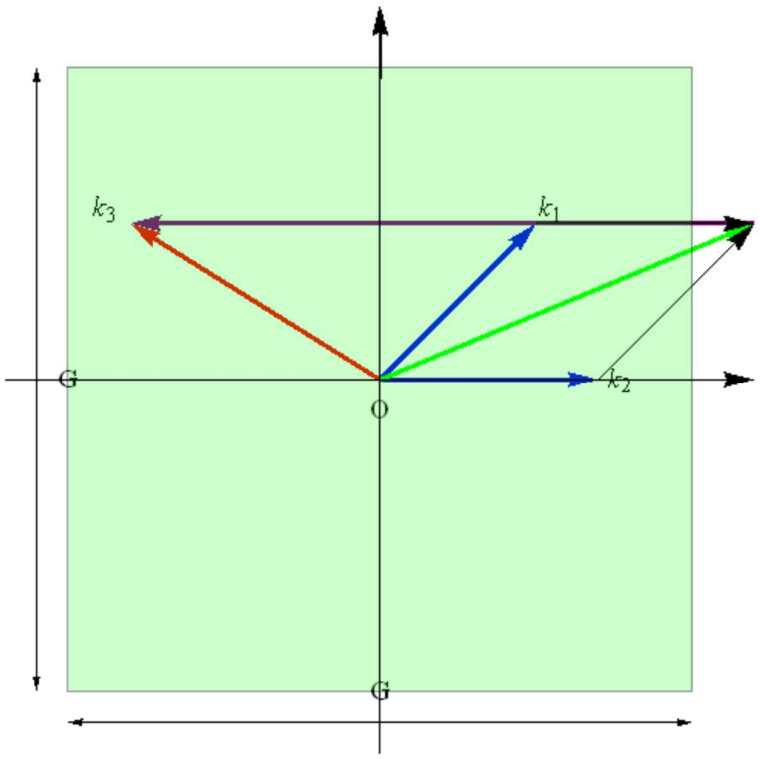


Fig.4 Umklapp process. $\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{G}$.

Thus $\boldsymbol{k}_3$ must be large enough for its energy to be equal to the sum of energies of $\boldsymbol{k}_1$ and $\boldsymbol{k}_2$. But the sum of the energies must go beyond the first Brillouin zone if we are to have the umpklapp processes at al. so that k_3 cannot be very much less in length than $G/2$. In the Debye model, this means that

$$k_3 \geq \alpha k_D ,$$

where α is a fraction, of the order of 1/2 or 2/3 (see the Appendix). In other words,

$$\hbar\omega_3 = \hbar v k_3 \geq \alpha\hbar v k_D = \alpha k_B \Theta .$$

Note that

$$\hbar\omega_D = \hbar v k_D = k_B \Theta$$

The probability of the occurrence of the umklapp process is given by

$$n(\boldsymbol{q}_1)n(\boldsymbol{q}_2) \approx \exp(-\frac{\hbar\omega_1}{k_B T})\exp(-\frac{\hbar\omega_2}{k_B T}) = \exp(-\frac{\hbar\omega_3}{k_B T}) \approx \exp(-\frac{\alpha\Theta}{T}).$$

at low temperatures since

$$< n(\omega) >= \frac{1}{\exp(\beta\hbar\omega) - 1} \approx \exp(-\beta\hbar\omega).$$

The effective relaxation time must vary as

$$\tau \propto \exp(\frac{\alpha\Theta}{T}).$$

The mean free path of the phonon increases very rapidly with decreasing temperature. sufficiently low temperatures.

$$l = v\tau = \exp(\frac{\alpha\Theta}{T})$$

Since $c \propto T^3$, the thermal conductivity is assumed to have the form

$$\kappa = (\frac{T}{\Theta})^3 \exp(\frac{\alpha\Theta}{T})$$

(c) Expression of κ at low temperatures ($T \ll \Theta$)

The low temperature thermal conductivity is limited by temperature-independent scattering processes determined by the geometry and the purity of the sample. The mean free path is independent of temperature.

$$l = D,$$

where D is the size of the system. Since $c \propto T^3$, we have

$$\kappa = \frac{1}{3}cvl \propto T^3$$

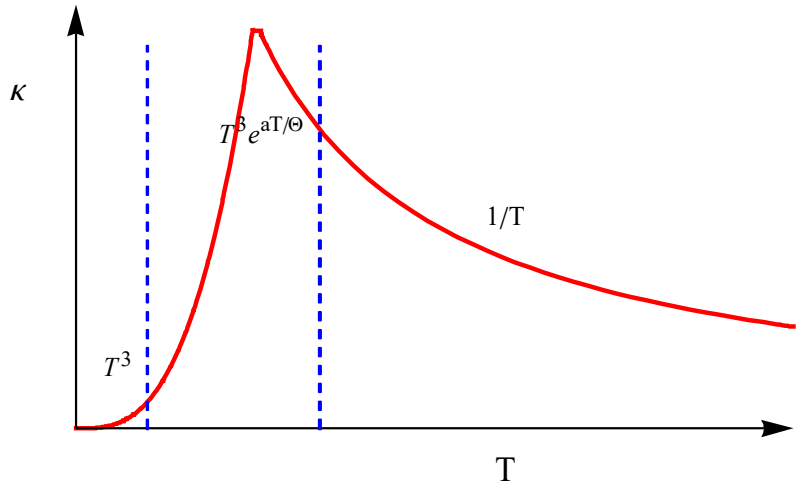


Fig.5 Schematic diagram for the T dependence of the thermal conductivity of insulator.

4. Experimental results of thermal conductivity (Cochran)

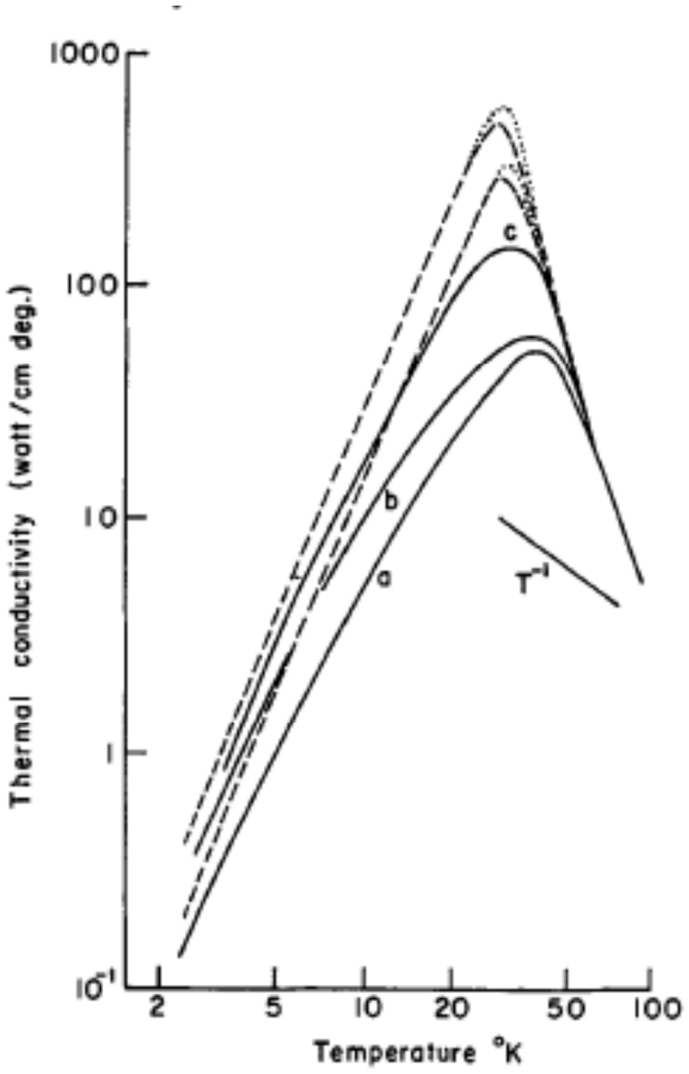


Fig.6 The thermal conductivity of some artificial sapphire crystals according to Berman. Curve a (1.5 mm diameter). Curve b (3.0 mm diameter). Curve c (crystal from a different source, 2.5 mm diameter). The broken lines give the conductivity of a and b expected if only boundary and umklapp processes contributed to the resistance.

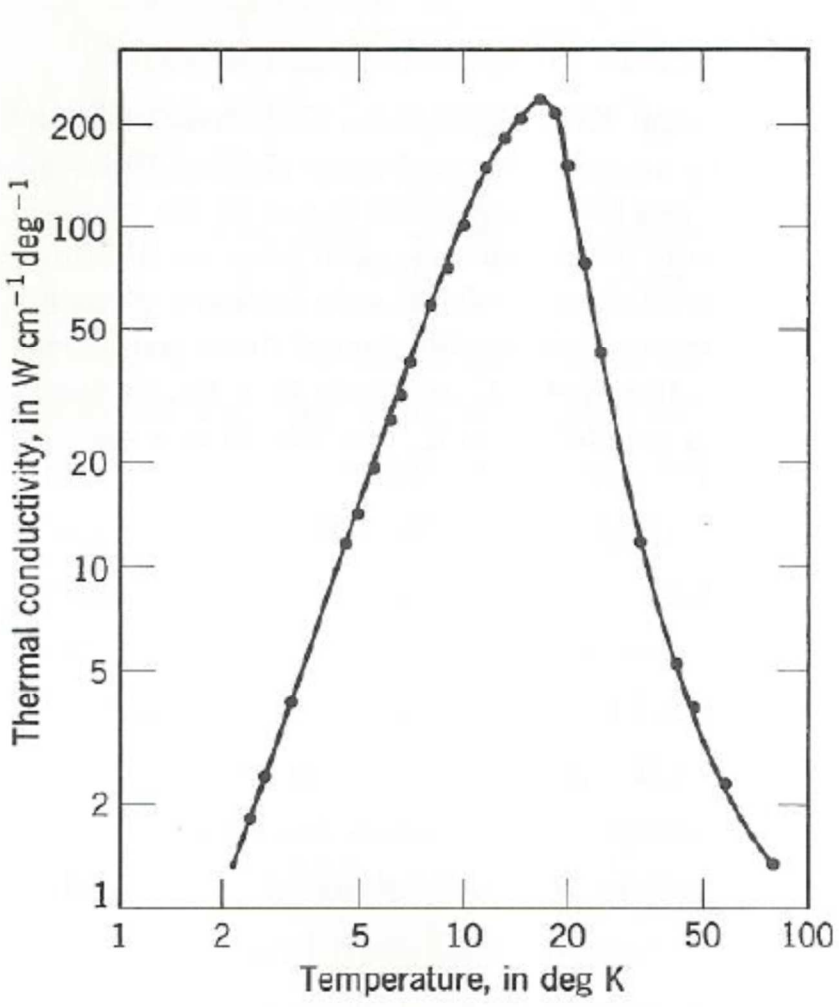


Fig.7 Thermal conductivity of a highly purified crystal of NaF crystal (H.E. Jackson, C.T. Walker, and T.F. McNelly, Phys. Rev. Letters **25**, 26 (1970).

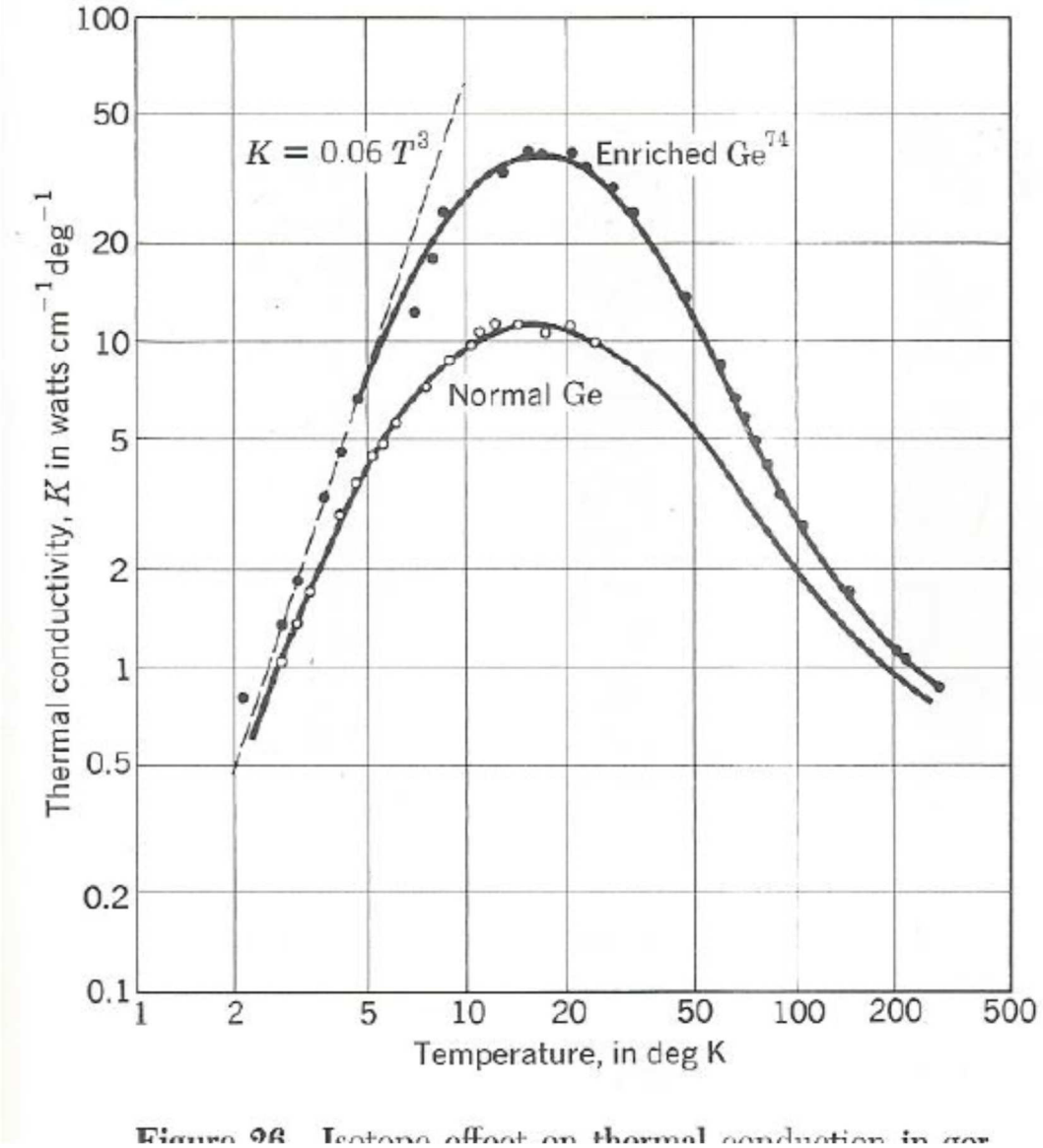


Fig.8 Isotope effect on thermal conduction in Ge, amounting to a factor of three at the conductivity maximum. The enriched specimen is 96 % Ge^{74}, natural Ge is 20% Ge^{70}, 27 % Ge^{72}, and 8 % Ge^{73}, 37% Ge^{74}, and 8% Ge^{76} (T.H. Geballe and G.W. Hull, Phys. Rev. 110, 773 (1958).

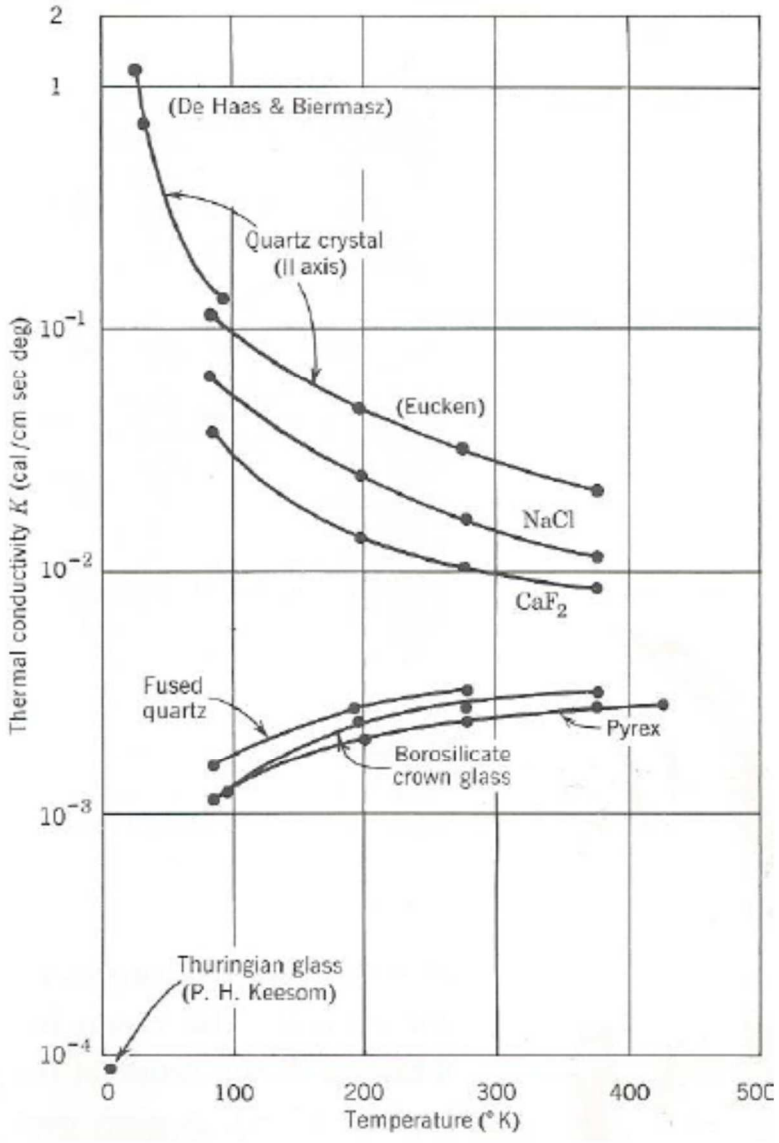
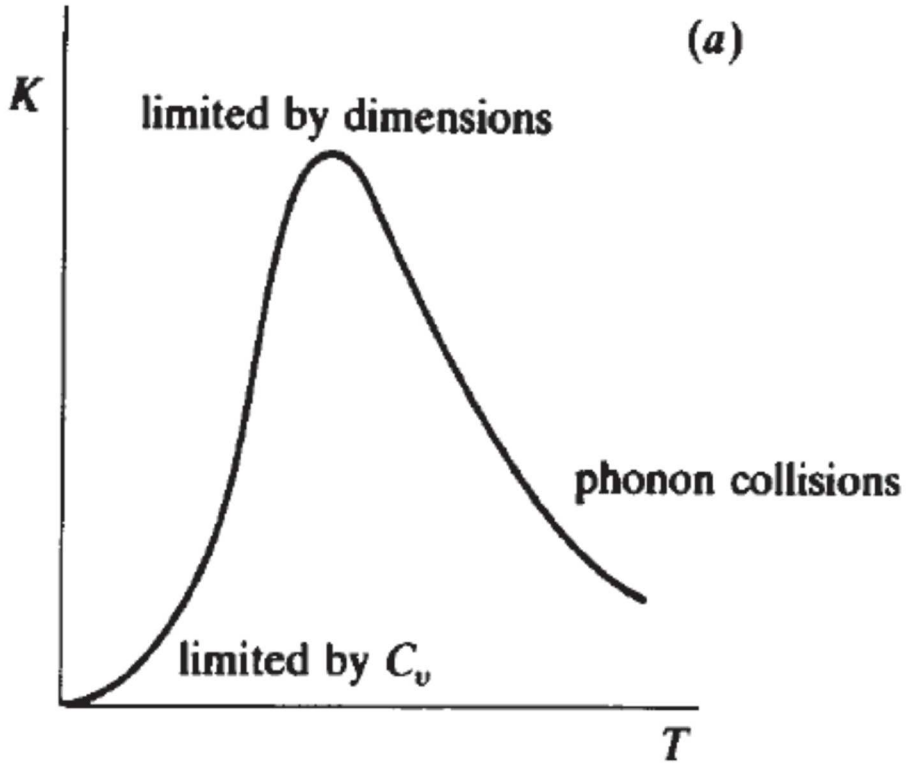


Fig.9 Temperature dependence of the thermal conductivity of various crystals and glasses.


(a)
K
limited by dimensions
phonon collisions
limited by C_v
T

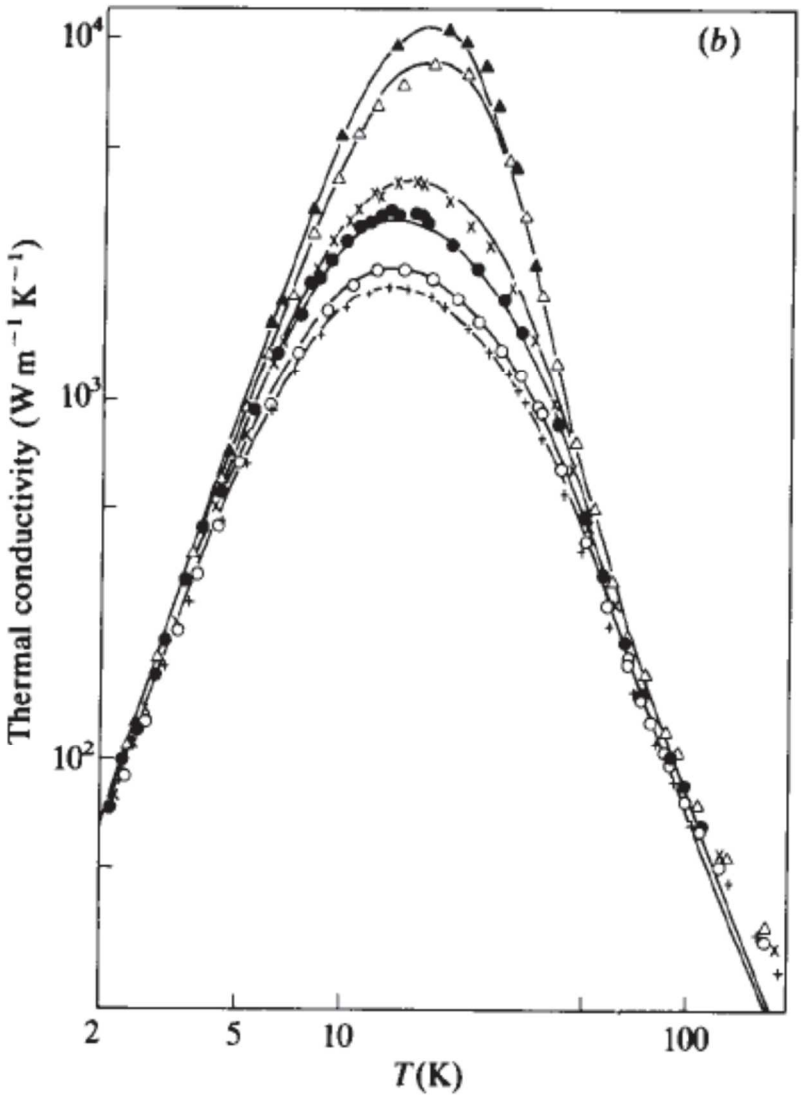
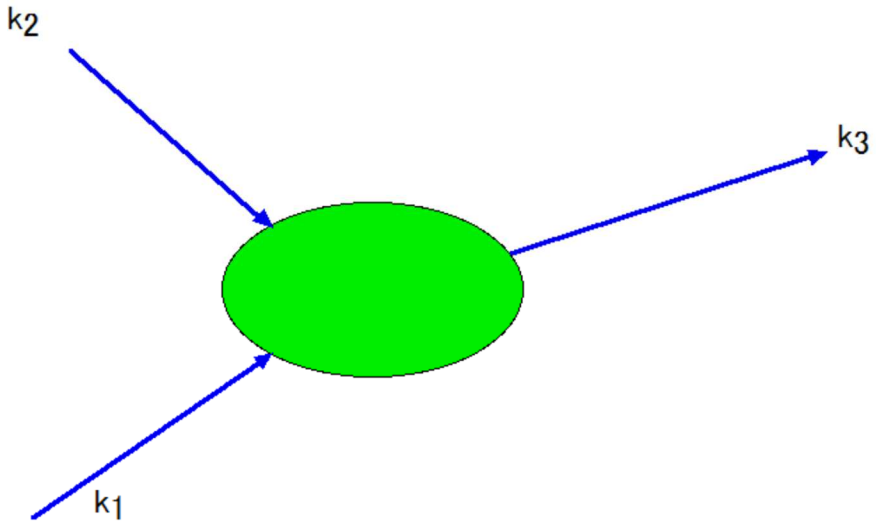


Fig.10 (a) The principal form for the variation of thermal conductivity. (b) Experimental data for LiF crystals containing different amount of the isotope ^{6}Li. 0.02% (▲). 0.01% (Δ). 4.6% (x). 9.4% (●). 25.4% (○), 50.1% (+). (Berman and Brock, 1965).

5. Three phonon processes



If the Hooke's law were rigorously obeyed in a solid, and the potential energy of an atom at location $\boldsymbol{r}$ (whose equilibrium position is $\boldsymbol{r}_0$) could be expressed by

$$V(\boldsymbol{r}) = V(\boldsymbol{r}_0) + A(\boldsymbol{r}-\boldsymbol{r}_0)^2 + V_a(\boldsymbol{r}-\boldsymbol{r}_0)$$

where

$$V_a(\boldsymbol{r}) = A(\boldsymbol{r}-\boldsymbol{r}_0)^3 + ...$$

The anharmonic potential V_a provide a coupling between phonons. We consider the case when two phonons are scattered inside the system. When the outgoing wavevector of phonon is k_3, we get the scattering amplitude as

$$\begin{aligned} S &= \int d\boldsymbol{r} e^{(-i\boldsymbol{k}_1\cdot\boldsymbol{r}+i\omega_1 t)} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}+i\omega_2 t)} V_a(\boldsymbol{r}) e^{(i\boldsymbol{k}_3\cdot\boldsymbol{r}-i\omega_3 t)} \\ &= e^{-i(\omega_3-\omega_1-\omega_2)t} \sum_G V_{aG} \int d\boldsymbol{r} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}_2\cdot\boldsymbol{r}} e^{i\boldsymbol{G}\cdot\boldsymbol{r}} e^{i\boldsymbol{k}_3\cdot\boldsymbol{r}} \end{aligned}$$

or

$$\begin{aligned} e^{-i(\omega_3-\omega_1-\omega_2)t} \int d\boldsymbol{r} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} e^{-i\boldsymbol{k}_1\cdot\boldsymbol{r}} V_a(\boldsymbol{r}) e^{i\boldsymbol{k}_3\cdot\boldsymbol{r}} &= e^{-i(\omega_3-\omega_1-\omega_2)t} \sum_G V_{a\boldsymbol{G}} \int d\boldsymbol{r} e^{i(\boldsymbol{k}_3+\boldsymbol{G}-\boldsymbol{k}_1-\boldsymbol{k}_2)\cdot\boldsymbol{r}} \\ &= e^{-i(\omega_3-\omega_1-\omega_2)t} \sum_G V_{a\boldsymbol{G}} \delta(\boldsymbol{k}_3+\boldsymbol{G}-\boldsymbol{k}_1-\boldsymbol{k}_2) \end{aligned}$$

where $V_{a(}\boldsymbol{r})$ is a periodic potential energy arising from the anharmonic terms

$$V_a(\boldsymbol{r}) = V_a(\boldsymbol{r} + \boldsymbol{T}),$$

and $V_a(\boldsymbol{r})$ is described by

$$V_a(\boldsymbol{r}) = \sum_{\boldsymbol{G}} V_{aG} e^{i\boldsymbol{G}\cdot\boldsymbol{r}},$$

where $\boldsymbol{T}$ is the translation vector. The Fourier component V_{aG} is given by

$$V_{aG} = \frac{1}{\Omega}\int d\boldsymbol{r} V_a(\boldsymbol{r}) e^{-i\boldsymbol{G}\cdot\boldsymbol{r}},$$

where W is the volume of the system. From the above equations, we get the momentum conservation law,

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{G}.$$

Averaging of S over time t,

$$\int dt e^{-i(\omega_3 - \omega_1 - \omega_2)t},$$

yields to the energy conservation law,

$$\omega_3 = \omega_1 + \omega_2.$$

((**Note**)) In quantum mechanics, the second term of the potential is given by the matrix form

$$\langle f | H_2 | i \rangle \approx M_2 (a_{-\mathbf{k}s}{}^{+} + a_{\mathbf{q}s})(a_{-\mathbf{k}'s'}{}^{+} + a_{\mathbf{k}'s'}),$$

where M_2 is a constant, $a_{\mathbf{ks}}$ is the annihilation operator for the phonon with the wavevector $\boldsymbol{k}$ and polarization vector $\boldsymbol{s}$, and $a_{\mathbf{ks}}{}^{+}$ is the creation operator for the phonon with the wavevector $\boldsymbol{k}$ and polarization vector $\boldsymbol{s}$. The Hamiltonian H_2 contributes to the two-phonons process;

$$\omega_1 = \omega_2, \qquad \boldsymbol{k}_2 = \boldsymbol{k}_1 + \boldsymbol{G}.$$

On the other hand, the third term (anharmonic term) of the potential is given by the matrix form

$$\langle f | H_3 | i \rangle \approx M_3 (a_{-\mathbf{q}s}{}^{+} + a_{\mathbf{q}s})(a_{-\mathbf{q}'s'}{}^{+} + a_{\mathbf{q}'s'})(a_{-\mathbf{q}''s'}{}^{+} + a_{\mathbf{q}'s'}).$$

where M_3 is a constant. This Hamiltonian H_3 contributes to the three-phonons process;

$$\omega_3 = \omega_1 + \omega_2, \quad \boldsymbol{k}_3 = \boldsymbol{k}_1 + \boldsymbol{k}_2 + \boldsymbol{G}.$$

Therefore, the contribution of the anharmonic potential is inevitable for the three-phonons process.

((**Note**))
$V_a(\boldsymbol{r})$ is proportional to the matrix form of the Hamiltonian H_3. Here we discuss qualitatively the three phonon processes semi-classically.

6. Normal process

The N processes ($\boldsymbol{G} = 0$) is defined by

$$\boldsymbol{k}_3 = \boldsymbol{k}_1 + \boldsymbol{k}_2,$$

where $\boldsymbol{k}_1$, $\boldsymbol{k}_2$, and $\boldsymbol{k}_3$ are the wavevectors in the first Brillouin zone. In this process, the phonon energy is conserved. The scattering merely redistributes the energy into different phonon modes without altering the total flow. In this sense, the N processes do not contribute to the thermal resistivity. The total crystal momentum

$$\boldsymbol{J} = \sum_k \hbar \boldsymbol{k} n_k,$$

will remain unchanged by the N process.

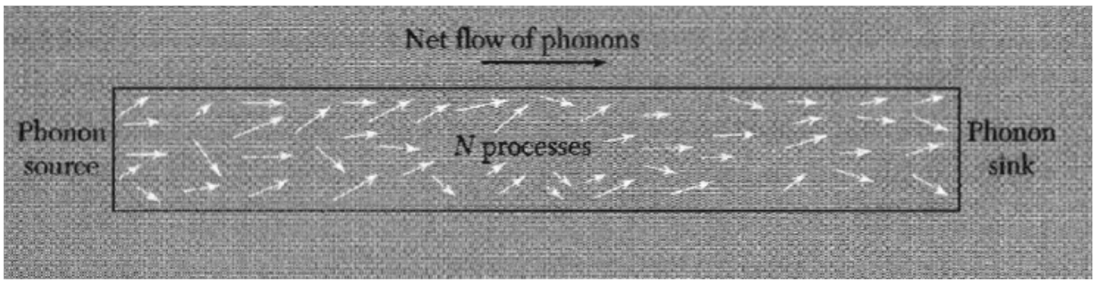


Fig. Normal process.

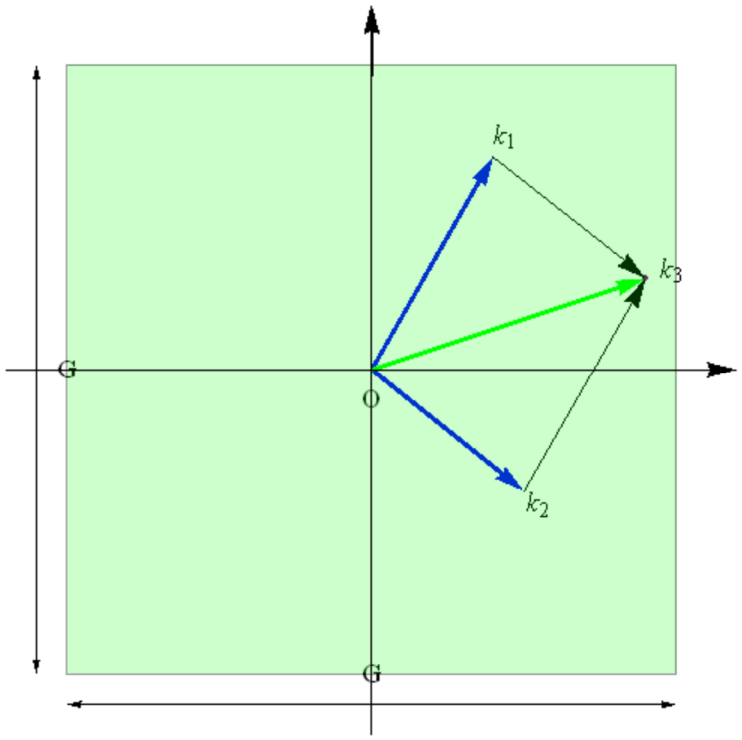
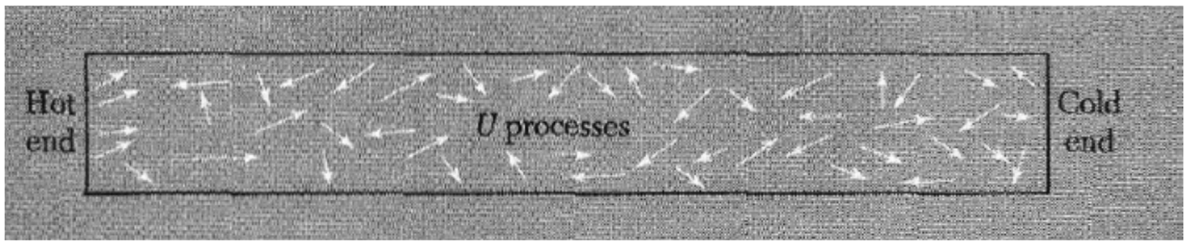


Fig. Normal process. $\mathbf{k}_3 = \mathbf{k}_1 + \mathbf{k}_2$,

7. Umklapp process



Here are examples of umklapp process in the 2D squarelattice Brillouin zone. The important three-phonon processes that cause thermal resistivity are of the form

$$\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{G},$$

where $\boldsymbol{G}$ is the reciprocal lattice vector. These processes discovered by Peierls, are called umklapp processes. For the umpklapp process as well as the normal process, the energy must be conserved, so that

$$\omega_1 + \omega_2 = \omega_3$$

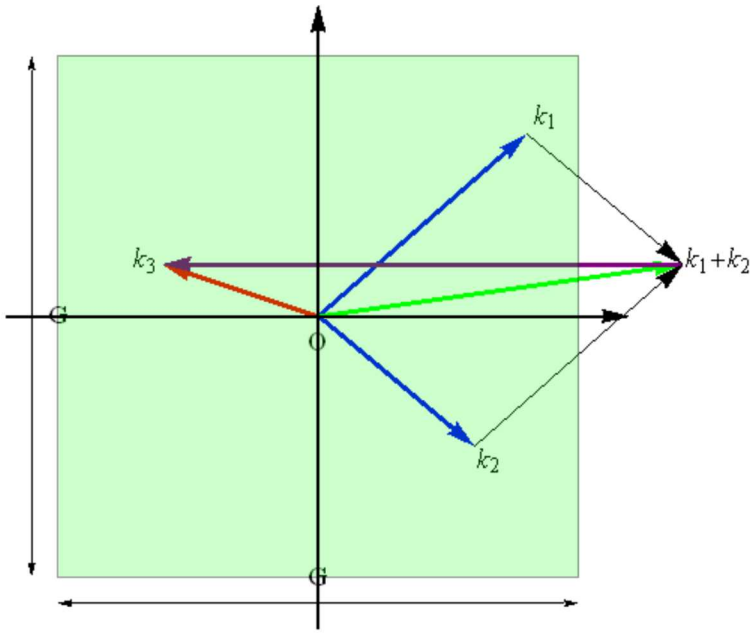
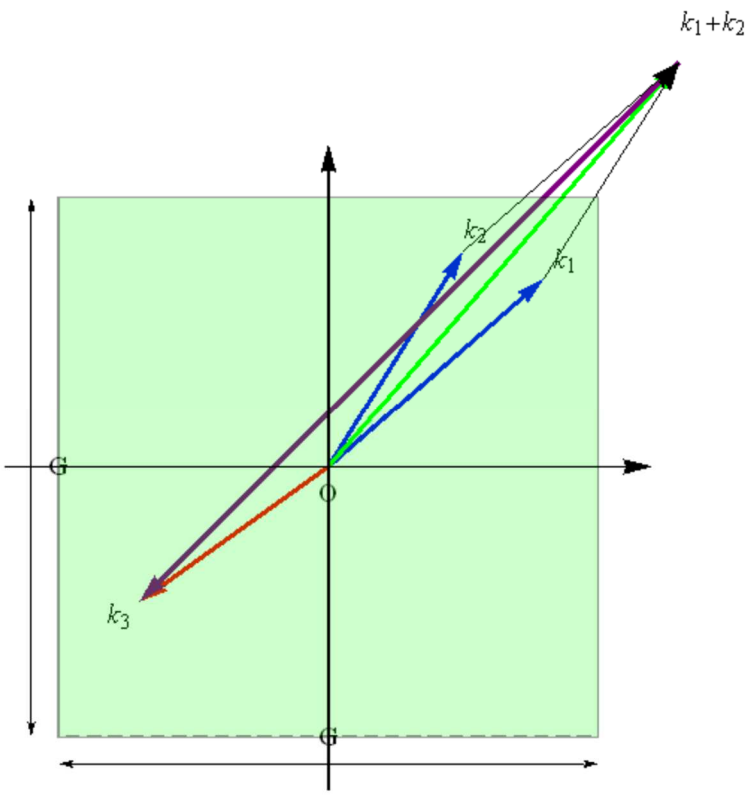
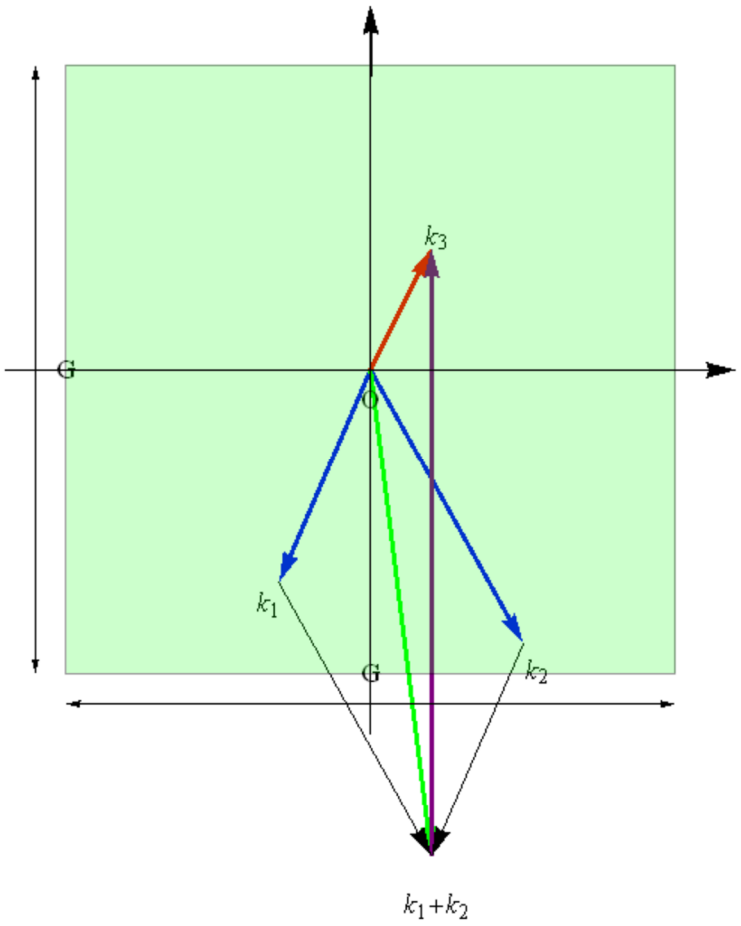
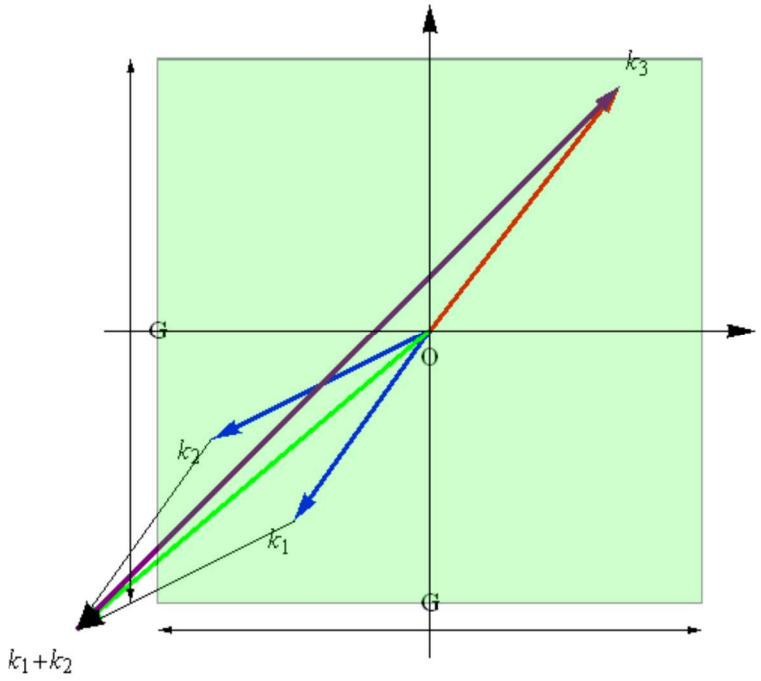
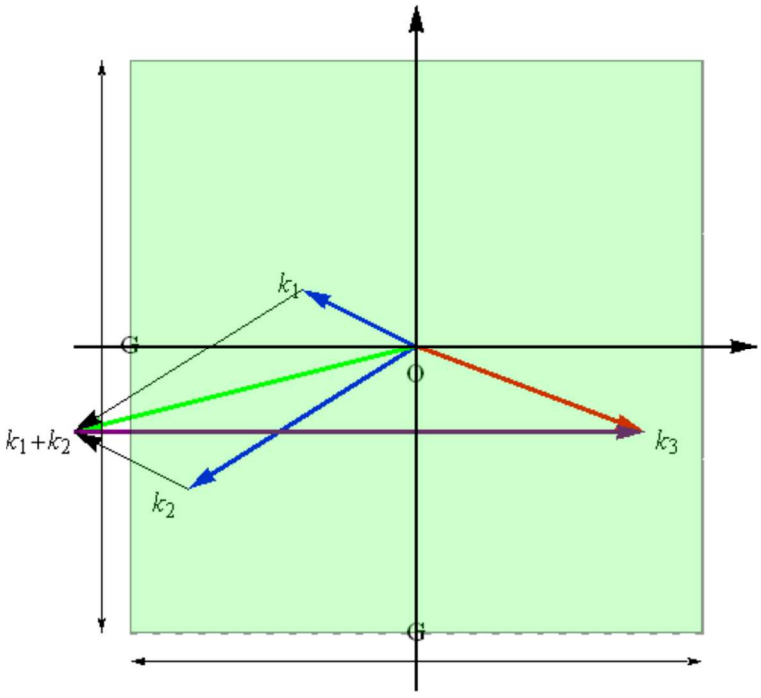


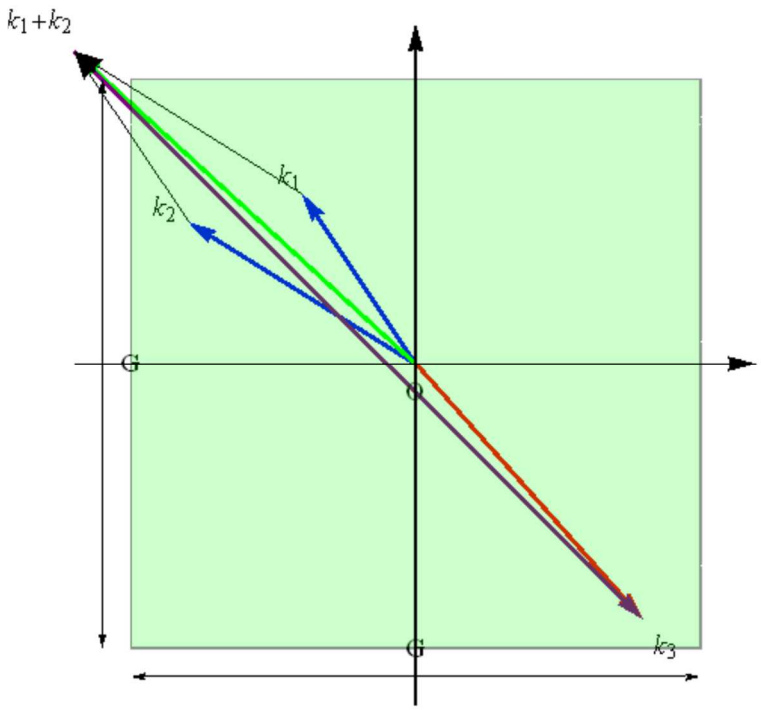
Fig. Umklapp process. $\boldsymbol{k}_1 + \boldsymbol{k}_2 = \boldsymbol{k}_3 + \boldsymbol{G}$. The square (green region) represents the first Brillouin zone. In the umklapp process, the direction of the x-component of the phonon flux is reversed.


k_1+k_2
k_2
k_1
G
O
k_3
G


k_3
G
O
k_1
G
k_2
k_1+k_2


k_3
G
O
k_2
k_1
G
k_1+k_2


k_1
G
O
k_1+k_2
k_3
k_2
G



8. Umklapp process in the 1D system

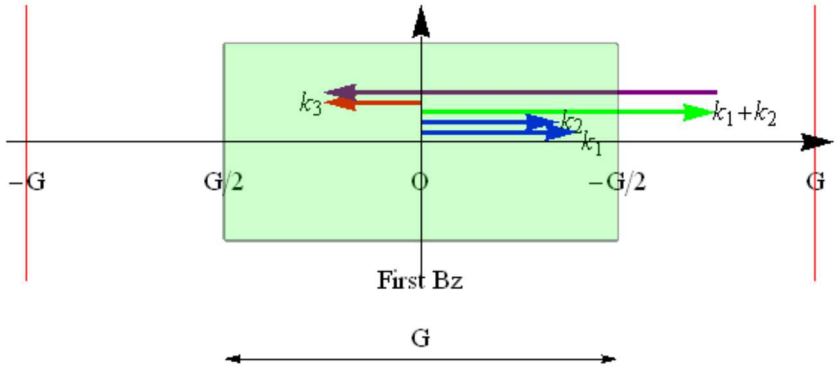
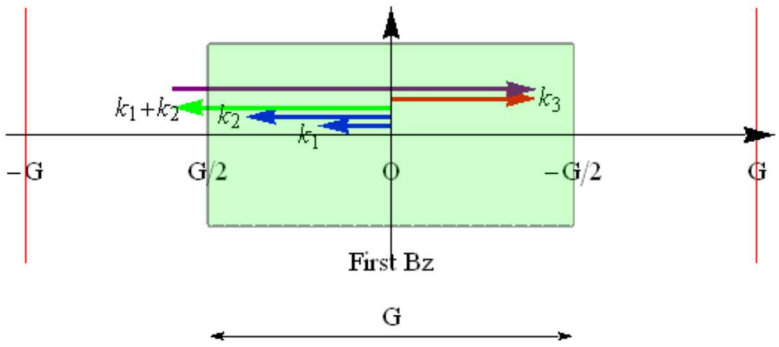


Fig. Umklapp process for the one dimensional system. The green zone is the first Brillouin zone.



The momentum conservation:

$$k_1 + k_2 = k_3 + nG$$

where G is the reciprocal lattice vector ($G = 2\pi/a$), $n = \pm 1$ (umklapp process) and $n = 0$ (normal process).

The energy conservation:

$$\omega_1 + \omega_2 = \omega_3$$

where

$$\omega_1 = \omega_m \left|\sin(\frac{k_1 a}{2})\right|, \qquad \omega_2 = \omega_m \left|\sin(\frac{k_2 a}{2})\right|, \qquad \omega_3 = \omega_m \left|\sin(\frac{k_3 a}{2})\right|$$

For simplicity, we use the following notation

$$\frac{k_1}{G} = x, \qquad \frac{k_2}{G} = y, \qquad \frac{k_3}{G} = z$$

Then we have two equations,

$$x + y = z + n$$

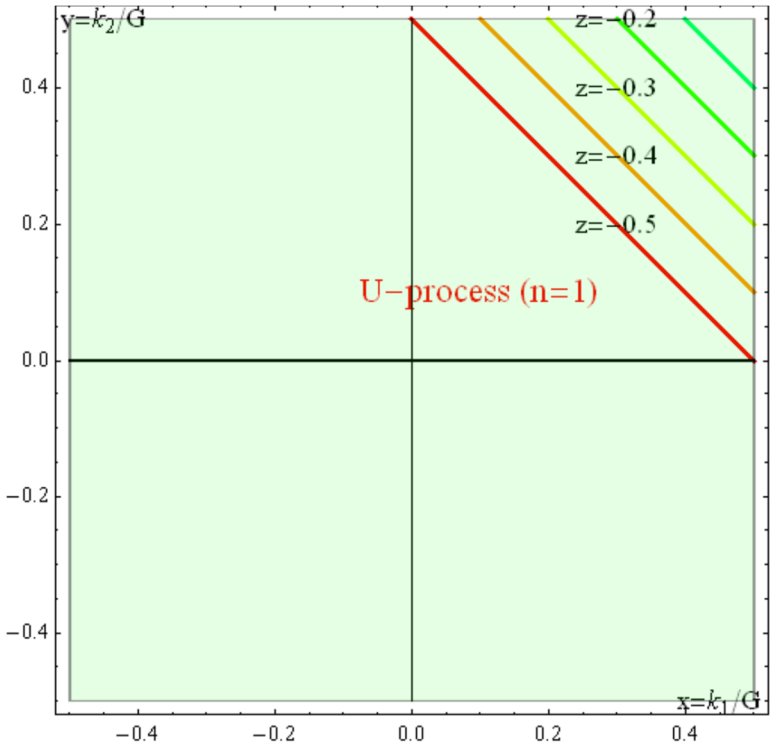


Fig. Umklapp process with $n = 1$ which appears for $x + y > 1/2$. The straight lines with z = -0.5, -0.4, -0.3, -0.2, and -0.1 are shown. $x = k_1/G$. $y = k_2/G$, and $z = k_3/G$. The momentum conservation; $x + y = z + n$, with $n = 0$ (the N process) and $n = \pm 1$ (the U process). The region with the green zone is the first Brillouin zone ($|x| < 1/2$ and $|y| < 1/2$).

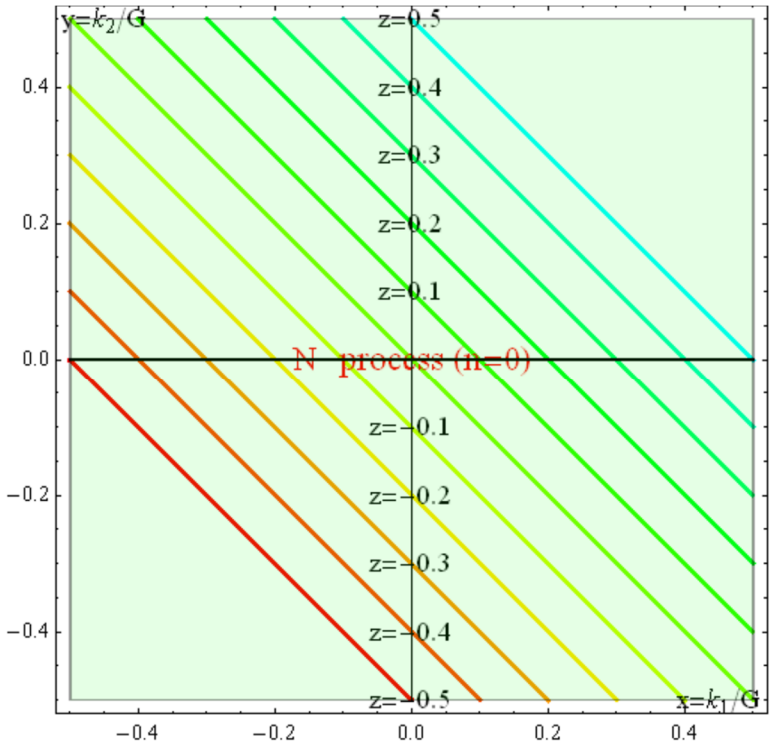


Fig. Normal process with n = 0, which appears for -1/2<x + y<1/2. The straight lines with z = -0.5, -0.4, -0.3, .., 0.4, and 0.5 are shown.

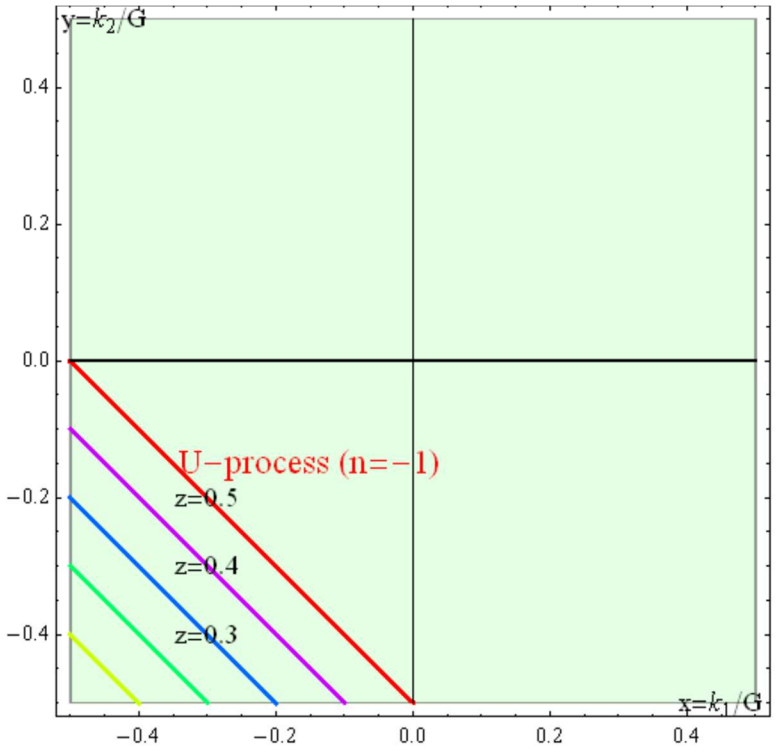


Fig. Umklapp process with n = -1, which appears for x+y<-1/2. The straight lines with z = 0.5, 0.4, 0.3, 0.2, and 0.1 are shown.

Here we use the dispersion relations for the longitudinal acoustic (LA) and transverse acoustic (TA) waves as,

$$\omega_L = \omega_0 \left|\sin(\pi x)\right|, \qquad \text{for the LA wave}$$

$$\omega_T = a\omega_0 \left|\sin(\pi x)\right| \qquad \text{for the TA wave}$$

where a is lower than 1 and ω_0 is constant, reflecting that the velocity of the LA wave is larger than that of the TA wave.

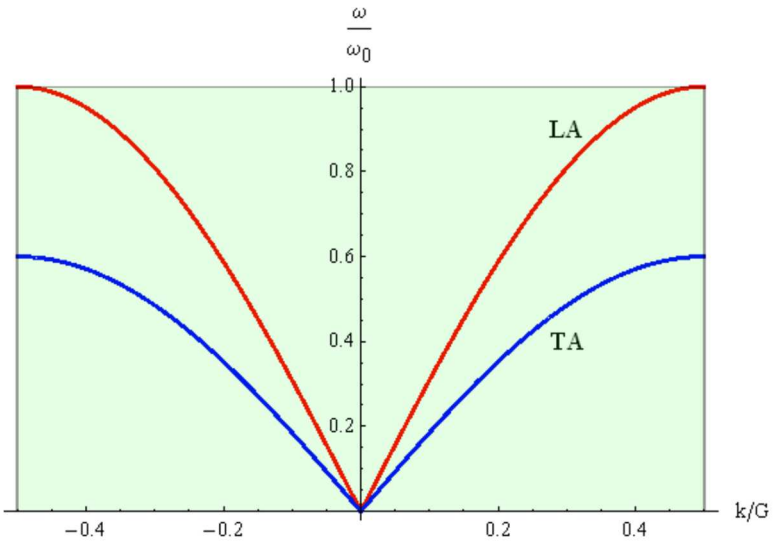


Fig. Dispersion relation of the LA phonon ($\omega = \omega_0|\sin(\pi k/G)|$) and TA phonon ($\omega$ = a $\omega_0|\sin(\pi k/G)|$). a = 0.6.

For the case of $L + T \rightarrow L$, we have

$$|\sin(\pi x)| + a|\sin(\pi y)| = |\sin(\pi z)|$$

where

$$|x| < \frac{1}{2}, \qquad |y| < \frac{1}{2}, \qquad |z| < \frac{1}{2}$$

(in the first Brillouin zone), where a is changed as a parameter ($0<a<1$)

((**Rule-1**))

There is no process in which all three phonons belong to the same polarization branch of the spectrum. (Ziman Electrons and Phonons).

$L + L \rightarrow L$ (not allowed), $T + T \rightarrow T$ (not allowed),

(a) For the case of $L + L \rightarrow L$, we have

$$|\sin(\pi x)| + a|\sin(\pi y)| = |\sin(\pi z)|$$

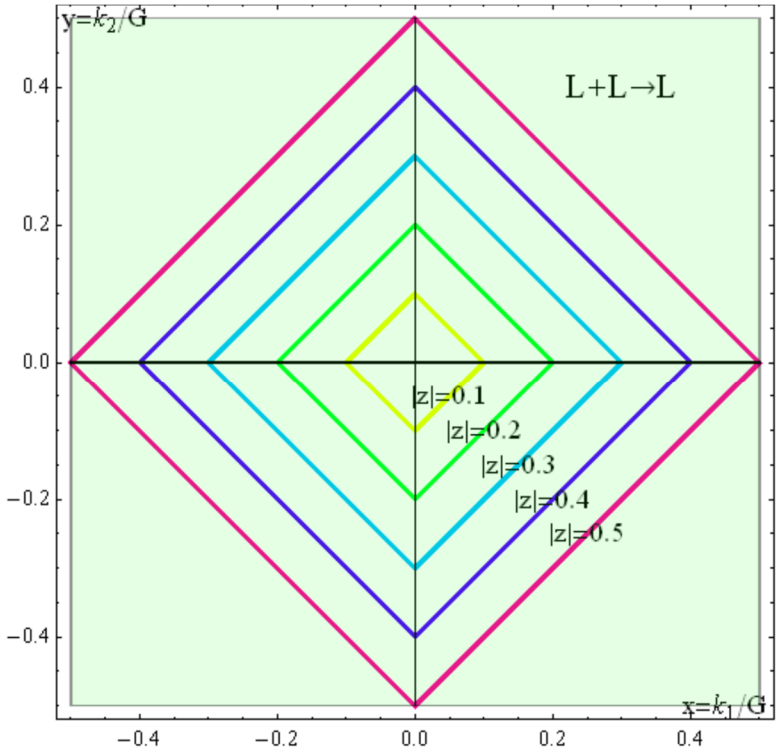


Fig. ContourPlot of $\omega_1(L)+\omega_2(L)=\omega_3(L)$ in the x-y plane. The parameter z is changes for $|z|<1/2$. No intersection is seen between the ContourPlot and the U-process denoted by $x+y=z+n$ (n = ±1).

In this case, the U-process does not occur. Only the N process exists.

(b) The case of $T+T\rightarrow T$

We have

$$a|\sin(\pi x)|+a|\sin(\pi y)|=a|\sin(\pi z)|$$

or

$$|\sin(\pi x)|+|\sin(\pi y)|=|\sin(\pi z)|$$

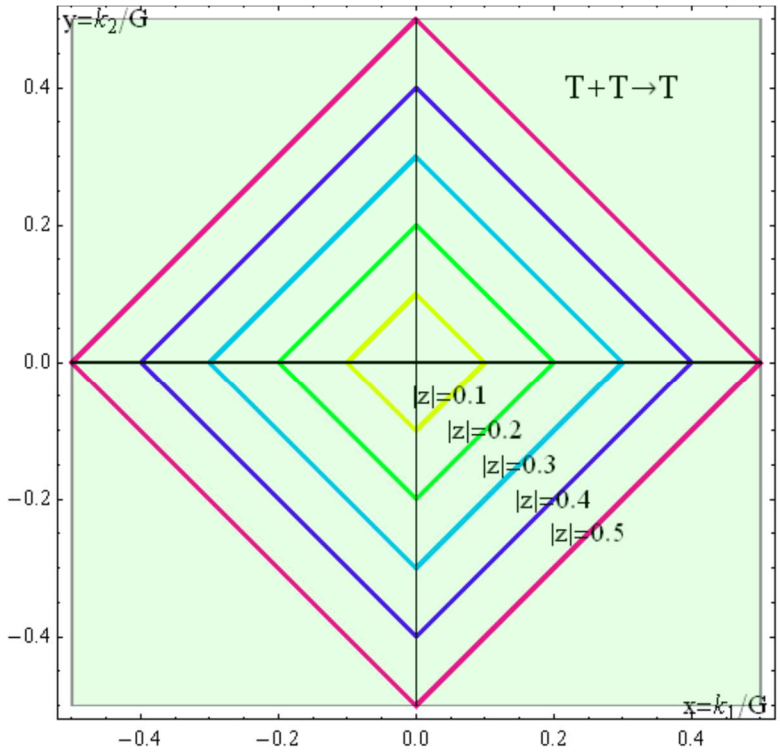


Fig. ContourPlot of $\omega_1(T)+\omega_2(T)=\omega_3(T)$ in the x-y plane. The parameter z is changes for $|z|<1/2$. No intersection is seen between the ContourPlot and the U-process denoted by $x+y=z+n$ (n = ±1).

((**Rule-2**))

The created phonon must lie in a higher branch than one at least of the destroyed phonons.

(c) The case of $T+L\rightarrow L$

We have

$$a\left|\sin(\pi x)\right|+\left|\sin(\pi y)\right|=\left|\sin(\pi z)\right|$$

with a = 0.6

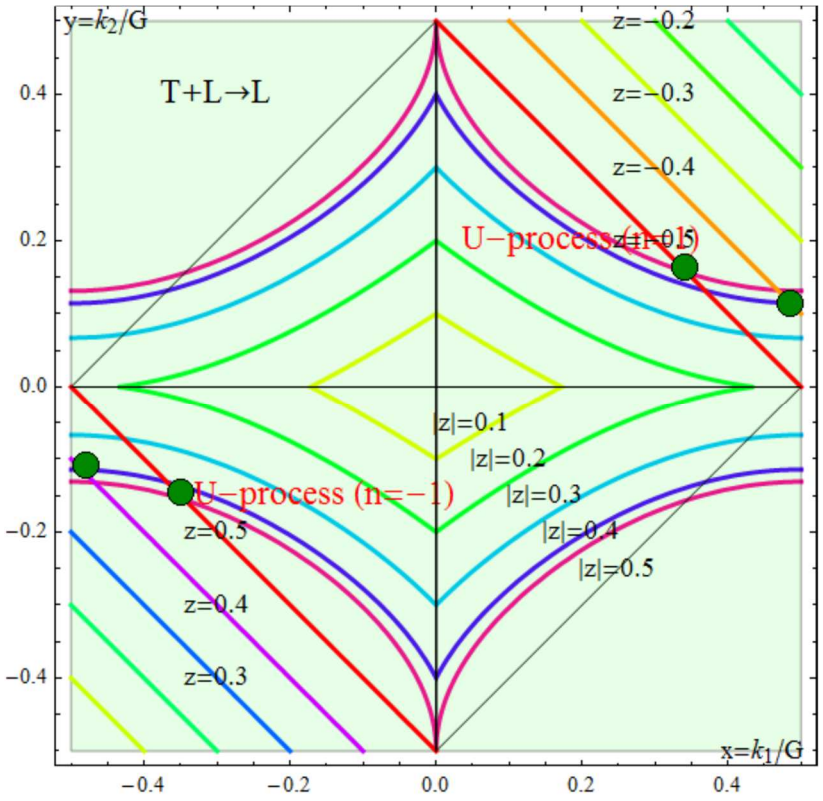


Fig. ContourPlot of $\omega_1(T)+\omega_2(L)=\omega_3(T)$ in the x-y plane. a = 0.6. The parameter z is changes for $|z|<1/2$. The intersections (denoted by Green circles,) is seen between the ContourPlot and the U-process denoted by $x+y=z+n$ ($n=\pm1$).

(d) The case of $T+T\rightarrow L$

We have

$$a|\sin(\pi x)|+a|\sin(\pi y)|=|\sin(\pi z)|$$

with a = 0.6

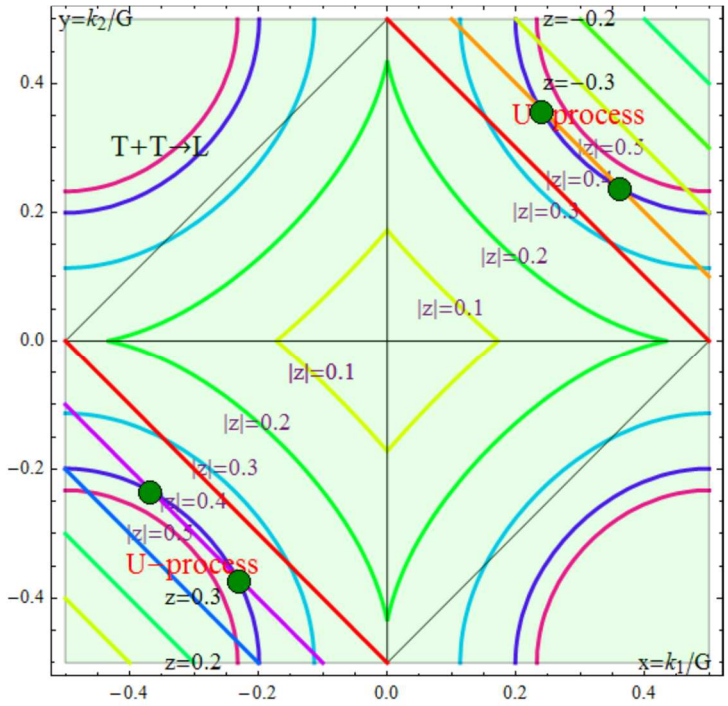


Fig. ContourPlot of $\omega_1(T)+\omega_2(T)=\omega_3(T)$ in the x-y plane. a = 0.6. The parameter z is changes for $|z|<1/2$. The intersections (denoted by Green circles) is seen between the ContourPlot and the U-process denoted by $x + y = z + n$ ($n = \pm 1$).

9. Thermal conductivity for electron in metal (Cochran)

The contribution of the thermal conductivity by electron is determined by an equation similar to that of phonon. The electron specific heat is small compared with the lattice specific heat except at low temperatures. However, the velocity of the electrons is two or three orders of magnitude greater than phonon velocities since only those electrons with wavevectors near the Fermi surface contribute. The relaxation time for electron collision is determined by interaction with the boundaries, with impurities and imperfections, with phonons and with other electrons. Detailed calculations give the result that for pure metals the electron contribution to the thermal conductivity is generally at least an order of magnitude greater than the phonon contribution over the whole temperature range, so that the latter contribution can be neglected. In this situation both charge current and heat current are carried by the electrons only.

REFERENCES

C. Kittel, Introduction to Solid State Physics, Eighth edition (John-Wiley & Sons, 2005).
R.E. Peierls, Quantum Theory of Solids (Oxford, 1955).

N.W. Ashcroft and N.D. Mermin, Solid State Physics (Harcourt College, 1972)
J.M. Ziman, Principles of The Theory of Solids, second edition (Cambridge, 1972).
W. Cochran, The Dynamics of Atoms in Crystals (Edward Arnold, 1973).
R Levy, Principles of Solid State Physics (Academic, 1968).
R. Berman, Thermal Conduction in Solids (Oxford, 1976).
P.G. Klemens,"Thermal Conductivity and Lattice Vibration Modes," in Solid State Physics vol. 7, edited by F. Seitz and D. Turnbull (Academic Press, 1958).

Appendix Evaluation of k_D

The cut-off wave number in the Debye model is given by

$$k_D = \left(6\pi^2 \frac{N}{V} \right)^{1/3}$$

We consider a simple cubic,

$V = Na^3$ for sc crystal.

Then we have

$$k_D = \left(6\pi^2 a^{-3}\right)^{1/3} = \left(6\pi^2\right)^{1/3} a^{-1} = \frac{3.89778}{a}.$$

or

$$k_D = \frac{(6\pi^2)^{1/3}}{\pi}\frac{\pi}{a} = 1.2407\ \frac{\pi}{a}$$

The Brillouin zone is $\frac{G}{2} = \frac{\pi}{a}$. Thus k_D is a little larger than $G/2$.