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SPONTANEOUS EMISSION OF PHONONS BY CARRIERS IN A PERFECT LATTICE AT $0^{o}K$

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A charge carrier in a perfect semiconductor at $0^{o}K$ will spontaneously emit phonons, when its speed exceeds the speed of sound. The average force due to spontaneous emission is evaluated for both normal and Umklapp processes. An approximate solution of the Boltzmann equation shows, that in the vicinity of the speed of sound the excess velocity is proportional to the fourth root of the applied electric field.

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INTRODUCTION

FOR an electron in a perfect semiconductor the mobility due to phonon scattering is usually assumed to depend on temperature as $\mu \sim T^{-3/2}$. In the derivation of this law [1] the changes of the electron energy during the scattering process are neglected. The emission and absorption processes therefore enter into the Boltzmann equation in a simmetric way, and the contribution of the spontaneous emission, which dominates at very low temperatures, is lost. In the present work the effect of the spontaneous emission alone, in the absence of phonons on the electron dynamics is studied.

In metals the resistivity due to the phonon interaction follows a T^5 dependence. This law takes into account the spontaneous emission; at low temperatures the spontaneous emission processes in the perturbed fermi distribution are supressed by the exclusion principle for small currents.

THE MODEL

Consider one Bloch electron in a perfect lattice. It is coupled to lattice vibrations; the matrix element for the transition of the electron from state k to k' under emission of a phonon of wave vector $\underline{q}$ is given by [2]

$$M(\underline{k};\underline{k}') = (n_q+1)^{\frac{1}{2}} \, (2\pi\hbar/2\rho V\omega_q)^{\frac{1}{2}} \, q \, \varepsilon_1 \, \delta_{\underline{\ell},\underline{k}-\underline{k}'-q} \, , \qquad (1)$$

where ρ is the density of the crystal, $n_{\underline{q}}$ the initial number of phonons in the state $\underline{q}$, V the volume of the crystal, ω_q the frequency of the phonon, $\underline{l}$ a vector of the reciprocal lattice, and ε_1 the coupling constant.

The temperature is mantained equal to zero. Therefore $n_{\underline{q}} = 0$, and only the spontaneous emission processes will contribute. To avoid difficulties from the exclusion principle, one electron only is considered.

The assumption of a moving electron excludes such insulators in which carriers become trapped by the deformation of the lattice [3]. It applies to the usual semiconductors with carriers of high mobility. Furthermore, the assumption that $n_{\underline{q}} = 0$ at all times eliminates the description of phonon amplification, which has actually been realized by the acceleration of a large number of charge carriers [3, 4].

TREATMENT WITH AN AVERAGE FORCE

For an estimate of the electric field necessary to mantain an electron in a state $\underline{k}$ we shall sum over the momentum losses per unit time, which on the average occur by spontaneous emission of phonons. The probability per unit time of a transition from $\underline{k}$ to k' is given by the quantum mechanical formula

$$P(\underline{k};\underline{k}') = (2\pi/\hbar)|M(\underline{k};\underline{k}')|^2 \, \delta(\varepsilon_{\underline{k}}-\varepsilon_{\underline{k}'}-\hbar\omega_{\underline{q}}) \; .$$

For the calculation we shall assume a scalar effective mass of the electron, i.e. $\varepsilon_{\underline{k}} = \hbar^2k^2/2m^*$, a linear phonon dispersion

$\omega_{\underline{q}} = cq$, and p = 3 phonon polarizations. The force on the electron is the momentum loss per unit time

$$F_{\underline{k}} = \sum_{\underline{k}'} p\ P(\underline{k};\underline{k}')\ \hbar(\underline{q}+\underline{\ell})\ .$$

With (1) and the replacement $\sum_{\underline{k}'} = \sum_{\underline{q}\underline{\ell}} = \left[V/(2\pi)^3\right]\int d^3q \sum_{\underline{\ell}}$ this becomes

$$F_{\underline{k}} = A\hbar\sum_{\underline{\ell}} \int q(\underline{\ell}+\underline{q})\,\delta\left[\hbar^2\underline{k}^2/2m^* - (\hbar^2/2m^*)(\underline{k}-\underline{q}-\underline{\ell})^2 - \hbar cq\right]\, d^3q\,, \qquad (2)$$

where $A = p\,\mathcal{E}_1^2/4\pi\rho c$ combines the constants which do not depend on $\underline{q}$.

A. Normal Processes, $\underline{\ell} = 0$

Introducing the angle θ between the vectors $\underline{k}$ and $\underline{q}$, and the de Broglie wave vector of an electron which travels with the speed of sound $\gamma = m^*c/\hbar$, the force is

$$F_{\underline{k}} = (2\pi A m^*/\hbar k)\int_0^\infty q^3 dq \int_{-1}^{1} \cos\theta\,\delta\left[\cos\theta - (q+2\gamma)/2k\right]\, d(\cos\theta)\ . \qquad (3)$$

From the properties of the δ-function, one integration consists in the replacement

$$\cos\theta = (q+2\gamma)/2k\ ,$$

which is possible within the limits

$$q_M = 2(k-\gamma) \qquad \text{for} \qquad \cos\theta = +1$$

$$q_m = 0 \qquad \text{for} \qquad \cos\theta = \gamma/k = c/v$$

Spontaneous emission can only occur when $\gamma/k < 1$, that is, when the speed of the electron $\hbar k/m^*$ is larger that the speed of sound c. The emission is limited to a cone given in the laboratory system by the angles

$$\theta_M = \cos^{-1} 1 = 0 \quad \text{and} \quad \theta_m = \cos^{-1}(v/c),$$

and in a system moving with the electron by the angles

$$\alpha_M = \pi \quad \text{and} \quad \alpha_m = \pi/2 + \theta_m \ .$$

This emission of phonons by a supersonic electron is analogous to Čerenkov radiation. (Fig. 1).

The expression (3) can be integrated:

$$F_{\underline{k}} = (2\pi Am^*/\hbar k)\int_0^{2(k-\gamma)} q^3(q+2\gamma)/2k \, dq$$

$$F_{\underline{k}} = (8\pi Am^*/5\hbar k^2)(k-\gamma)^4(4k+\gamma) \text{ for } \gamma/k < 1, \tag{4}$$

and $F_{\underline{k}} = 0$ otherwise.

B. Umklapp Processes, $\underline{\ell} \neq 0$

These contributions depend on the details of the crystal structure. We shall evaluate a case in which the umklapp process is most efficient, namely when $\underline{\ell}$ lies in the direction of $\underline{k}$. (Fig. 2).

Equation (2) then reads

$$F_{\underline{k}}^{\underline{\ell}} = [2\pi Am^*/\hbar(\ell-k)]\int q^2 dq\,|(\ell+q\cos\theta)\,\delta[\cos\theta+(q^2+2q\gamma+\ell^2-2\ell k)/2q(\ell-k)]\,d(\cos\theta),$$

or after integrating over $\cos\theta$

$$F_{\underline{k}}^{\underline{\ell}} = \left[\pi Am^*/\hbar(\ell-k)^2\right]\int_{q_-}^{q_+} q^2(\ell^2-q^2-2q\gamma)dq = \left[\pi Am^*/\hbar(\ell-k)^2\right]\left[\tfrac{1}{3}\ell^2 q^3 - \tfrac{1}{5}q^5 - \tfrac{1}{2}\gamma q^4\right]_{q_-}^{q_+} .$$

The limits of integration $q_{\pm} = \ell - k - \gamma \pm \left[(k+\gamma)^2 - 2\ell\gamma\right]^{\frac{1}{2}}$ correspond to the possible emissions with $\cos\theta = -1$. The transition can only occur when these limits are real, i.e. when $k \geqslant (2\ell\gamma)^{\frac{1}{2}} - \gamma$.

The ratio $F_{\underline{k}}^{\ell}/F_{\underline{k}}$ is plotted in Fig. 3 for the value $\gamma/\ell = (10^5 \text{cm}^{-1}/10^8 \text{ cm}^{-1}) = 10^{-3}$. It is seen that unklapp processes in this case occur only for electrons with 44 times the spead of sound, which, as will be seen later, would require a field of order 10^3 Volt/cm. The spontaneous emission of optical phonons sets in at electron energies which usually lie still higher.

DISTRIBUTION FUNCTION

The above treatment is inconsistent. The electron will not stay in the state $\underline{k}$, but make transitions. It is therefore necessary to introduce a statistical distribution $f(\underline{k})$, which is the probability that the electron occupies the state $\underline{k}$. It satisfies a Boltzmann equation. Once $f(\underline{k})$ is known, the average velocity of the electron can be calculated as a function of the applied field.

The Boltzmann equation for a stationary distribution

$$(eE/\hbar)\, \partial f(\underline{k})/\partial k_x = A\int q f(\underline{k}+\underline{q})\, \delta\left[\hbar^2(\underline{k}+\underline{q})^2/2m^* - \hbar^2\underline{k}^2/2m^* - \hbar c q\right] d^3q$$

$$- A\int q f(\underline{k})\, \delta\left[\hbar^2\underline{k}^2/2m^* - \hbar^2(\underline{k}-\underline{q})^2/2m^* - \hbar c q\right] d^3q \quad (5)$$

states that the change of $f(\underline{k})$ per unit time due to an electric field E in x direction is compensated by the transitions into and out of a state k.

Transitions into a given k are possible from the points of a rotationally simmetric surface in k-space. The corresponding analytical expression follows from the first δ-function in (5):

$$q = 2(\gamma - k \cos\theta) .$$

Similarly the surface into which a given k can radiate is given by

$$q = 2(k \cos\theta - \gamma) .$$

Note in Fig. 4 that in the limit when $k \rightarrow \gamma$, the transitions occur radially. For an electron in a state k, which lies near the sphere $k = \gamma$ in the direction of the electric acceleration, both this acceleration and the spontaneous transitions correspond to radial motions. Provided that the distribution has a sufficiently small angular spread, so that $\cos\nu \simeq 1$, where $\nu = \measuredangle(k, eE)$, it is the balance of these two opposite radial motions which determine the current.

We shall limit the problem to a region near the γ sphere. As long as $\cos\nu \simeq 1$, the distribution function will be a product of a radial and an angular function, where the radial function alone is important for the current. It is therefore sufficient to estimate the angular spread.

For this we assume that a spontaneous emission from k changes the angle ν by $\pm\eta$, where actually $\eta = [(k-\gamma)/\gamma]^{3/2}$, and that the subsequent electric acceleration contributes to ν with $-\nu(k-\gamma)/\gamma$. Such a sequence reduces ν when $|\nu| > \eta\gamma/(k-\gamma) =$

$= [(k- \ )/\gamma]^{\frac{1}{2}}$. For $(k-\gamma)/\gamma = 0.1$ the angle will therefore stay within 0.3 so that cos 0.3 = 0.94 is not much different from 1.

PROJECTED BOLTZMANN EQUATION

We introduce the dimensionless variables of Fig. 5; where γ has been used as a unit in k-space, and neglect in the following terms of order ξ^4. A projected transition rate is obtained by integrating $P(\xi;\sigma,\eta)$ over the plane σ = const.:

$$P(\xi;\sigma) = 2\pi \int P(\xi;\sigma,\eta)\eta \, d\eta \ .$$

Using for this the relation

$$\eta = (\xi - \sigma)(\xi + \sigma)^{\frac{1}{2}} \ ,$$

the projected Boltzmann equation is obtained

$$\begin{aligned} df(\sigma)/d\sigma &= \frac{1}{4} B \int_0^\infty (\sigma - \xi)^2 f(\xi) d\xi - \frac{2}{3} B\sigma^3 f(\sigma) & \sigma > 0 \\ df(\sigma)/d\sigma &= \frac{1}{4} B \int_{-0}^\infty (\sigma - \xi)^2 f(\xi) d\xi & \sigma < 0 \end{aligned} \qquad (6)$$

where $B = 8\pi A m^* \gamma^3/\hbar e E$ is dimensionless.

It is noteworthy that B disappears from the equation (6) with the transformation $s = B^{1/4}\sigma$, $x = B^{1/4}\xi$.

$$\begin{aligned} df(s)/ds &= \frac{1}{4} \int_s^\infty (s-x)^2 f(x)\, dx - \frac{2}{3} s^3 f(s) & s > 0 \\ df(s)/ds &= \frac{1}{4} \int_{-s}^\infty (s-x)^2 f(x)\, dx \ . & s < 0 \end{aligned} \qquad (7)$$

The mean velocity

$$\langle v\rangle = c(1+\langle\sigma\rangle) = c(1 + \langle s\rangle B^{-1/4}) \qquad (8)$$

therefore again shows the $E^{1/4}$ dependence implied in eq. (4) for $k \rightarrow \gamma$.

An asymptotic solution of (7) for large s is $f(s)=\exp\left[-s^4/6\right]$, which shows a very rapid decay. For s = 0 eq. (7) shows that $\left[df(s)/ds\right]_{s=0} > 0$ and $\left[d^2f(s)/ds\right]_{s=0} < 0$. More information about f(s) may be obtained by iteration procedures. Starting with $f(x) = 1/a$ for $0 < x < a$ and $f(x) = 0$ otherwise, we obtain after one step

$$f(s) = \left[\frac{1}{6}(a^4 - s^4) - \frac{1}{48}(a-s)^4\right]\frac{5}{a^5} \qquad 0 < s < a$$

$$f(s) = \left[\frac{1}{6}(a^4 + s^4) - \frac{1}{48}(a-s)^4\right]\frac{5}{a^5} \qquad -a < s < 0 \qquad (9)$$

$$f(s) = 0 \qquad |s| > a ,$$

where the constants of integration have been chosen so that f(s) is continuous for s = 0 and vanishes at symetric points $\pm$ a. Note that with the approximate solution (9) $df(0)/ds$, $d^2f(0)/ds^2$, and $d^3f(0)/ds^3$ are continuous at s = 0, as required by (7) for the exact solution.

The parameter a can be determined by some aditional requirement. A physical condition is that the total momentum irradiated by the distribution per unit time equals the force on the charge. From (4) this is given by

$$\frac{B}{5\gamma^3}\int_{k>\gamma} k^{-2}(k-\gamma)^4\,(4k+\gamma)\,f(\underline{k})\cos\varphi\; d^3k = 1 ,$$

where $\varphi = \measuredangle(\underline{k}, e\underline{E})$. Similarly, the total energy irradiated per unit time is equal to the energy dissipated by the electric field, if

$$\frac{B}{\gamma^2} \int_{k>\gamma} k^{-1}(k-\gamma)^4 \, f(\underline{k}) \, d^3k = \int kf(\underline{k}) \cos\varphi \, d^3k \ .$$

In the one dimensional case both equation read to lowest order in ξ

$$\int_0^a f(s) \, s^4 ds = \int_{-a}^a f(s) ds \ ,$$

which is satisfied with (9) and $a = 2.32$. This determine the mean value of s

$$\langle s \rangle = \int_{-a}^a sf(s) \, ds = \frac{a}{6} = 0.38 \ .$$

Owing to the rough calculation this value may be in error by as much as 20%. The velocity of the electron by (8) is

$$\langle v \rangle = c(1 + 0.38 \, B^{-1/4}) \ .$$

CONDITIONS ON A MEASUREMENT

Although this improved treatment changes the earlier result (4) only slightly, the effect on the electric field is considerable owing to the $E^{1/4}$ dependence. For an order of magnitude estimate, we insert numerical values, which may be typical for Germanium, although the use of a scalar effective mass is a considerable source of error. Let $\varepsilon_1 = 4.8$ ev., $c = 3.9 \; 10^5$ cm/sec., $m^* = 0.3$ m, $\rho = 5.46$ gr/cm^3. Then $\gamma = 10^5$ cm^{-1}, $A = 0.66 \; 10^{-29}$ erg cm^4/sec., $B = 2.7 \; 10^{-2}$ Volt cm^{-1}/E. A mean velocity $\langle v \rangle =$

$= 1.1$ is sustained by an electric field $E = 1.3\ 10^{-4}$ Volt/cm. Typical emitted phonons then have a wave vector $q = 0.1\gamma = 10^4\ cm^{-1}$. Therefore a relaxation time between emissions τ is given by $eE\tau = \hbar q$, from which $\tau = 4.5\ 10^{-8}$ sec. This corresponds to a mean free path for spontaneous phonon emission $\lambda = 1.1\ c\tau = 2\ 10^{-2}$ cm. This requires that a sample used for observation be sufficiently pure, so that the density N of scattering centers with a cross section S satisfy $NS \ll \lambda^{-1}$. In order that phonons of wave vector q are not excited thermally, the temperature must be less than $\hbar cq/k_B = 3\ 10^{-2}\ {}^oK$.

For a ten times higher field $E = 1.3\ 10^{-3}$ Volt/cm, we obtain $\langle v \rangle = 1.18$, $\tau = 8.10^{-9}$ sec., $\lambda = 3.7\ 10^{-3}$ cm, $T < 5\ 10^{-2}\ {}^oK$, where, however, the velocity may already exceed the range of validity of this approximation.

The values show that an observation should be rather delicate.

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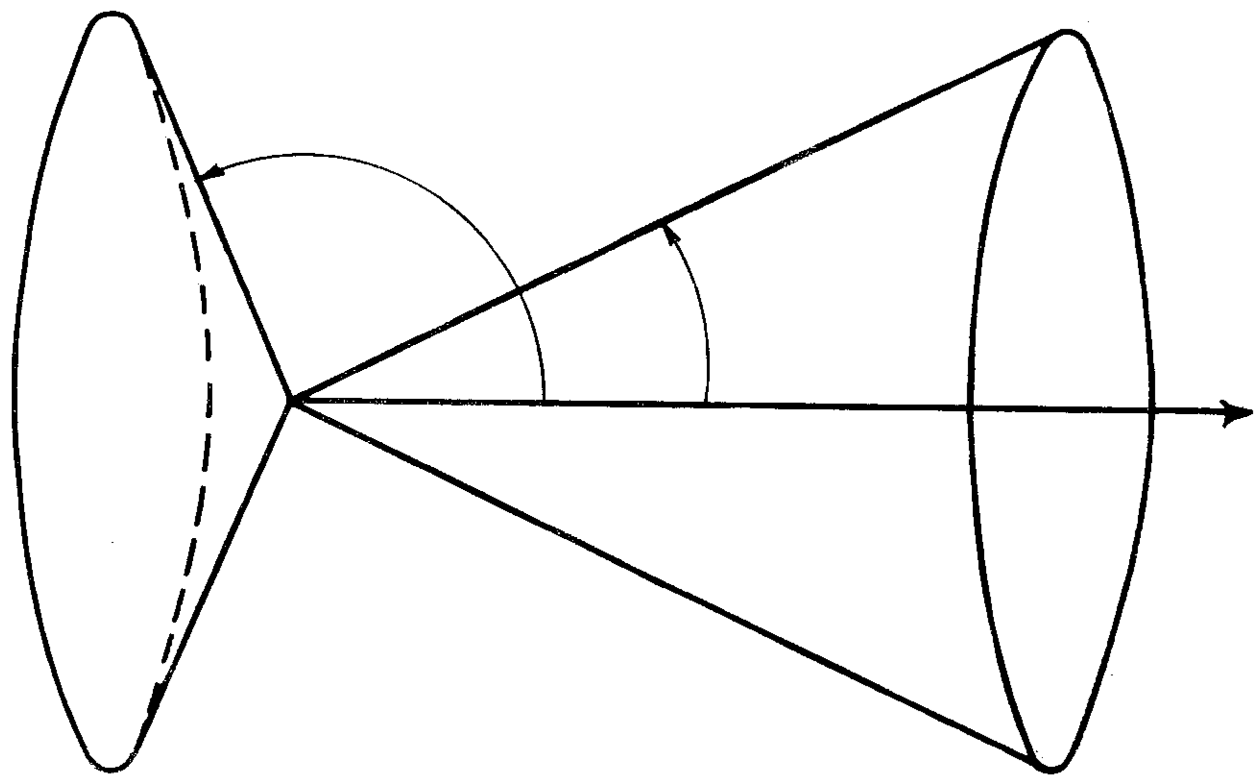

Fig. 1: Angle of the Čerenkov cone in the laboratory system (θ_m) and the moving system of coordinates (α_m).

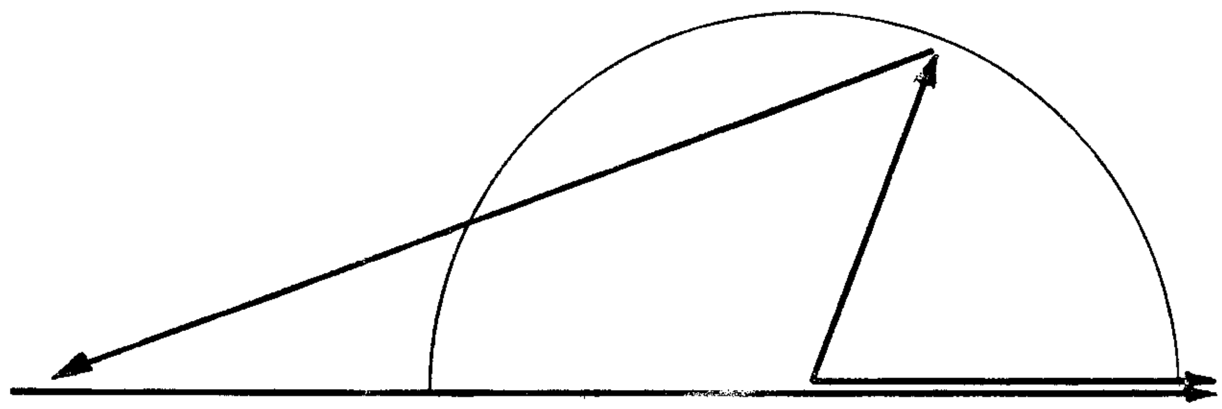

Fig. 2: Momentum conservation in an Umklapp process.

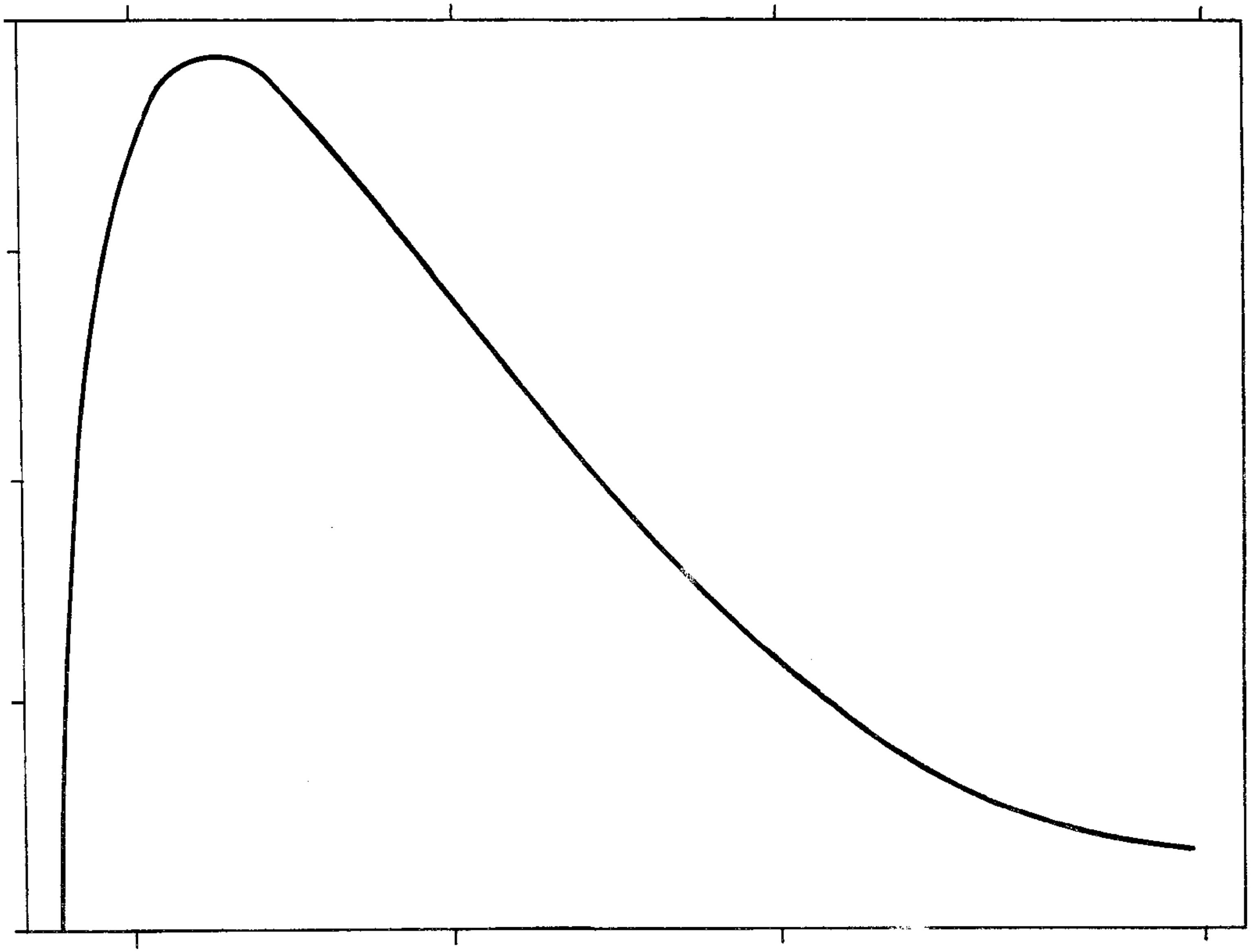

Fig. 3: Ratio of the mean force due to Umklapp processes to the mean force due to the normal processes.

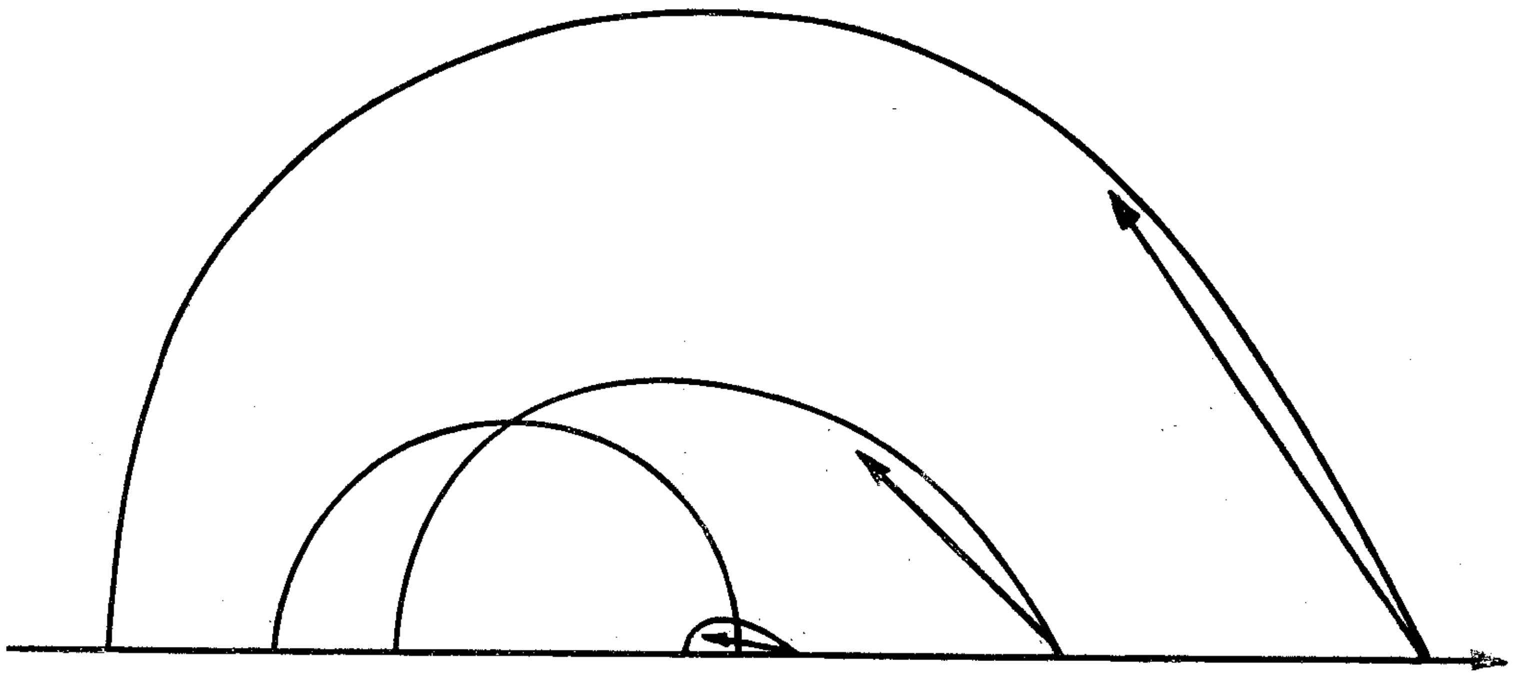

Fig. 4: Transitions occur from any point $\underline{k}$, where $k > \gamma$, to the corresponding rotationally symmetric surface shown.

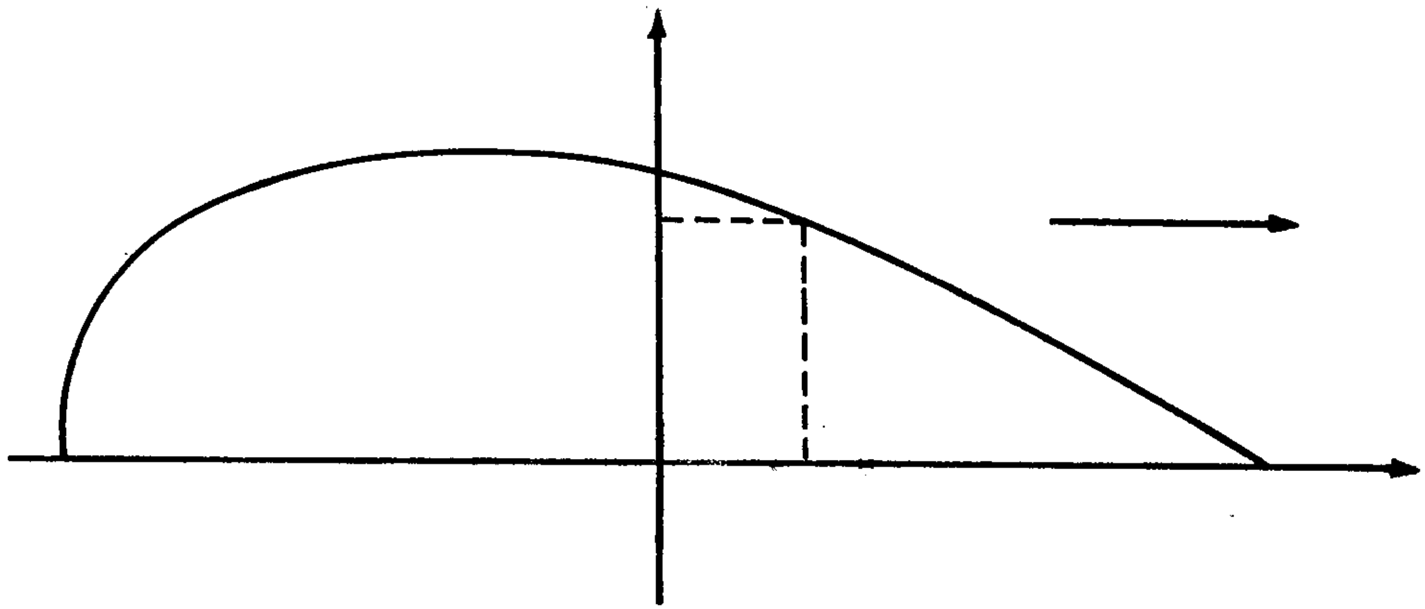

Fig. 5: Dimensionless units in **k**-space.

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