SC

PECULIARITIES OF THE ELECTRON-PHONON INTERACTION DURING CHANGE OF TOPOLOGY OF THE FERMI SURFACE IN METALS

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ABSTRACT

The necessary background material for the analysis of the electron phonon interaction with respect to the absorption coefficient and change in incident phonon frequency is discussed in the first and second chapters of this thesis. At the end of the second chapter the Migdal-Kohn anomalies for a spherical Fermi surface is discussed. Experimental varification and phisical sense of these anomalies is also presented here.

An investigation of the change in the phonon spectrum due to the Migdal-Kohn anomalies for some important cases of change in topology of the Fermi surface in metals is done in chapter three. In general it is found that the anomalies in Γ and $\Delta\omega$ depend on the changes of the Fermi surface topology caused at phase transition of order $2\frac{1}{2}$. Also it is noted that the singularities in Γ and $\Delta\omega$ are interdependent as can be predicted by the Kramer's and Kronig relations.

INTRODUCTION

A clear majority of the elements in the periodic table are metals. Together with their alloys they form a great multitude of substances with very diverse properties. Metals differ from each other and to a great extent from the nonmetals in their electrical properties, heat conductivity, optical properties, magnetic and mechanical properties.

Despite all these diversified properties there is a common characteristic which allows all metals to be described from a single standpoint. This is the energy spectrum of electrons in metals or the dependence of the energy "ε" of the electrons on their momenta "$\vec{p}$".

According to the modern views, a metal may be regarded as a combination of a system of positively charged oscillating ions which form a quasi-periodic space-structure (cystalline) and a system of relatively free valence electrons filling the lattice. The difference between any two metals may be related to the difference in valence electrons of atoms, the peculiarities of their electronic structure and the symmetry of the crystal lattice. Thus, a metal can be thought as a "sea" of valence electrons moving in a cystalline lattice of ions. These electrons are often called conduction electrons.

A convinient method for the description of the energy spectrum of the electrons in metals is through the introduction of a

Fermi surface for metals. This is the surface which separates the region occupied by electrons from the region free from electrons at 0 degree Kelvin (absolute zero temperature). The Fermi surface is one of the constant energy surfaces of the metal $\varepsilon(\vec{p}) = \varepsilon$. It can have a simple shape as in metals of the first group Na, K, and Rb and the noble metals silver and gold or a very complex shape as in lead.

A.R. Mackintosh says "Few people would define a metal as a solid with a Fermi surface." This definition represents a profound advance in the understanding of why metals behave as they do. The concept of the Fermi surface as developed by quantum physics provides a precise explanation of the main physical properties of metals.

Delineating the Fermi surface of a specific metal is an intricate problem in solid state physics. Experimental methods for studying the energy spectrum and determination of Fermi surface of metals are mostly based on investigation of various physical effects in metals occurring in the presence of an external magnetic field (eg. Brandt and Chudinov, 1975). A feature of all these methods is the use of strong magnetic fields in which cyclic motion of current carriers is observed. This is linked with that the nature of cyclic motion is determined by the topology and shape of the Fermi surface and therefore allows a certain information on that surface to be obtained.

Another promising method to determine this surface is based on peculiarities of electron-phonon interaction which is to be discussed in greater detail in chapters 2 and 3. A.B. Migdal (1958) and W. Kohn (1959) independently showed that the electron-phonon interaction brings about a logarithmic singularity at $q = 2P_F$ where q is the phonon momentum and P_F is the Fermi momentum which is equal to $\sqrt{2m\varepsilon_F}$. This singularity if observed offers a direct information of the radius of the spherical Fermi surface in momentum space.

The aim of the thesis is to investigate the change of the phonon spectrum due to the Migdal-Kohn singularities in some important cases of variation of topology of the Fermi surface in metals (Lifshits 1960):

a) appearance of a new cavity

b) breaking of the connecting neck.

A digression on the energy spectrum of the electrons in metals is necessary. It is extremely important to device scientific models to be able to describe the properties of metals. The free electron model for example helps us to describe the heat capacity, thermal conductivity, electrical conductivity, magnetic susceptibility and electrodynamics of metals eventhough it fails to help us with other large questions like the distinction between metals, semiconductors and dielectrics; the occurence of the positive values of the Hall Coefficient etc. Therefore, important attempts to improve this model have been made and will continue to be until a well established and consistent theory is developed.

It was possible to go much further with the theory after the fundamental work of Bloch and Peierls in which the concept of free-electrons was developed significantly (Lifshitz and Kaganov, 1960). In Bloch's theory the interaction of the conduction electron with the crystalline medium was described by introducing a periodic potential to take into account the symmetry of the lattice.

The study of the motion of particles in a periodic field led to the explanation of the band theory of metals. Detailed investigation of the energy spectrum of electrons in metals indicates that the electrons in crystals are arranged in energy bands separated by regions in energy for which no electron states exist. Such forbidden regions are called energy gaps or forbidden bands.

One of the most important consequences of the band theory was the distinction between metals, semimetals, semiconductors and dielectrics using a criterion the filling of the zones in the ground state. Metals corrospond to materials having a partially filled zone (eg. see diagram from Kittle (1976)).

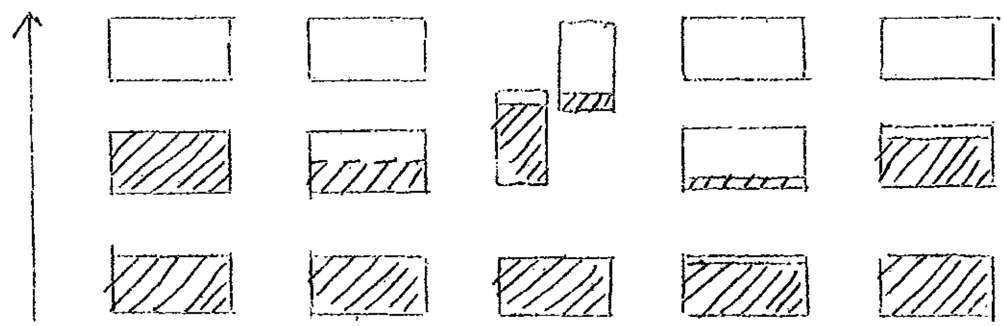

Fig.1. Schematic diagram of energy bands of different substances

The Bloch model which is formulated as a one-electron problem in a crystalline medium is not without its limitations. For example it is not clear whether or not a consistent inclusion of electron interactions will cause fundamental changes in the concepts of the band theory (Lifshitz and Kaganov, 1960).

A new approach to the problem of the electron theory of metals is based on the general idea that energy spectrum in metals have several branches. Each branch being a quantised system has its characteristic quasi-particles which carry definite energy and momentum. The simplest examples of such elementary excitations or quasi-particles are the system of valence electrons (which are treated as an ideal gas of charged Fermi quasiparticles), phonons in crystals, spin waves (magnons) in ferromagnets, excitons in semi-conductors and dielectrics etc. Depending on the statistics of the quasiparticles which produce the energy spectrum of the system, we say that the spectrum is a Bose or Fermi Spectrum.

The energy spectrum of the individual quasiparticle is a periodic function of the quasi-momentum $\vec{p}$ and single valued for each band "s" unless there is overlapping of bands. That is $\varepsilon_s(\vec{p}) = \varepsilon_s(\vec{p} + 2\pi\hbar\vec{b})$ or using the wave vector notation

$$\varepsilon_s(\vec{k}) = \varepsilon_s(k + 2\pi\vec{b}) .$$

For every band "s" we have minimum and maximum values of the energy and these values are followed by the forbidden bands. That is

$$\varepsilon_{min} < \varepsilon_s(\vec{p}) < \varepsilon_{max}$$

For example a plot of energy versus wave vector for an electron in a monatomic linear lattice gives the following diagram:

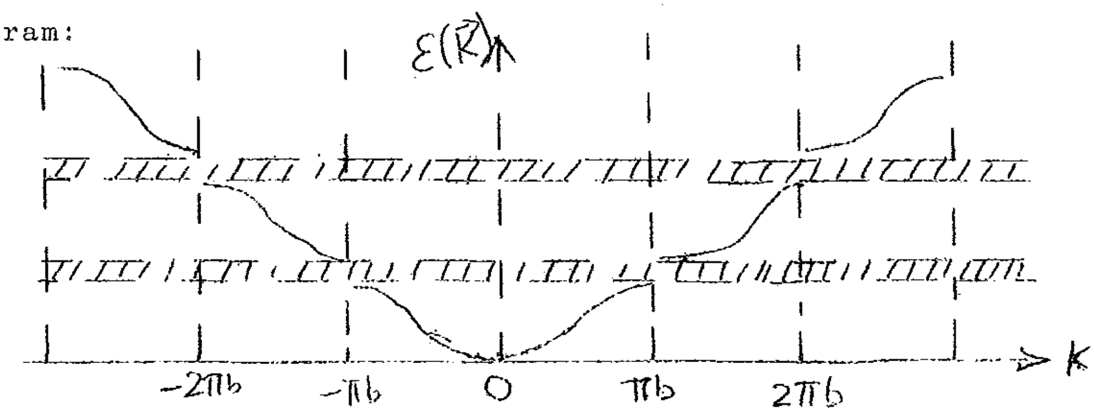

Fig.2. Energy spectrum of one dimensional monatomic lattice, shadded region is a forbidden band.

The zero slope of the energy spectrum at the zone boundaries follows from the two requirements that

$$\varepsilon_s(\vec{p}) = \varepsilon_s(-\vec{p}) \quad \text{symmetric dispersion law}$$

and

$$\varepsilon_s(\vec{p}) = \varepsilon_s(\vec{p} + 2\pi\hbar\vec{b}) \quad \text{periodic dispersion law}$$

Thus, the group velocity $V_g = \dfrac{\partial \varepsilon_s(\vec{p})}{\partial p} = 0$ at zone boundaries.

CHAPTER 1

THERMODYNAMICAL PROPERTIES OF METALS AND GEOMETRY

1.1 Geometry of Isoenergetic Surfaces

Consider the dispersion law $\varepsilon_s(\vec{p})$ of an electron. It is already stated that $\varepsilon_s(\vec{p})$ attains its minimum and maximum values for definite values of the quasimomentum $\vec{p}$. What is the shape of $\varepsilon_s(\vec{p}) = \varepsilon =$ constant, which is an isoenergetic surface of the electron in momentum space? To answer this question we have to expand $\varepsilon_s(\vec{p})$ about the minimum (or maximum) energy for a specific band s. If we disregard cases of degeneracy, the expansion has the following form (Lifshitz and Kaganov, 1960)

$$\varepsilon_s(\vec{p}) = \varepsilon_{min} + \frac{\partial \varepsilon_s(\vec{p})}{\partial \vec{p}}(p-p_{min}) + \tfrac{1}{2}\frac{\partial^2 \varepsilon_s(\vec{p})}{\partial p_i \partial p_k}(p_i - p_{imin})(p_k - p_{kmin})$$

$$= \varepsilon_{min} + \tfrac{1}{2}\left.\frac{\partial^2 \varepsilon_s(p)}{\partial p_i \partial p_k}\right|_{p=p_{min}}(p_i - p_{imin})(p_k - p_{kmin}) \qquad (1)$$

$\left.\dfrac{\partial^2 \varepsilon_s(\vec{p})}{\partial p_i \partial p_k}\right|_{p=p_{min}}$ is a symmetric tensor of the second rank.

The components of the tensor have the dimension of the reciprocal mass. For this reason the tensor is called the reciprocal effective mass tensor and is denoted by

$$M_{ik}^{-1} = \frac{\partial^2 \varepsilon_s(\vec{p})}{\partial p_i \partial p_k} \qquad (2)$$

M_{ik}^{-1} can be diagonalized and thus $\varepsilon_s(\vec{p})$ is reduced to the form

$$\varepsilon_s(\vec{p}) = \mathcal{E}_{min} + \frac{(p_1 - p_{1min})^2}{2m_1} + \frac{(p_2 - p_{2min})^2}{2m_2} + \frac{(p_3 - p_{3min})^2}{2m_3} . \quad (3)$$

If $\mathcal{E}_s(\vec{p})$ is referred to the minimum, we get a simpler equation

$$\varepsilon_s'(\vec{p}) = \varepsilon_s(\vec{p}) - \varepsilon_{min} = \frac{p_1^{\,2}}{2m_1} + \frac{p_2^{\,2}}{2m_2} + \frac{p_3^{\,2}}{2m_3} . \quad (4)$$

The principal values of the tensor m_1, m_2 and m_3 are positive when the expansion is about the minimum and negative when it is about the maximum. Equation (4) is the equation of an ellipsoid whose semi-axes are respectively equal to

$\sqrt{2m_1\varepsilon'}$, $\sqrt{2m_2\varepsilon'}$, $\sqrt{2m_3\varepsilon'}$. Thus, the surfaces of constant energy ε = constant, near the extremal points for electrons in a crystal are ellipsoidal surfaces. In the particular case when $m_1 = m_2 = m_3$ the ellipsoid degenerates into a sphere.

When the components m_1, m_2 and m_3 are positive (expansion about ε_{min}) an electron in the lattice behaves qualitatively like a free electron ie. its kinetic energy and velocity in an electric field increases in the direction of the acting force. If the components of the tensor are negative the electron is accelerated in the direction opposite to that of the external force and thus behaves as a negative mass particle and it is called hole-like (Brandt and Chudinov, 1975).

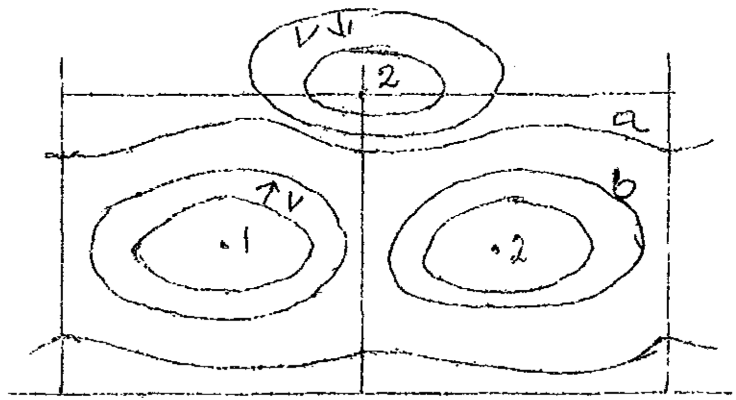

Fig.3. Open (a) and closed (b) isoenergetic surfaces near ε_{min} (1) and ε_{max} (2).

Any closed energy surface in momentum space near a minimum point encloses a region in the momentum space in which the energy is less than its value on the surface, while near a maximum point any point within has greater energy than the surface. This means that in the first case the velocity is directed along the external normal to the surface of constant energy and along the inward normal in the second case. Sine $\varepsilon_s(\vec{p})$ is periodic in reciprocal space (momentum space) the surfaces described above are repeated periodically over the whole reciprocal lattice.,

It is obvious that between these surfaces which are topologically simple there must be more complicated surfaces like open surfaces which extend throughout the whole reciprocal lattice for otherwise it would be impossible to have a continuous transition from surfaces surrounding minimum points to surfaces surrounding maximum points (Fig.3).

1.2 Change in Topology of Isoenergetic Surfaces

If metals are subjected to external pressure, the accompanying change in interatomic separations modifies the entire energy structure of the metal (Lifshits, 1960). However, if there is no change in the symmetry of the metal as a result of the external pressure there exists a quantitative change in the structure of the isoenergetic surfaces up to some critical pressure P_c. A qualitative change occurs at the critical pressure and the topology of the isoenergetic surface is changed. Some of the common changes are

a) appearance of a spherical isoenergetic surface

b) appearance (or disappearance) of ellipsoidal isoenergetic surfaces (Fig.4a)

c) breaking of necks (Fig.4b)

Fig.4a. Appearance of a new sheet of a constant energy-surface

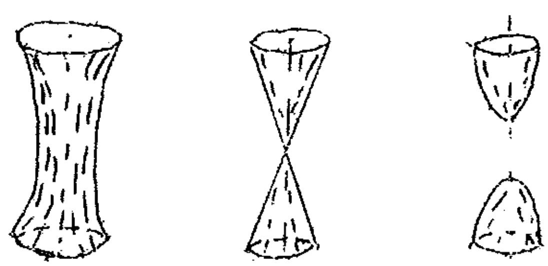

Fig.4b. Breaking up of a "bridge" on the isoenergetic surface.

The dispersion law $\varepsilon_s(p)$ near the critical points in the above transitions are given by

$$a)\quad \varepsilon_s(\vec{p}) = \varepsilon_c + \frac{p^2}{2m} \tag{5a}$$

$$b)\quad \varepsilon_s(\vec{p}) = \varepsilon_c + \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3} \tag{5b}$$

$$c)\quad \varepsilon_s(\vec{p}) = \begin{cases} \varepsilon_c + \dfrac{p_1^2}{2m_1} + \dfrac{p_2^2}{2m_2} - \dfrac{p_3^2}{2m_3}, & \varepsilon_s(\vec{p}) > \varepsilon_c \qquad (5c_1) \\[2ex] = \varepsilon_c \quad \text{or} \quad \dfrac{p_1^2}{2m_1} + \dfrac{p_2^2}{2m_2} - \dfrac{p_3^2}{2m_3} = 0 & \qquad (5c_2) \\[2ex] = \varepsilon_c + \dfrac{p_1^2}{2m_1} + \dfrac{p_2^2}{2m_2} - \dfrac{p_3^2}{2m_3}, & \varepsilon_s(\vec{p}) < \varepsilon \qquad (5c_3) \end{cases}$$

The Fermi surface is one of the isoenergetic surfaces in metals. So it can pe subjected to such types of transitions as a result of external pressure which may be caused by external electric, magnetic or acoustic fields and even mechanical forces reasonably enough not to cause change in symmetry in the crystal.

The above changes in topology of isoenergetic surfaces are known to be accompanied by singularities in the density of electron states as is shown in the next section.

1.3 Van Hove Singularities

Now let us find an expression for the density of states $\nu_s(\varepsilon)$ which determines the number of electron states per unit interval of energy.

The total number of quantum states per primitive cell is given by (in momentum space)

$$n_{\vec{p}} = \frac{2V}{(2\pi\hbar)^3} \int_{cell} d^3p \quad . \tag{6}$$

The total number of electron states for the energy $\varepsilon_s(\vec{p}) \leq \varepsilon$ is given by

$$N_s = \frac{2V}{(2\pi\hbar)^3} \int_{\varepsilon_s(\vec{p}) \leq \varepsilon} d^3p$$

$$= \frac{2V}{(2\pi\hbar)} \int_{\varepsilon_s(p) \leq \varepsilon} dp_1 dp_2 dp_3 \quad .$$

For an ellipsoidal surface $\varepsilon_s(\vec{p})$,

$$\int dp_1 dp_2 dp_3 = \frac{4}{3}\pi \ (2m_1 2m_2 2m_3)^{\frac{1}{2}} \ (\varepsilon-\varepsilon_{min})^{3/2}$$

and thus $N_s = \frac{2V}{(2\pi\hbar)^3} \ \frac{4}{3}\pi \ 2^{3/2} \ (m_1 m_2 m_3)^{\frac{1}{2}} \ (\varepsilon-\varepsilon_{min})^{3/2}$.

But $$\nu_s(\varepsilon) = \frac{dN_s}{d\varepsilon} \quad , \tag{7}$$

$$\nu_s(\varepsilon) = \frac{\sqrt{2}\,V}{\pi^2\hbar^3} \ (m_1 m_2 m_3)^{\frac{1}{2}} (\varepsilon-\varepsilon_{min})^{\frac{1}{2}} \quad , \tag{8}$$

This expression for the density of states gives

$$\nu_s(\varepsilon) = \frac{\sqrt{2}\ V}{\pi^2 \hbar^3} m^{3/2}\ \varepsilon^{\frac{1}{2}} \tag{9}$$

for the special case of spherical isoenergetic surface. Similar analysis of $\nu_s(\varepsilon)$ near maximum critical point ε_{max} gives,

$$\nu_s(\varepsilon) = \frac{\sqrt{2}\ V}{\pi^2 \hbar^3} (|m_1||m_2||m_3||)^{\frac{1}{2}} (\varepsilon_{max} - \varepsilon)^{\frac{1}{2}} \tag{10}$$

If we differentiate equations 8 and 10 with respect to energy we get a root type of singularities in the density of states $\nu(\varepsilon)$. Such singularities are called Van Hove singularities and are common to all quasiparticles (Van Hove, 1953).

The density of states $\nu(\varepsilon)$ can now be expressed as a sum of smooth part ν_o and singular part $\delta\nu$ ie.

$$\nu(\varepsilon) = \nu_o(\varepsilon) + \delta\nu(\varepsilon) \tag{11}$$

Where $\delta\nu(\varepsilon)$ is given by equation (8) for $\varepsilon > \varepsilon_{min}$ and by equation (10) for $\varepsilon < \varepsilon_{max}$. It is obvious that $\delta\nu(\varepsilon)$ should be zero for both $\varepsilon < \varepsilon_{min}$ and $\varepsilon > \varepsilon_{max}$.

For the case of breaking of necks or transition from hyperboloid of one sheet to hyperboloid of two sheets through the critical conical point $\varepsilon = \varepsilon_c$ of figure 4b we obtain similar singularities in $\nu(\varepsilon)$ as is shown below.

Consider first the hyperboloid of one sheet in Fig.4b. Calculation of the volume bounded by the surface

$$\varepsilon = \varepsilon_c + \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - \frac{p_3^2}{2m_3} \text{ and the surface}$$

$p_3 = p_o$ = constant gives

$$V_p = \int_{-p_o}^{p_o} d\,p = \int_{-p_o}^{p_o} \pi (2m_1)^{\frac{1}{2}}(2m_2)^{\frac{1}{2}}(\varepsilon-\varepsilon_c + \frac{p_3^2}{2m_3})\, dp_3$$

$$= 4\ (m_1 m_2)^{\frac{1}{2}}(\varepsilon-\varepsilon_c)p_o + \frac{2\pi(m_1 m_2)^{\frac{1}{2}}}{2m_3}\frac{p_o^3}{3},\ \varepsilon > \varepsilon_c \qquad (12)$$

If $\varepsilon < \varepsilon_c$ then we have hyperboloid of two sheets and $|p_3|_{min} \neq 0$.

$$V_p = \int_{+|p_3|min}^{p_o} d^3p + \int_{-p_o}^{-|p_3|min} d^3p$$

$$= 4\pi(m_1 m_2)^{\frac{1}{2}}(\varepsilon-\varepsilon_c)p_o + \frac{2\pi p_o^3}{3}\frac{(m_1 m_2)^{\frac{1}{2}}}{m_3} + \frac{8\pi}{3}(2m_1 m_2 m_3)^{\frac{1}{2}}(\varepsilon-\varepsilon_c)^{3/2}$$

$$\text{for } \varepsilon < \varepsilon_c \qquad (13)$$

Thus, $\nu(\varepsilon) = \frac{dN\varepsilon}{d\varepsilon}$

$$= \frac{d}{d\varepsilon}\ \{ \frac{2V}{(2\pi\hbar)^3}V_p \}$$

$$\doteq \begin{cases} \frac{2V}{(2\pi\hbar)^3}\, 4\pi(m_1 m_2)^{\frac{1}{2}}p_o\ , & \varepsilon > \varepsilon_c \\ \frac{2V}{(2\pi\hbar)^3}\, 4\pi(m_1 m_2)^{\frac{1}{2}}p_o + \frac{\sqrt{2}V}{\pi^2\hbar^3}(m_1 m_2 m_3)^{\frac{1}{2}}(\varepsilon_c-\varepsilon)^{\frac{1}{2}}, & \varepsilon < \varepsilon_c \end{cases}$$

The non-smooth part of the density of states for the case of breaking of necks is then identical to that of appearance (disappearance) of new isoenergetic surface equation (10).

1.4 Electron Phase Transitions of Order $2\frac{1}{2}$

It is shown in the previous section that for certain critical values of energy $\varepsilon = \varepsilon_c$ for which the topology of isoenergetic surfaces change (for example an open surface changes to a closed surface by disruption of a neck or a new splitting off region of surfaces appear) there corresponds peculiarities (root singularities) in the density of electron states. These anomalies are called electron phase transitions of Order $2\frac{1}{2}$ or Lifshitz Transitions after their discoverer (Lifshitz, 1960). At the point of such a transition the electron dynamics also possesses some peculiar features which lead to anomalies of the electron characteristics of the metal (thermodynamic and kinetic). It will be discussed in latter sections that such transitions create anomalies in the absorption coefficient and change in the phonon spectrum of an incident sound.

1.5 Anomalies in Thermodynamic Quantities as a Result of $2\frac{1}{2}$ Order Phase Transitions

It was found out that the singular part of $\nu(\varepsilon)$, the density of states, is given by

$$\delta\nu(\varepsilon) = \begin{cases} 0 & \varepsilon > \varepsilon_c \\ \alpha|\varepsilon-\varepsilon_c|^{\frac{1}{2}} & \varepsilon < \varepsilon_c \end{cases} \qquad (14)$$

where $\qquad = \frac{\sqrt{2}V}{\pi^2\hbar^3}\,(m_1 m_2 m_3)^{\frac{1}{2}}$.

The thermodynamic potential Ω has also smooth part and singular part as is the case for any other thermodynamic quantity. ie.

$\Omega = \Omega_o + \delta\Omega$. This function is related to the number of electrons and the chemical potential ξ of the electrons in the metal by the equation

$$N = -\frac{d\Omega(\xi)}{d\xi} \quad . \tag{15}$$

It is a standard equation in statistical physics that

$$\Omega = -T\int_0^\infty \nu(\varepsilon)\,\ln(1+e^{\frac{\xi-\varepsilon}{T}})d\varepsilon \ . \tag{16}$$

Limiting ourselves to the singular part we get

$$\begin{aligned}\delta\Omega &= -T\int_0^\infty\delta\nu(\varepsilon)\,\ln(1+e^{\frac{\xi-\varepsilon}{T}})d\varepsilon\\ &= -T\int_0^\infty\ln(1+e^{\frac{\xi-\varepsilon}{T}})dN(\varepsilon)\\ &= -T\,\ln(1+e^{\frac{\xi-\varepsilon}{T}})\delta N(\varepsilon)\Big|_0^\infty-\int_0^\infty\delta N(\varepsilon)\,\frac{e^{\frac{\xi-\varepsilon}{T}}}{1+e^{\frac{\xi-\varepsilon}{T}}}d\varepsilon\\ &= -\int_0^\infty\frac{\delta N(\varepsilon)}{e^{\frac{\xi-\varepsilon}{T}}+1}d\varepsilon \quad .\end{aligned}$$

But $\delta N(\varepsilon) = \frac{2}{3}\alpha\,(\varepsilon-\varepsilon_c)^{3/2}$ from equation (12). So

$$\delta\Omega = -\frac{2}{3}\alpha\int_{\varepsilon_c}^\infty\frac{(\varepsilon-\varepsilon_c)^{3/2}}{e^{\frac{\varepsilon-\xi}{T}}+1}\,d\varepsilon \quad .$$

Letting $z = \xi-\varepsilon_c$ and $\varepsilon-\varepsilon_c = x$ and considering the cases $z < 0$ and $z > 0$ we get

i) $z < 0$, $\delta\Omega = -\frac{2}{3}\alpha\int_0^\infty\frac{x^{3/2}dx}{e^{\frac{x+|z|}{T}}}$

for $T \ll |z|$ we have $e^{\frac{|z|}{T}} \gg 1$ and thus

$$\delta\Omega = -\frac{2}{3}\alpha\, e^{-\frac{|z|}{T}} \int_0^\infty \frac{x^{3/2}}{e^{\frac{x}{T}}}\, dx$$

Substitute $\frac{x}{T} = y^2$, $dx = 2Tydy$, and integrate to get

$$\delta\Omega = -\frac{\sqrt{\pi}}{2}\alpha\, e^{-\frac{|z|}{T}}\, T^{5/2}$$

ii) $z > 0$ $\quad \delta\Omega = -\frac{2}{3}\alpha \int_0^\infty \frac{x^{3/2}dx}{e^{\frac{x-z}{T}}+1}$

Considering again $T \ll |z|$ and using Sommerfeld's Integral $\int_0^\infty \frac{f(\varepsilon)d\varepsilon}{e^{\frac{\varepsilon-\xi}{T}}+1} \simeq \int_0^\xi f(\varepsilon)d\varepsilon + \frac{\pi^2 T^2}{6} f'(\xi)$

we get

$$\delta\Omega = \frac{-2}{3}\alpha\left(z^{5/2}\left(\frac{2}{5}\right) + \frac{\pi^2T^2}{6}\,\frac{3}{2}\,z^{\frac{1}{2}}\right)$$

$$= \frac{-4}{15}\alpha\, z^{5/2} - \frac{\pi^2}{6}\alpha\, T^2\, z^{\frac{1}{2}} \quad .$$

The combined result is then

$$\delta\Omega = \begin{cases} -\frac{\sqrt{\pi}}{2}\alpha\, e^{-\frac{|z|}{T}}T^{5/2} & z < 0 \\ -\frac{4}{15}\alpha\,|z|^{5/2} - \frac{\pi^2}{6}\alpha\, T^2|z|^{\frac{1}{2}} & z > 0 \quad . \end{cases} \tag{17}$$

For $T = 0$,

$$\delta\Omega = \begin{cases} 0 & z < 0 \\ -\frac{4}{15}\alpha|z|^{5/2} & z > 0 \end{cases} \tag{18}$$

The power of z in equation (18) is related to the name $2\frac{1}{2}$ Order phase transition. The second derivatives of Ω at the point of "electron transition" $z = 0$ have a vertical break. While the third derivatives go to infinity as $z^{-\frac{1}{2}}$ (Lifshitz 1960). Besides singularities in Ω we have also similar situation in the specific heat C_v, compressibility K and other thermodynamic quantities. In $2\frac{1}{2}$ order phase transitions no change in symmetry of the crystal takes place but only change in topology of the Fermi surface or other isoenergetic surfaces as is stated in section 1.2.

CHAPTER 2

ELECTRON-PHONON INTERACTIONS

2.1 Phonons

In a large crystalline solid body say an elastic continuum mechanical vibrations of the atoms take the form of waves. It is reasonable to expect and quantum mechanics tells us that the energy in such waves must be quantised. Using de-Broglie ideas of wave-particle duality it is convinient to associate a particle with a quantum of excitation in such a wave. For vibration in a crystal, such a quantum is called phonon in analogy with the photon which represents a quantum in electromagnetic field.

The phonon is one of the elementary excitations that contribute to the total energy spectrum in the crystal discussed in the introduction. To each phonon we associate a wave vector $\vec{k}$ and frequency $\omega(\vec{k})$. To each wave we can assign an oscillator and to each oscillator an energy $\hbar\omega(\vec{k})$ and momentum $\vec{p} = \hbar \vec{k}$. Phonons are bosons and thus have to obey the Bose-Einstein Distribution function

$$f = \frac{1}{e^{\frac{\hbar\omega}{kT}} - 1} \qquad (19)$$

the chemical potential "ξ" being zero for phonons.

The number of phonons in a crystal is dependent on the temperature of the crystal. At high temperatures $N \alpha T$ and at low temperature $N \alpha (\frac{T}{T_o})^{3/2}$ where T_o is called the degeneracy temperature of the crystal (Kaganov, 1981).

We can directly measure dispersion law for phonons $\varepsilon(\vec{k})$ by inelastic scattering of slow neutrons in crystals (Brockhouse, 1961).

The neutron makes the atoms of the crystal to swing thus exciting sound waves (creating phonons) thereby decreasing its energy. The change in neutron momentum and energy are related to the phonon momentum and energy by the conservation laws applied to the crystal as a whole (Brockhouse etal, 1962).

2.2 Collision between Electrons and Phonons

Phonons interact with each other, with electrons and with other quasiparticles in the solid. The most common effect of the electronphonon interaction is seen in the temperature dependence of the electrical resistivity, which for example for pure copper is 1.55 microhm-cm at 0°C and 2.28 microhm-cm at 100°C (Kittel, 1976). The electrons are scattered by the phonons, and the higher the temperature the more phonons there are and hence more scattering.

A more subtle effect of the electron-phonon interaction is the apparent increase in electron mass in metals and insulators because the electron drags the heavy ion cores along with it (Kittel, 1976).

Another important application of electron phonon interaction worth mentioning in here is the direct amplification of acoustic phonons by drifting electrons in piezoelectric crystals (Elliott and Gibson, 1974).

As temperature decreases to 0°K thermal motion is almost suppressed minimizing the electron phonon interaction and the electrical resistance is now caused by defects in the crystal. At higher temperatures electrons interact with phonons in one of the following ways.

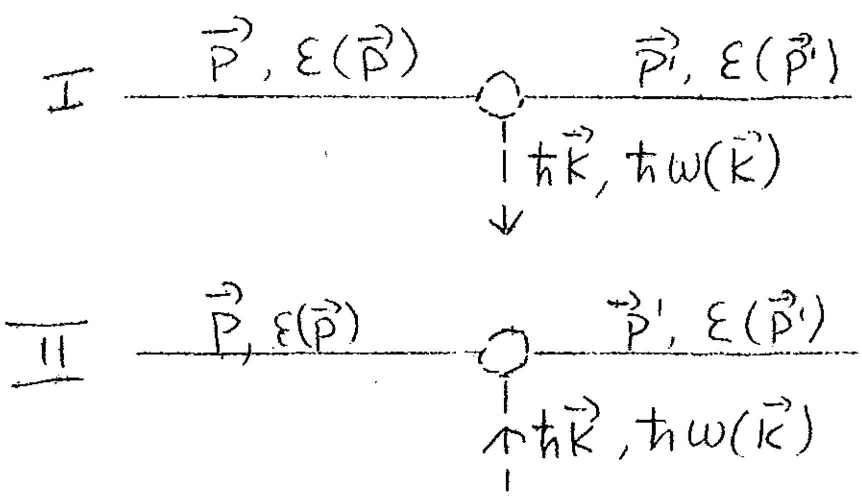

Fig.5. Emmission(I)and absorption (II) of phonons by electrons

Solid lines symbolize electrons and dashed lines, phonons (Kaganov, 1981). The lines are labeled with the momenta and energies of the electrons and phonons with primed quantities after the collision.

In the first process there is no collision at all but the electrons create phonons. In the second process there is a collision resulting in the absorption of a phonon. Conservation of energy equation is the same for both processes (eg. see Kaganov, 1981),

$$\varepsilon(\vec{p}) + \hbar\,\omega = \varepsilon(\vec{p} + \hbar\,\vec{k}). \tag{20}$$

Near the Fermi surface h can be ignored compared with ε_F to get

$$\varepsilon_F(\vec{p}) = \varepsilon(\vec{p} + \hbar\,\vec{k}) \tag{21}$$

Equation (21) implies that the two processes in Figure 5 are allowed if $\varepsilon(\vec{p}) = \varepsilon_F$ and $\varepsilon(\vec{p} + \hbar\,\vec{k}) = \varepsilon_F$ simultanecusely. If $h\vec{k}$ is small compared to $\vec{p}$ as is usually the case, then using Taylor expansion we get (eg. see Abrikosov, 1972)

$$\varepsilon(\vec{p} + \hbar\vec{k}) = \varepsilon(\vec{p}) + \hbar\vec{k}.\ \frac{\partial\varepsilon(\vec{p})}{\partial p}\ \text{, resulting in}$$

$$\varepsilon(\vec{p} + \hbar\vec{k}) = \varepsilon(\vec{p}) + \hbar\vec{k}.\vec{v} \tag{22}$$

Near the Fermi surface $\varepsilon_F(\vec{p}) = \varepsilon_F(\vec{p}) + \hbar\vec{k}.\vec{V}_F$ giving,

$$\hbar k V_F \cos\theta = 0. \tag{23}$$

In general if $\hbar\omega$ is not to be ignored we have

$$\varepsilon(\vec{p}) + \hbar\omega = \varepsilon(\vec{p}) + \hbar\vec{k}.\vec{v} \quad \text{, and thus}$$

$$\hbar\omega = \hbar\, kV_F \cos\theta \text{ near Fermi surface.} \tag{24}$$

Since $\frac{\omega}{k} = s$ which is the speed of sound we finally get

$$V_F \cos\theta = s. \tag{25}$$

Analysis of equations (23) and (25) leads to the conclusion that the electrons interacting with the phonons have velocities perpendicular to the wave vector of the phonons of the incident sound (Note that in equation (23) $V_F \sim 10^8 \frac{cm}{sec}$ and $s \sim 10^5 \frac{cm}{sec}$ $\cos\theta \ll 1$ $\theta \sim \pi/2$). Thus the effective belt where the interacting electrons are located is almost perpendicular to the incident phonon wave vector.

2.3 Absorption Coefficient Γ and Change in Phonon Frequency $\Delta\omega$

Now let us make use of the free electron model of metals to analyse electron-phonon interaction in further detail. Consider an incident sound into a metal box at $T = 0$. The collision between a phonon and an electron within the box obeys the momentum conservation law

$$\vec{P}_{1i} + \vec{P}_{2i} = \vec{P}'_{1f} + \vec{P}_{2f} + \hbar\,\vec{G} \tag{26}$$

where $\vec{G} = \begin{cases} 0 & \text{for Normal Process} \\ \neq 0 & \text{for Umklapp Process} \end{cases}$

(Note that here momentum is not conserved in the collision but it is in the crystal).

If the mean free path "ℓ" of the electrons is very small compared with the phonon-wavelength λ then the descreteness of ℓ will not be felt by the phonon and thus can be said that there is no interaction. If $\ell >> \lambda$, there is interaction resulting in absorption or emission of a phonon by an excited electron.

Introduce

Γ	as absorption coefficient
$\vec{P}$	as electron momentum
$\vec{q}$	as phonon momentum
$\varepsilon(\vec{p})$	as electron energy
ε_F	as Fermi Energy
f_p	as Fermi Dirac Distribution function
$\Delta\omega$	as change in phonon frequency..

An electron can absorb or emit a phonon if there is a free state in the adjacent state to where the transition occurs.

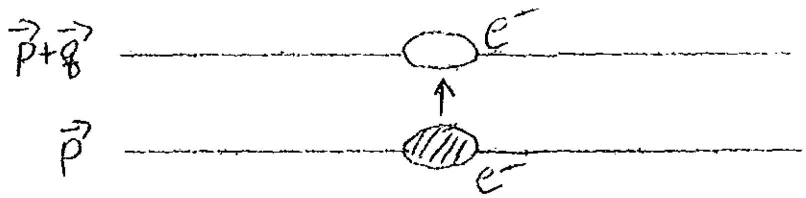

Fig.6. Transition from $\vec{p}$ to $\vec{p}+\vec{q}$ or the reverse can take place only if one of the states is empty.

In calculating the transition rate of electrons from state $\vec{p}$ to state $\vec{p}+\vec{q}$, one must multiply by the Fermi Dirac Distribution functions $f_{\vec{p}}(1-f_{\vec{p}+\vec{q}})$ to account for the probability that the initial state is occupied $f_{\vec{p}}$ and the final state is unoccupied $1-f_{\vec{p}+\vec{q}}$. The reverse process may take place in the above process and its probability of occurence is $f_{\vec{p}+\vec{q}}(1-f_{\vec{p}})$.

If there is equilibrium between the two processes then there is no net absorption or creation of phonons. If on the other hand there is <u>no</u> equilibrium then using quantum statistics and perturbation theory one can show that (Akhiezer etal, 1957)

$$\Gamma = \int |M|^2 \{f_{\vec{p}}(1-f_{\vec{p}+\vec{q}})-f_{\vec{p}+\vec{q}}(1-f_{\vec{p}}) x \delta(\varepsilon_{\vec{p}}+\hbar\omega-\varepsilon\vec{p}+\vec{q}) \ d^3p$$

$$= \int |M|^2 \ (f_{\vec{p}}-f_{\vec{p}+\vec{q}}) \ \delta(\varepsilon_{\vec{p}} + \hbar\omega-\varepsilon_{\vec{p}+\vec{q}}) \qquad (27)$$

For the change in phonon spectrum

$$\Delta\omega = \fint \frac{|M|^2(f_{\vec{p}} - f_{\vec{p}+\vec{q}})}{\varepsilon_{\vec{p}} + \hbar\omega - \varepsilon_{\vec{p}+\vec{q}}} d^3p \qquad \text{see} \tag{28}$$

for example Kaganov M.I. and Semenenko, (1966).

The symbol $\fint$ denotes the principal value of the integral, and $|M|^2$ is the square of the matrix element of the two states which includes factors of the type $\frac{2\pi}{\hbar}$

An alternative expression for $f_{\vec{p}} - f_{\vec{p}+\vec{q}}$ is that

$$f_{\vec{p}} - f_{\vec{p}+\vec{q}} \approx -\hbar\omega\frac{\partial f_{\vec{p}}}{\partial\varepsilon} \approx \delta(\varepsilon_{\vec{p}} - \varepsilon_F)\,\hbar\omega \tag{29}$$

and

$$\delta(\varepsilon_{\vec{p}} + \hbar\omega - \varepsilon_{\vec{p}+\vec{q}}) \approx \frac{1}{\hbar}\,\delta(\omega - \vec{K}.\vec{V}) \tag{30}$$

Equations (29) and (30) are obtained under the assumption that $\hbar\omega \ll \varepsilon_F$ and $T \to 0$.

The quantum formulas for $\Delta\omega$ and Γ are related mathematically as is shown in Semenenko's article, (1967).

$$\begin{aligned}\Delta\omega &= \fint \frac{|M|^2(f_{\vec{p}} - f_{\vec{p}+\vec{q}})}{\varepsilon_{\vec{p}} + \hbar\omega - \varepsilon_{\vec{p}+\vec{q}}} d^3p \\ &= \fint \frac{|M|^2(f_{\vec{p}} - f_{\vec{p}+\vec{q}})\ \delta(\varepsilon_{\vec{p}} - {}_{\vec{p}+\vec{q}} + \hbar\omega - \varepsilon)}{\varepsilon} d\varepsilon\, d^3p \\ &= \fint_{\varepsilon_{min}}^{\varepsilon_{max}} \frac{\Gamma(\vec{q}, \hbar\omega - \varepsilon)}{\varepsilon} d\varepsilon\end{aligned} \tag{31}$$

where $(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}} + \hbar\omega)_{min} = \varepsilon_{min}$

and

$(\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}} + \hbar\omega)_{max} = \varepsilon_{max}$

2.4 Migdal-Kohn Anomalies for Spherical Fermi Surface of Metals.

Consider now the absorption coefficient and change in phonon frequency when $T \to 0$ and $\hbar\omega << \varepsilon_F$. Assume also that the energy spectrum $\varepsilon(\vec{p})$ is isotropic in momentum space ie. $\varepsilon(\vec{p}) = p^2/2m$. Equation (27) will now be simplified to the expression

$$\Gamma = \hbar\omega \int |M|^2 \ \delta(\varepsilon_{(\vec{p})} - \varepsilon_F)\delta(\varepsilon_{\vec{p}+\vec{q}} - \varepsilon_F) \ d^3p \ . \qquad (32)$$

Equation (32) will vanish unless

$$\varepsilon_{(\vec{p})} = \varepsilon_F$$

and $\varepsilon_{(\vec{p}+\vec{q})} = \varepsilon_F$ are satisfied simultaneousely.

Thus,

$$\frac{p^2}{2m} = \varepsilon_F = \frac{(\vec{p}+\vec{q})^2}{2m}.$$

The intersection of these two surfaces consists of allowed values of phonon momentum q.

There cannot be any intersection if $q > 2p_F$.

The matrix element $|M|^2$ depends on the curve of intersection. Assuming this to be $|M_o|^2$

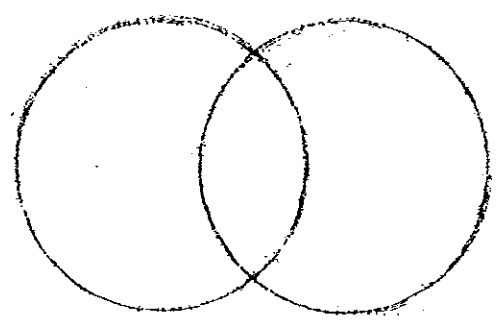

Fig.7. Two intersecting spherical Fermi surfaces

we then have

$$\Gamma = \hbar\omega|M_o|^2 \int \delta(\varepsilon(\vec{p})-\varepsilon_F)\ \delta(\varepsilon_{(\vec{p}+\vec{q})}-\varepsilon_F)d^3p$$

$$= \hbar\omega|M_o|^2 \int \delta(\frac{p^2}{2m} - \varepsilon_F)\delta(\frac{(\vec{p}+\vec{q})^2}{2m} - \varepsilon_F)\ d^3p$$

$$= \hbar\omega|M_o|^2(2m)\int \delta(p^2-p_F^2)\,\delta\left[(\vec{p}+\vec{q})^2 - p_F^2\right]d^3p$$

Using spherical coordinates to evaluate the integral we get

$$d^3p = p^2dpd\phi \ \sin\theta\, d\theta \tag{33}$$

$$\Gamma = \hbar\omega|M_o|^2(2m)^2\int_0^{p_F}\int_0^{2\pi}\int_0^{\pi}\delta(p^2-p_F^2)\ \delta(p^2+2pq\cos\theta+q^2-p_F^2)\ \times$$

$$\times\ p^2\sin\theta\ dpd\theta d\phi$$

Integration with respect ϕ gives 2π. To integrate with respect to θ substitute first $\cos\theta$ by x. Then $-\sin\theta d\theta = dx$ and the limits of integration will now be from 1 to -1 with respect to χ

$$\Gamma = 2\pi\hbar\omega\ |M_o|^2(2m)\int_{-1}^{1}\int_0^{p_F}\delta(p^2-p_F)p^2dp \quad \times$$

$$\times\,\delta(p^2+2pq\ x + q^2 - p_F^2)dx$$

$$= \frac{2\pi\hbar\omega|M_o|^2(2m)^2}{2q}\int_0^{p_F} p\delta(p^2-p_F^2)dp, \quad \text{with } \left|\frac{p_F^2-p^2-q^2}{2pq}\right| < 1$$

$$= \begin{cases} \dfrac{2\pi m^2\hbar\omega\ |M_o|^2}{q} & \text{if } q < 2p_F \\ 0 & \text{if } q > 2p_F \end{cases} \tag{34}$$

The absorption coefficient is thus constant for a non zero but specific value of q as far as $q < 2p_F$ and zero if $q > 2p_F$.

The phonon frequency ω can be expressed as the sum of a smooth part ω_0 and singular part $\Delta\omega$, where $\Delta\omega$ is given by equation (28).

$$\Delta\omega = \int \frac{|M|^2 f_p d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}} - \int \frac{|M|^2 f_{\vec{p}+\vec{q}}\, d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}}$$

$$= |M_0|^2 \int_{\varepsilon_{\vec{p}} < \varepsilon_F} \frac{d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}} - |M_0|^2 \int_{\varepsilon_{\vec{p}+\vec{q}} < \varepsilon_F} \frac{d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}}$$

Consider now $I_1 = \int_{\varepsilon_{\vec{p}} < \varepsilon_F} \frac{d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}}$

$$I_1 = \int_{\varepsilon_{\vec{p}} < \varepsilon_F} \frac{d^3p}{\frac{p^2}{2m} - \frac{(p^2 + 2\vec{p}.\vec{q} + q^2)}{2m}}$$

There is no loss of generality if we assume $\vec{q}$ to be directed along the p_z axis. Let the angle between $\vec{p}$ and $\vec{q}$ be θ.

$$I_1 = -2m \int \frac{p^2 \sin\theta d\theta d\phi dp}{2pq\cos\theta + q^2}$$

$$= -\frac{2\pi m}{q} \int_0^{p_F} p \ln \left|\frac{2p+q}{2p-q}\right| dp$$ after integration with respect to ϕ and θ . Note that the logarithmic

function is smooth around the singularity of the denominator. ie.

$$\int_{-1}^{1} \frac{dx}{Ax+B} = \frac{1}{A} \quad \ell n\,|Ax+B|\Big|_{x=-1}^{x=x_0-\varepsilon} + \quad \ell n\,|Ax+B|\Big|_{x=x_0+\varepsilon}^{1}$$

$$= \frac{1}{A} \quad \ell n\left|\frac{A+B}{B-A}\right|$$

Evaluation of the above integral I_1 leads to the expression (Dwight, 1961)

$$I_1 = \frac{2\pi m}{q} \left\{ \frac{4p_F{}^2-q^2}{8} \ell n \left|\frac{2p_F-q}{2p+q}\right| - \frac{qp_F}{2} \right\} \qquad (35)$$

Similarly

$$I_2 = -\int_{\varepsilon_{\vec{p}+\vec{q}} < \varepsilon_F} \frac{d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}}$$

Introduce new variable letting $\vec{P} = \vec{p}+\vec{q}$

$d^3P = d^3p$ since the Jacobian is 1.

$$I_2 = -\int_{|\vec{P}|<P_F} \frac{d^3P}{\varepsilon(\vec{P}-\vec{q}) - \varepsilon(\vec{P})}$$

, we can now use the old variable, small $\vec{p}$.

$$I_2 = -2m\int_{|p|<p_F} \frac{d^3p}{(p-q)^2 - p^2},$$ using equation (33),

we have

$$I_2 = -2m \int_0^{p_F} p^2 dp \int_{-1}^{1} \frac{dx}{2pqx-q^2} \int_0^{2\pi} d\phi$$

$$= \frac{2\pi m}{q} \int_{|p|<p_F} p \, \ell n \left|\frac{2p-q}{2p+q}\right| dp$$

$$I_2 = \frac{2\pi m}{q} \left\{ \left(\frac{4p_F^2 - q^2}{8}\right) \ell n \left|\frac{2p_F-q}{2p_F+q}\right| - \frac{qp_F}{2} \right\}$$

which is identical to equation (35) of I_1.

Combining we get

$$\Delta\omega = \frac{4\pi m}{q} |M_o|^2 \left\{ \frac{(4p_F^2-q^2)}{8} \ell n \left|\frac{2p_F-q}{2p_F+q}\right| - \frac{qp_F}{2} \right\} . \tag{36}$$

Equation (36) can be re-written as

$$\Delta\omega = \frac{\pi m |M_o|^2}{2q} \{(2p_F+q)(2p_F-q) \ell n \left|\frac{2p_F-q}{2p_F+q}\right|\} - 2\pi m |M_o|^2 p_F.$$

The last term can be included with the smooth part of $\omega = \omega_o + \Delta\omega$. The last expression of $\Delta\omega$ is of the form

$$\Delta\omega \sim x \, \ell n \, x \quad \text{where} \quad x = 2p_F - q$$

$$\lim_{x\to 0} \Delta\omega \sim \lim_{x\to 0} \frac{\ell n \, x}{1/x} \sim \lim_{x\to 0} \frac{1/x}{-1/x^2} \to 0$$

This shows that $\Delta\omega$ is a continuous function.

Consider the group velocity which is defined as

$$V_g = \hbar \frac{d(\Delta\omega)}{dq} = \hbar \frac{d(\Delta\omega)}{dx} \frac{dx}{dq} = -\hbar \frac{d(\Delta\omega)}{dx}$$

$$V_g \sim -\hbar \ln|x| - \hbar$$

$$\lim_{x\to 0} V_g \sim \infty$$

It is evident that there is a kink in the phonon dispersion law which results in infinite group velocity.

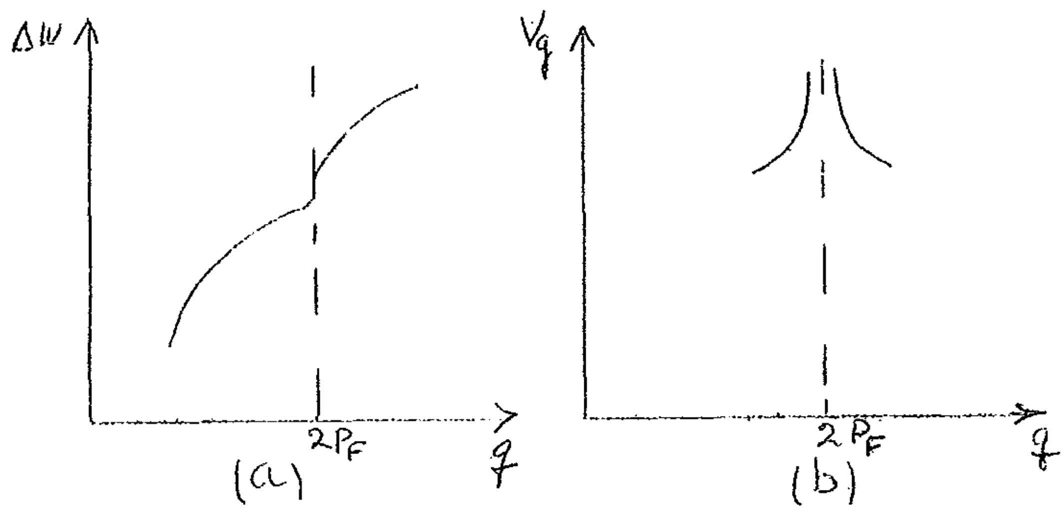

Fig.8. Dispersion curves for the phonon frequency (a) and group velocity (b) for spherical Fermi surface.

The above kink in the phonon dispersion law leads to the expectation of the appearance of the image of the Fermi surface of the metal concerned.

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$$V_g \sim - \hbar \, \ell n|x| - \hbar$$

$$\lim_{x\to 0} V_g \sim \infty$$

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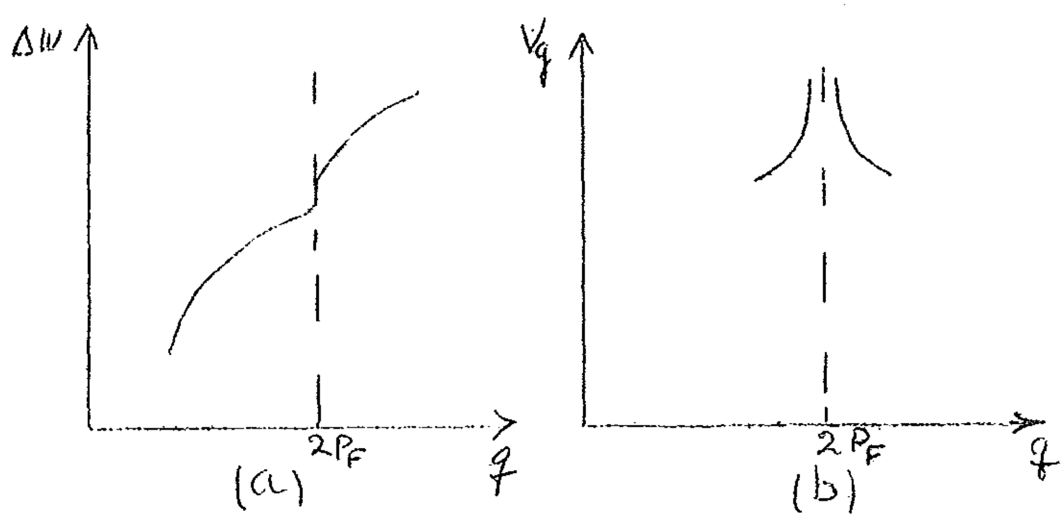

Fig.8. Dispersion curves for the phonon frequency (a) and group velocity (b) for spherical Fermi surface.

The above kink in the phonon dispersion law leads to the expectation of the appearance of the image of the Fermi surface of the metal concerned.

This behaviour of the phonon spectrum at about $q = 2p_F$ was first discovered theoretically by Migdal (1958) and then Kohn (1959) independently. Its experimental confirmation was first provided by Brockhouse etal (1961) for lead. The magnitude of the kink is supposed to be very small as estimated by Kohn himself and Taylor (1963) especially for metals having almost spherical Fermi surface (Woll and Kohn, 1962). Afanasev and Kagan (1962) have shown that the relative kinks of different Fermi surfaces are as plotted below:

a → spherical

b → cylinderical

c → nearly plane

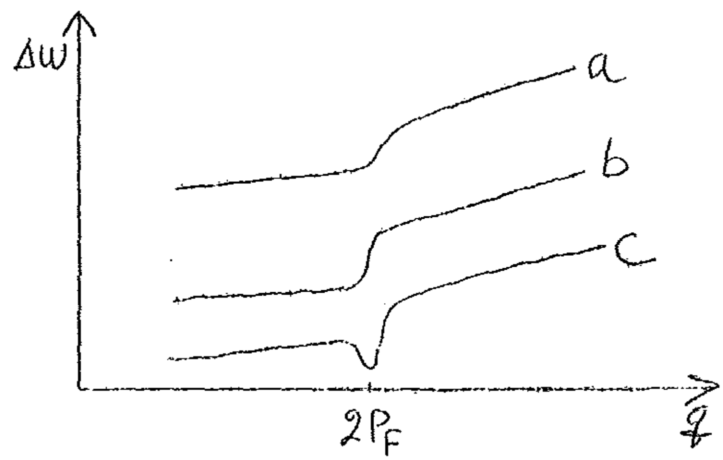

Fig.9. Relative kinks in phonon dispersion curve for different Fermi surface.

2.5 Physical Sense of the Migdal-Kohn Anomalies

A more physical relationship between the absorption coefficient and change in the phonon frequency can be arrived at using the well known Kramers and Kronig relations when applied to the dielectric function $\varepsilon(q,\omega)$.

The dielectric function $\varepsilon(q,\omega)$, which is dependent on the phonon frequency ω and momentum q is given by

$$\varepsilon(q,\omega) = 1 + \frac{4\pi e^2}{q} \sum_K \frac{f_{\vec{p}} - f_{\vec{p}+\vec{q}}}{\varepsilon_{(\vec{p}+\vec{q})} - \varepsilon_{\vec{p}} - \hbar\omega + i\hbar\alpha} \tag{37}$$

impossing an oscillation of frequency ω, wave-vector q growing slowly with time constant α(Ziman, 1979). The function $\varepsilon(q,\omega)$ is sometimes called Lindhards dielectric function. It is a complex function, the imaginary part being related to the absorption coefficient Γ and the real part to the change in phonon frequency. This relationship will become obvious in later sections were we will find that the singularities for $\varepsilon(q,\omega)$, $\Delta\omega$ and Γ for a spherical Fermi surface are all at $q = 2p_F$. ie.

$$\varepsilon(q,0) = 1 + \frac{k_s^2}{q^2} F\left(\frac{q}{2p_F}\right) \tag{38}$$

(See Back Thor A, 1963).

Where k_s is the Fermi Thomas screening parameter and p_F is the Fermi radius in momentum space.

The function $F(\frac{q}{2p_F})$ or $F(x)$ is sketched below:

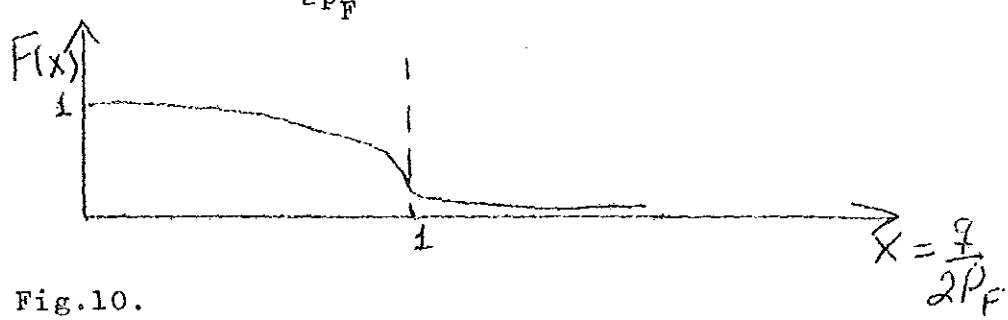

Fig.10.

$\varepsilon(q,\omega)$ being complex can be expressed as

$$\varepsilon(q,\omega) = \varepsilon'(q,\omega) + i\ \varepsilon''(q,\omega) \tag{39}$$

$\varepsilon'(q,\omega)$ and $\varepsilon''(q,\omega)$ inturn are related by Kramer's and Kronig Relations:

$$\varepsilon' = \frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\varepsilon''(x)dx}{x-\omega} \tag{40}$$

$$\varepsilon'' = -\frac{P}{\pi} \int_{-\infty}^{\infty} \frac{\varepsilon'(x)dx}{x-\omega} \tag{41}$$

Equation (40) is related to $\Delta\omega$ and equation (41) to Γ.

The similarity in the logarithmic singularity between Γ, $\Delta\omega$ and $\varepsilon(q,\omega)$ indicates that the cause is related with the response of the conduction electrons to the motion of ions. At $q = 2p_F$ the conduction electrons fail to screen out the ionic electrostatic field and thus the anomaly is created. Kohn's approach (1959) to this problem of the phonon spectrum is based on the dielectric function where as Migdal (1958) followed field theoretical methods. The quantities Γ, $\Delta\omega$ and $\varepsilon(q,\omega)$ behave like the function $F(x)$ sketched in Figure 10 at about $q = 2p_F$.

CHAPTER 3

MIGDAL-KOHN ANOMALIES FOR THE CASE OF CHANGE IN TOPLOGY OF FERMI SURFACE OF METALS

3.1 Appearance (Disappearance) of Spherical Cavity.

The anomalous dependence of the sound absorption coefficient Γ and change in the phonon frequency $\Delta\omega$ on $z = \varepsilon_F - \varepsilon_c$, where ε_F is the Fermi energy and ε_c is the critical energy at which the topology of the Fermi-surface changes is calculated in this section near $z = 0$ (see Fig.4a).

In equation (32), $\varepsilon_{\vec{p}} = \varepsilon_c + \frac{p^2}{2m}$

and

$$\delta(\varepsilon_{\vec{p}} - \varepsilon_F) = \delta\left(\frac{p^2}{2m} - z\right)$$

and

$\delta(\varepsilon_{\vec{p}+\vec{q}} - \varepsilon_F) = \delta\left(\frac{(p+q)^2}{2m} - z\right)$. This simplification is assuming that $\hbar\omega << z$ and $T = 0$ since we are interested in the rough estimation of the singularities as in section 2.4. Thus,

$$\Gamma = \hbar\omega|M_o|^2 \int \delta\left(\frac{p^2}{2m} - z\right)\delta\left(\frac{p^2+2pq\cos\theta+q^2}{2m} - z\right)d^3p$$

$$= (2m)^2\hbar\omega\,|M_o|^2 \int\delta(p^2 - p_z^2)\,\delta(p^2+2pq\cos\theta+q^2-p_z^2)\,p^2\,d\Omega\,dp$$

$$= 2\pi(2m)^2\hbar\omega|M_o|^2\left\{\int_o^{p_z}\int_{-1}^{1}\delta(p^2+2pqx+q^2-p_z^2)\,dx\;\delta(p^2-p_z^2)\,p^2\,dp\right.$$

$$\doteq \frac{2\pi m^2\hbar\omega|M_o|^2}{q}\int_o^{p_z}\delta(p^2-p_z^2)\;d(p^2)$$ where the condition

of integration is $|x| \leq 1$ or

$$\left| \frac{p_z^2 - p^2 - q^2}{2pq} \right| \leq 1$$

$$\Gamma = \begin{cases} \dfrac{2\pi\hbar\omega m^2 |M_o|^2}{q} & q < 2p_z \\ 0 & q > 2p_z \end{cases} \tag{42}$$

$\Delta\omega$ for the appearance or disappearance of a spherical Fermi surface is, from equation (28),

$$\Delta\omega = |M_o|^2 \int_{\varepsilon(\vec{p}) < \varepsilon_F} \frac{d^3p}{\varepsilon(\vec{p}) - \varepsilon(\vec{p}+\vec{q})} - |M_o|^2 \int_{\varepsilon_{\vec{p}+\vec{q}} < \varepsilon_F} \frac{d^3p}{\varepsilon(\vec{p}) - \varepsilon(\vec{p}+\vec{q})}$$

$$= |M_o|^2 \int_{\frac{p^2}{2m} < z} \frac{d^3p}{\frac{p^2}{2m} - \frac{p^2}{2m} - \frac{2pq\cos\theta}{2m} - \frac{q^2}{2m}}$$

$$- |M_o|^2 \int_{\frac{(\vec{p}+\vec{q})^2}{2m} < z} \frac{d^3p}{\frac{p^2}{2m} - \frac{(\vec{p}+\vec{q})^2}{2m}}$$

Consider the first integral and use equation (33)

$$I_1 = -2m \int_{|p| < p_z} \frac{p^2 dp \sin\theta d\theta d\phi}{2pq\cos\theta + q^2}, \quad \text{where } p_z = \sqrt{2mz}$$

$$= -\frac{4\pi m}{q} \int_0^{p_z} p^2 dp \int_0^{\pi} \frac{\sin\theta d\theta}{2p\cos\theta + q}$$

$$= -\frac{4\pi m}{2q} \left\{ \int_0^{p_z} p \ln|2p+q| dp - \int_0^{p_z} p \ln|2p-q| dp \right\}$$

$$= - \frac{2\pi m}{q} \left\{ \frac{4p^2 - q^2}{8} \ln|2p+q| - \frac{4p^2 - q^2}{8} \ln|2p-q| + \frac{pq}{2} \right\} \Big|_o^{p_z}$$

$$= \frac{2\pi m}{q} \left\{ \frac{4p_z{}^2 - q^2}{8} \ln\left|\frac{2p_z - q}{2p_z + q}\right| - \frac{p_z q}{2} \right\}$$

The 2^{nd} integral I_2 will yield

$$I_2 = \int_{|\vec{p}+\vec{q}| < p_z} \frac{d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}} \text{ , letting } \vec{P} = \vec{p}+\vec{q} \text{ we get}$$

$$I_2 = \int_{|\vec{P}| < p_z} \frac{d^3p}{\varepsilon(\vec{P}-\vec{q}) - \varepsilon(\vec{P})}$$

$$= \int_{|p| < p_z} \frac{d^3p}{\frac{(p-q)^2}{2m} - \frac{p^2}{2m}} = \frac{2m}{q} \int \frac{d^3p}{q - 2p \cos\theta}$$

$$I_2 = \frac{4\pi m}{q} \int p^2 dp \int_o^\pi \frac{\sin\theta \, d\theta}{q - 2p\cos\theta}$$

Following similar procedures we finally get

$$I_2 = - \frac{2\pi m}{q} \left[\frac{4p_z{}^2 - q^2}{8} \ln\left|\frac{q-2p_z}{q+2p_z}\right| - \frac{qp_z}{2} \right]$$

Combining I_1 and I_2 we have the final expression for $\Delta\omega$ as

$$\Delta\omega = |M_o|^2 I_1 - |M_o|^2 I_2$$

$$= \frac{4\pi m |M_o|^2}{q} \left\{ \frac{4p_z{}^2 - q^2}{8} \ln\left|\frac{q-2p_z}{q+2p_z}\right| - \frac{qp_z}{2} \right\} \qquad (43)$$

This result is identical in form to that of a normal spherical Fermi surface (no transition of order $2\frac{1}{2}$) treated before in section 2.4. So the conclusion given there applies also to this section.

arance (Disappearance) of Ellipsoidal Cavity.

his case the energy spectrum is given by equation
i.e.

$$\varepsilon(\vec{p}) = \varepsilon_c + \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3}$$

$$\varepsilon(\vec{p}+\vec{q}) = \varepsilon_c + \frac{(p_1+q_1)^2}{2m_1} + \frac{(p_2+q_2)^2}{2m_2} + \frac{(q_3+p_3)^2}{2m_3}$$

oduce now new variables P and Q defined by

$$P_1 = \frac{p_1}{\sqrt{m_1}}, \quad P_2 = \frac{p_2}{\sqrt{m_2}}, \quad P_3 = \frac{p_3}{\sqrt{m_3}}$$

$$Q_1 = \frac{q_1}{\sqrt{m_1}}, \quad Q_2 = \frac{q_2}{\sqrt{m_2}} \text{ and } Q_3 = \frac{q_3}{\sqrt{m_3}}, \text{ so that}$$

$$P^2 = \frac{p_1^2}{m_1} + \frac{p_2^2}{m_2} + \frac{p_3^2}{m_3}$$

$$Q^2 = \frac{q_1^2}{m_1} + \frac{q_2^2}{m_2} + \frac{q_3^2}{m_3} \qquad (44)$$

the equations (27) and (28) will have the form using
new variables

$$= (m_1 m_2 m_3)^{\frac{1}{2}} |M_o|^2 \hbar\omega \int \delta\left(\frac{P^2}{2} - z\right) \delta\left(\frac{P^2}{2} + \frac{Q^2}{2} + PQ\cos\theta - z\right) d^3p \qquad (45)$$

$$\omega = -|M_o|^2 (m_1 m_2 m_3)^{\frac{1}{2}} \int_{|\vec{P}| < 2z} \frac{P^2 \sin\theta\, d\theta\, dP\, d\phi}{\vec{P}\cdot\vec{Q} + \frac{Q^2}{2}}$$

$$-|M_o|^2 (m_1 m_2 m_3)^{\frac{1}{2}} \int_{P<2z} \frac{P \sin\theta\, d\theta\, dP\, d\phi}{\left(\frac{\vec{P}-\vec{Q}}{2}\right)^2 - \frac{P^2}{2}} \qquad (46)$$

where $d^3p = (m_1m_2m_3)^{\frac{1}{2}} \quad d^3P$

$$= (m_1m_2m_3)^{\frac{1}{2}} \quad P^2\sin\theta dPd\theta d\phi \; .$$

$$\therefore \quad \Gamma = 4|M_o|^2(m_1m_2m_3)^{\frac{1}{2}} \hbar\omega\int\delta(P^2-2z)x$$

$$x \;\; (P^2+Q^2+2PQ\chi-2z)P^2dPdxd\phi$$

$$= \frac{4\pi|M_o|^2(m_1m_2m_3)^{\frac{1}{2}}\hbar\omega}{Q} \quad \tfrac{1}{2}\int\delta(P^2-2z)d(P^2)$$

where $\int_0^{2\pi} d\phi = 2\pi$ and $\int_{-1}^{1} \delta(p^2+Q^2+2PQx-2z)dx = \frac{1}{2PQ}$

under the condition that $|x| \leqslant 1 \iff \left|\frac{2z-P^2-Q^2}{2PQ}\right| \leqslant 1$

$$\Gamma = \begin{cases} \dfrac{2\pi|M_o|^2(m_1m_2m_3)^{\frac{1}{2}}\hbar\omega}{Q} \;, & Q \leqslant 2\sqrt{2z} \\[2ex] 0 & Q > 2\sqrt{2z} \end{cases} \qquad (47)$$

The first part of equation (46) can be evaluated in a similar fashion as in section 3.1.

$$I_1 = -2|M_o|^2(m_1m_2m_3)^{\frac{1}{2}} \int \frac{P^2\sin\theta d\theta dPd\phi}{2PQ\cos\theta+Q^2}$$

$$= -2|M_o|^2(m_1m_2m_3)^{\frac{1}{2}} \left[\int_{|P|<2z} P^2 \int_{-1}^{1} \frac{dx}{2PQx+Q^2} \int_0^{2\pi} d\phi\right]$$

$$= \frac{-2\pi|M_o|^2(m_1m_2m_3)^{\frac{1}{2}}}{Q} \int_{|\vec{p}|<2z} P \;\ln\left|\frac{2P+Q}{2P-Q}\right| dP$$

$$= \frac{2\pi|M_o|^2(m_1m_2m_3)^{\frac{1}{2}}}{Q} \left[\frac{8z-Q^2}{8} \ln\left|\frac{2\sqrt{2z}-Q}{2\sqrt{2z}+Q}\right| - \frac{Q\sqrt{2z}}{2}\right.$$

Similarly I_2 gives an identical result.

Thus

$$\Delta\omega = \frac{4\pi |M_o|^2 (m_1 m_2 m_3)^{\frac{1}{2}}}{Q} \left[\frac{8z-Q^2}{8} \ln \left|\frac{2\sqrt{2z}-Q}{2\sqrt{2z}+Q}\right| - \frac{Q\sqrt{2z}}{2}\right] \quad (48)$$

The anisotropy of Γ and $\Delta\omega$ is now obvious from the results of equations (47) and (48) because of the Q dependence.

$$\vec{Q} = \left(\frac{q_1}{\sqrt{m_1}}, \frac{q_2}{\sqrt{m_2}}, \frac{q_3}{\sqrt{m_3}}\right).$$

and

$$\vec{q} = q \sin\theta \cos\phi \vec{i} + q \sin\theta \sin\phi \vec{j} + q \cos\theta \vec{k}.$$

$$|\vec{Q}| = q\left(\frac{\sin^2\theta \cos^2\phi}{m_1} + \frac{\sin^2\theta \sin^2\phi}{m_2} + \frac{\cos^2\theta}{m_3}\right)^{\frac{1}{2}}.$$

The critical value of $|\vec{Q}|$ is $2\sqrt{2z}$ which corrosponds to the critical value of the phonon momentum $q = 2\sqrt{2M^*z}$ with M^* being the effective mass.

$$M^* = \frac{m_1 m_2 m_3}{m_2 m_3 \sin^2\theta \cos^2\phi + m_1 m_3 \sin^2\theta \sin^2\phi + m_1 m_2 \cos^2\theta} \quad (49)$$

Thus for the case of appearance (disappearance) of ellipsoidal cavity the singularities of Γ and $\Delta\omega$ are anisotropic because of the θ and ϕ dependence of the effective mass. Information about the relationship between the principal values of the effective mass tensor may be extracted from investigation of the Migdal-Kohn anomalies.

Besides the logarithmic singularity in $\Delta\omega$ we have now additional root singularity in equation (48).

3.3 Peculiarities of the Migdal-Kohn Anomalies for Breaking of Necks.

Refering back to figure 4b we will now analyse the singularities in the phonon frequency for the unparted hyperboloid ($z>0$) and for the parted hyperboloid ($z<0$). For rough estimation $\hbar\omega$ is ignored, $T=0$ is assumed and integration with respect to δ-function is used since it is easier to treat.

$$\Delta\omega = \int \frac{|M_o|^2 (f_{\vec{p}} - f_{\vec{p}+\vec{q}})\, d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}}$$

$$= |M_o|^2 \hbar\omega \int \frac{\delta(\varepsilon_{\vec{p}} - \varepsilon_F)\; d^3p}{\varepsilon_{\vec{p}} - \varepsilon_{\vec{p}+\vec{q}}} \qquad (50)$$

Consider now the following cases:

Case 1 $\quad \vec{q} = (0,0,q)$

Case 2 $\quad \vec{q} = (0,q,0)$ or $(q,0,0)$

Case 3 $\quad \vec{q} = (0, q\sin\theta, q\cos\theta)$

Z may be greater than or less than zero for each case.

Case 1a $\quad q = (0,0,q)$ and $Z>0$.

The energy spectrum is

$$\varepsilon(\vec{p}) = \varepsilon_c + \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} - \frac{p_3^2}{2m_3} = \varepsilon_c + \frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_\parallel}$$

$$\varepsilon_{(\vec{p}+\vec{q})} = \varepsilon_c + \frac{p_\perp^2}{2m_\perp} - \frac{(p_3+q)^2}{2m_\parallel}$$

where $m_1 = m_2 = m_\perp$ and $m_3 = m_\parallel$. There is no loss in generality in this assumption.

$$\Delta\omega = \hbar\omega |M_o|^2 \int \delta \frac{\left(\frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_\parallel} - z\right) p_\perp \, dp_\perp \, dp_3 d\phi}{\frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_\parallel} - \frac{p_\perp^2}{2m_\perp} + \frac{(p_3+q)^2}{2m_\parallel}}$$

Cylinderical coordinates are now being used instead of spherical coordinates because the figures considered have cylinderical symmetry.

$$\Delta\omega = \frac{2m_\perp \hbar\omega |M_o|^2 2m_\parallel}{q} \int \frac{\delta\left[p_\perp^2 - 2m_\perp\left(\frac{p_3^2}{2m_\parallel} + z\right)\right] p_\perp \, dp_\perp \, d\phi \, dp_3}{2p_3 + q}$$

$$= \frac{4\pi\hbar\omega |M_o|^2 m_\perp m_\parallel}{q} \int_{-p_o}^{p_o} \frac{dp_3}{2p_3+q}$$

$$\Delta\omega = \frac{2\pi\hbar\omega |M_o|^2 m_\perp m_\parallel}{q} \ \ell n \left| \frac{2p_o+q}{2p_o-q} \right| \qquad (52)$$

In the close vacinity of the critical point (since our interest is near $z = 0$) $p_o \ll q$ so there is no singularity in $\Delta\omega$ since the limit is zero. Besides there is no explicit dependence on z as in section 3.2. If z is assumed to be zero there is no change in equation (51).

Case 1b. After the rupture of the connecting neck that is for $z < 0$ we get

$$\Delta\omega = \hbar\omega |M_o|^2 \int \frac{\delta\left(\frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_\parallel} + |z|\right)}{\frac{2p_3 q + q}{2m_\parallel}} p_\perp \, dp_\perp \, d\phi \, dp_3$$

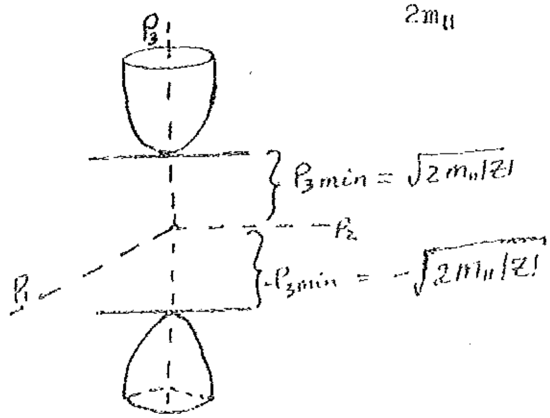

Fig.11 Hyperboloid of two sheets indicating p_{3min}.

$$\Delta\omega = \frac{\hbar\omega |M_o|^2 2\pi 2m_\parallel \;\; 2m_\perp}{2q} \left\{ \int_{-p_o}^{-\sqrt{2m_\parallel |z|}} \frac{dp_3}{2p_3+q} + \int_{\sqrt{2m_\parallel |z|}}^{p_o} \frac{dp_3}{2p_3+q} \right\}$$

$$= 2\pi\hbar\omega m_\perp m_\parallel \; |M_o|^2 \; \ln\left|\frac{2p_o - q}{2p_o + q}\right| + \ln\left|\frac{q - 2\sqrt{2m_\parallel |z|}}{q + 2\sqrt{2m_\parallel |z|}}\right| \qquad (52)$$

The first logarithmic expression in equation (52) is not an actual singularity since p_o can be taken arbitrary small as in case 1a, but the second one is important. It contains an explicit dependence on z and it is particularly important since $\Delta\omega$ is now proportional to $\ln|\chi|$ rather than

$x \ell n|x|$ as in previous sections. Thus, the singularity is now much stronger.

$$\lim_{x \to 0} \Delta\omega \to \infty \quad \text{logarithmically.}$$

The group velocity $V_g = \frac{\hbar d(\Delta\omega)}{dq}$ has hyperbolic singularity as $x \to 0$ since

$$V_g = \hbar d \frac{(\Delta\omega)}{dq} = -\frac{\hbar}{|x|}\left(\frac{d|x|}{dx}\right)$$

where $\frac{d|x|}{dx} = \begin{cases} 1 & \text{if } x > 0 \\ -1 & \text{if } x < 0 \end{cases}$

Such a behaviour in the phonon spectrum after the rupture of the neck is expected since Γ vanishes for this case (Davydov, 1976).

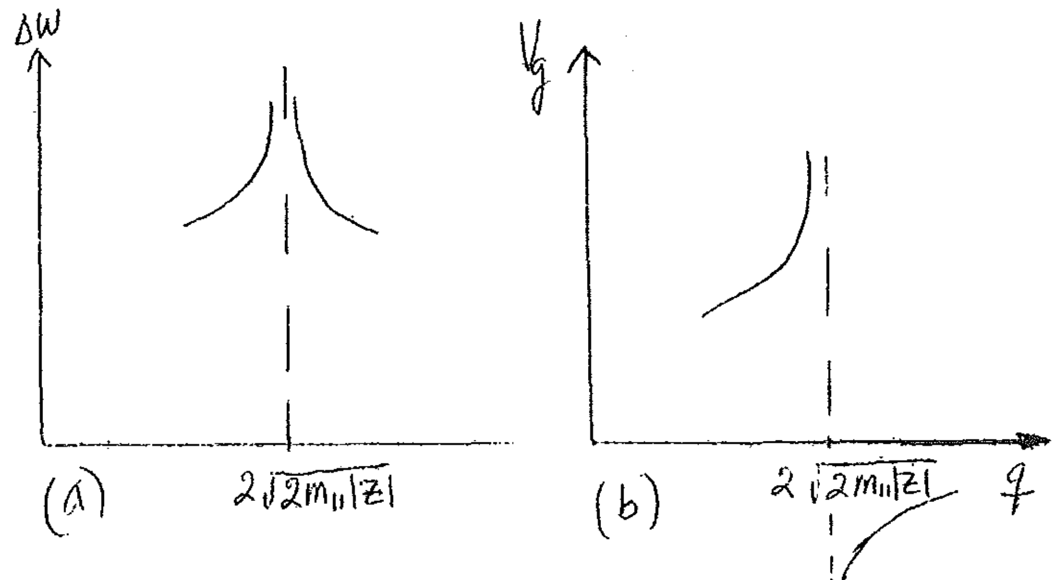

Fig.12. Migdal-Kohn singularities for the phonon frequency (a) and group velocity (b)

<u>Case 2.</u> Assume now the vector $\vec{q}$ to be perpendicular to the axis of the neck, say $\vec{q} = (q,0,0)$ in Fig.4b.

$$\Delta\omega = \hbar\omega|M_o|^2 \int \frac{\delta\left(\frac{p_\perp^2}{2m_\perp} - \frac{p_3^2}{2m_{\parallel}} - z\right) d^3p}{\frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \frac{p_3^2}{2m_3} - \frac{(p_1+q)^2}{2m_1} - \frac{p_2^2}{2m_2} + \frac{p_3^2}{2m_3}}$$

$$= \hbar\omega|M_o|^2(2m_\perp)^2 \int \delta \frac{\left(p_\perp^2 - 2m_\perp\left(\frac{p_3^2}{2m_{\parallel}} + z\right)p_\perp dp_\perp d\phi dp_3\right.}{-(2p_\perp q \cos\phi + q^2)}$$

$$= \frac{-\hbar\omega|M_o|^2(2m_\perp)^2}{q} \int \frac{dp_3 d\phi}{2\sqrt{2m_\perp\left(\frac{p_3^2}{2m_{\parallel}} + z\right)}\cos\phi + q}$$

after integrating with respect to $p_\perp$ using the identity

$$\int f(x)\ \delta(x-a)d(x) = f(a)\,.$$

To integrate with respect to ϕ we have to use the standard integral

$$\int_0^{2\pi} \frac{d\phi}{1+a\ \cos\phi} = \frac{2\pi}{\sqrt{1-a^2}} \qquad \text{see Dwight (1961),}$$

where $a = \frac{2}{q}\left[2m_\perp\left(\frac{p_3^2}{2m_{\parallel}} + z\right)\right]^{\frac{1}{2}} < 1$ and $a > 0$

$$\Delta\omega = -\frac{2\hbar\omega\ |M_o|^2 m_\perp^2}{q^2}\int dp_3 \int_o^{2\pi}\frac{d\phi}{1+a\cos\phi}$$

$$= -\frac{4\pi\hbar\omega|M_o|^2 m_\perp^2}{q^2}\int \frac{dp_3}{\left\{1-\frac{4}{q^2}\left[2m_\perp\left(\frac{p_3^2}{2m_{\parallel}}+z\right)\right]\right\}^{\frac{1}{2}}}$$

$$= -\frac{4\pi\hbar\omega|M_o|^2 m_\perp^2}{q^2}\int \frac{dp_3}{\left(1-\frac{8m_\perp}{q^2}z-\frac{4m_\perp}{q^2 m_{\parallel}}p_3^2\right)^{\frac{1}{2}}}$$

This integral should be reduced to the standard form

$\int\frac{dx}{(a^2-x^2)^{\frac{1}{2}}}$. To do this we have to limit the sign of z.

$$\Delta\omega = -\frac{4\pi\hbar\omega|M_o|^2 m_\perp^2}{q^2}\int \frac{dp_3}{\frac{2m_\perp^{\frac{1}{2}}}{qm_{\parallel}^{\frac{1}{2}}}\left\{\frac{q^2 m_{\parallel}}{4m_\perp}\left(\frac{1-8m_\perp z}{q^2}\right)-p_3^2\right\}}$$

$$= -\frac{2\pi m_\perp^{3/2}\ m_{\parallel}^{1/2}\ \hbar\omega|M_o|^2}{q}\,2\int_{p_3\min}^{p_3\max}\frac{dp_3}{\left\{\frac{m_{\parallel}\ q^2}{4m_\perp}\left(\frac{1-8m_\perp z}{q^2}\right)-p_3^2\right\}}$$

If $z > 0$, $\Delta\omega = -\frac{4\pi m_\perp^{3/2}\ \hbar\omega|M_o|^2 m_{\parallel}^{1/2}}{q}\int_0^{p_3\max}\frac{dp_3}{\left[p_3^2\max-p_3^2\right]^{\frac{1}{2}}}$

where $p_3\max = \frac{q}{2}\left(\frac{m_{\parallel}}{m_\perp}\right)^{\frac{1}{2}}\left(1-8\frac{m_\perp z}{q^2}\right)^{\frac{1}{2}}$. This value of $p_3\max$

is consistent with the above limitation namely

$$0 < a < 1 \quad \text{where} \quad a = \frac{2}{q}\left[2m_\perp\left(\frac{p_3^2}{2m_\parallel} + z\right)\right]^{1/2}$$

$p_3 max$ is obtained for max "a" ie.

$$\frac{2}{q}\left[2m_\perp\left(\frac{p_3^2 max}{2m_\parallel} + z\right)\right]^{\frac{1}{2}} = 1 \Rightarrow p_3 max = \frac{q}{2}\left(\frac{m_\parallel}{m_\perp}\right)^{\frac{1}{2}}\left(1 - \frac{8m_\perp z}{q}\right)^{\frac{1}{2}}$$

The result of the integration is

$$\Delta\omega = -\frac{4\pi m_\perp^{3/2}\hbar\omega|M_o|^2 m_\parallel^{\frac{1}{2}}}{q}\sin^{-1}\frac{p_3}{p_3 max}\Big|_0^{p_3 max}$$

$$= -\frac{2\pi^2 m_\perp^{3/2} m_\parallel^{1/2}\hbar\omega|M_o|^2}{q}, \quad z > 0 \quad \text{and} \quad \frac{1-8m_\perp z}{q^2} > 0 \qquad (9)$$

$\underline{z = 0}$, $$\Delta\omega = -\frac{4\pi m_\perp^{3/2}\hbar\omega|M_o|^2 m_\parallel^{1/2}}{q}\int_0^{p_o}\frac{dp_3}{\left[\frac{m_\parallel}{4m_\perp}q^2 - p_3^2\right]^{\frac{1}{2}}}$$

where $p_o^2 = \dfrac{m_\parallel q^2}{4m_\perp}$

$$\Delta\omega = -\frac{4\pi m_\perp^{3/2}\hbar\omega|M_o|^2 m_\parallel^{1/2}}{q}\sin^{-1}\frac{p_3}{p_o}\Big|_0^{p_o}$$

$$= -\frac{2\pi^2 m_\perp^{3/2} m_\parallel^{1/2}\hbar\omega|M_o|^2}{q}$$, The same as equation (9)

$\underline{Z < 0}$

$$\Delta\omega = -\frac{4\pi m_\perp^{3/2} m_\parallel^{1/2}\hbar\omega|M_o|^2}{q}\,2\int_{p_3 min}^{p_3 max}\frac{dp_3}{\left[p_3^2 max - p_3^2\right]^{\frac{1}{2}}}$$

where $p_3\ \max = \frac{q}{2}\left(\frac{m_{\parallel}}{m_{\perp}}\right)^{\frac{1}{2}}\left(1+\frac{8m_{\perp}|z|}{q^2}\right)^{\frac{1}{2}}$

and $p_3\ \min = \sqrt{2m_{\parallel}|z|}$

$$\therefore \qquad \Delta\omega = -\frac{4\ m_{\perp}^{3/2}m_{\parallel}^{\frac{1}{2}}|M_o|^2\hbar\omega}{q}\sin^{-1}\left(\frac{p_3}{p_3\max}\right)\Bigg|_{p_3\min}^{p_3\max}$$

$$\Delta\omega = -\frac{2\pi^2 m_{\perp}^{3/2}m_{\parallel}^{\frac{1}{2}}\ |M_o|^2\hbar\omega}{q} + \frac{4\ m_{\perp}^{3/2}m_{\parallel}^{\frac{1}{2}}|M_o|^2\hbar\omega}{q}\sin^{-1}\frac{2\sqrt{2m|z|}}{p_3\ \max} \qquad (54)$$

Equation (54) shows that there is a jump in the value of $\Delta\omega$ after the neck is brocken.

Case 3

Analysis of the Anomalies in $\Delta\omega$ for the case of Arbitrary Angle of the Phonon Momentum $\vec{q}$.

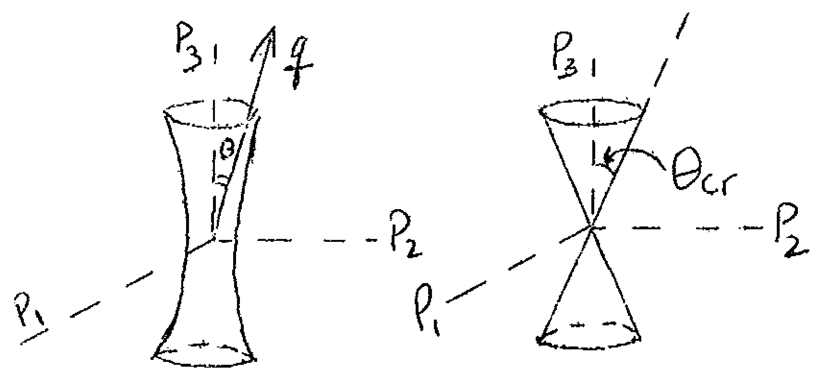

Fig.13. Rupture of the connecting neck of the Fermi surface

$$\frac{p_1^2}{2m_1}+\frac{p_2^2}{2m_2}-\frac{p_3^2}{2m_3}=z \quad , \quad z=\varepsilon_F-\varepsilon_c \quad , \quad \theta=\tan^{-1}\left(\frac{m_{\perp}}{m_{\parallel}}\right)^{\frac{1}{2}}$$

We can choose the direction of $\vec{q}$ to have no projection along the p_1 axis. ie. let

$$\vec{q} = (0,\ q\sin\theta,\ q\cos\theta) \tag{55}$$

The expression for $\Delta\omega$ will then be

$$\Delta\omega = \frac{\hbar\omega|M_o|^2 \int \delta\left(\frac{p_\perp^{\ 2}}{2m_\perp} - \frac{p_3^{\ 2}}{2m_\parallel} - z\right) p_\perp dp_\perp d\phi dp_3}{\frac{p_\perp^{\ 2}}{2m_\perp} - \frac{p_3^{\ 2}}{2m_\parallel} - \left[\frac{p_1^{\ 2}}{2m_\perp} + \left(\frac{p_2+q\sin\theta^2}{2m_\perp}\right) - \left(\frac{p_3+q\cos\theta^2}{2m_\parallel}\right)\right]}$$

$$= \frac{\hbar\omega|M_o|^2 2m_\perp}{2q} \int \delta \frac{\left[p_\perp^{\ 2} - 2m_\perp\left(\frac{p_3^{\ 2}}{2m_\parallel} + z\right)\right] d(p^{\ 2}) d\phi dp_3}{-p\frac{\sin\theta\sin}{m_\perp} + \frac{p_3\cos\theta}{m_\parallel} - \frac{q\sin^2\theta}{2m_\perp} + \frac{q\cos^2\theta}{2m_\parallel}}$$

Integration with respect to $p_\perp$ is based on the following property of the δ-function.

$\int F(x)\delta(x-a)dx = F(a)$ and the result is

$$\Delta\omega = \frac{m_\perp\hbar\omega|M_o|^2}{q} \int \frac{dp_3 d\phi}{\frac{-p_\perp\sin\theta}{m_\perp}\sin\phi + \frac{p_3\cos\theta}{m_\parallel} - \frac{q\cos^2\theta}{2m_\perp}(\tan^2\theta - \tan^2\theta_{cr})}$$

$$\Delta\omega = \frac{m_\perp \hbar\omega |M_o|^2}{q} \; I\,(q,\theta,z) \tag{56}$$

where

$$I(q,\theta,z) = \int \frac{dp_3 d\phi}{\frac{-p_\perp \sin\theta}{m_\perp} \sin\phi + \frac{p_3 \cos\theta}{m_{\parallel}} - \frac{q\ \cos^2\theta}{2m_\perp}(\tan^2\theta - \tan^2\theta_{cr})} \tag{57}$$

and

$$p_\perp = \left[2m_\perp \left(\frac{p_3}{2m_{\parallel}} + z\right)\right]^{\frac{1}{2}}$$

or

$$p_\perp = (2\ m_\perp\ z + p_3^2\ \tan^2\theta_{cr})^{\frac{1}{2}} \tag{58}$$

where

$$\theta_{cr} = \text{arc tan}\ \left(\frac{m_\perp}{m_{\parallel}}\right)^{\frac{1}{2}} \quad \text{(see Fig. 13)}$$

If $\theta = \theta_{cr}$, $I(q,\theta,z)$ will be independent on the phonon momentum $\vec{q}$. This means that the Migdal-Kohn singularity vanishes for this particular direction of the incident sound. We can investigate the behaviour of $I(q,\theta,z)$ as θ approaches θ_{cr} from both sides, ie. $\theta \to \theta_{cr}^{\pm}$. Here θ approaches θ_{cr} being less (θ_{cr}^{-}) or greater θ_{cr}^{+} respectively.

Equation (57) will have the form

$$I^{\mp}(q,\theta,z) = \int \frac{dp_3 d\phi}{\frac{-p_\perp \sin\theta_{cr}^{\mp}}{m_\perp}\sin + \frac{p_3\cos\theta_{cr}^{\mp}}{m_{\parallel}} - \frac{q\cos^2\theta_{cr}^{\mp}}{2m_\perp}\psi(\theta)}$$

(59)

where

$$\psi(\theta) = \tan^2\theta - \tan^2\theta_{cr}.$$

We can expand $\psi(\theta)$ about θ_{cr} to get

$$\psi(\theta) = \psi(\theta_{cr}) + \left.\frac{\partial\psi}{\partial\theta}\right|_{\theta=\theta_{cr}} (\theta-\theta_{cr}) + \cdots\cdots$$

$$= \frac{2\tan\theta_{cr}}{\cos^2\theta_{cr}} \Delta\theta$$

Where second order terms and above are neglected.

Equation (59) will now have the form

$$I^{\mp}(q,\theta,z) = \int \frac{dp_3 d\phi}{\frac{-p_\perp \sin\theta_{cr}^{\mp}}{m_\perp}\sin\phi + \frac{p_3\cos\theta_{cr}^{\mp}}{m_{\parallel}} - q\frac{\tan\theta_{cr}}{m_\perp}\Delta\theta}$$

in the limit as $\Delta\theta \to 0$.

$$I^{\mp}(q,\theta,z) = \int \frac{d\phi dp_3}{\frac{p_3\cos\theta_{cr}^{\mp}}{m_{\parallel}} - q\frac{\tan\theta_{cr}}{m_\perp}\Delta\theta - \frac{p\sin\theta_{cr}^{\mp}}{m_\perp}\sin\phi}$$

The integral over $d\phi$ is of the form

$$\int_0^{2\pi} \frac{d\phi}{1-a\sin\phi} \quad \text{and its value is} \quad \frac{2\pi}{(1-a^2)^{\frac{1}{2}}}$$

Thus

$$I^{\mp}(q,\theta,z) = 2\pi \int \frac{dp_3}{\left\{\left(\frac{p_3\cos^{\mp}_{cr}}{m_{\parallel}} - q\frac{\tan\theta_{cr}\,\Delta\theta}{m_{\perp}}\right)^2 - \frac{p_{\perp}{}^2\sin^2\theta^{\mp}_{cr}}{m_{\perp}{}^2}\right\}^{\frac{1}{2}}}$$

$$= 2\pi \int \frac{dp_3}{\left\{\left(\frac{\cos^2\theta^{\mp}_{cr}}{m_{\parallel}{}^2} - \frac{\sin^2\theta^{\mp}_{cr}\tan^2\theta_{cr}}{m_{\perp}{}^2}\right)p_3{}^2 - \frac{2q\tan\theta_{cr}\Delta\theta p_3\cos\theta^{\mp}_{cr}}{m_{\perp}\;m_{\parallel}} - \frac{2m_{\perp}z\sin^2\theta_{cr}}{m_{\perp}{}^2}\right\}^{\frac{1}{2}}} \qquad (60)$$

The above integral is of a standard form

$$\int \frac{dx}{(ax^2 + bx + c)^{\frac{1}{2}}}$$ and the result depends on the

sign of a, ie. on whether

$$\frac{\cos^2\theta^{\mp}_{cr}}{m_{\parallel}{}^2} - \frac{\sin^2\theta^{\mp}_{cr}\tan^2\theta_{cr}}{m_{\perp}{}^2} \qquad (61)$$

is greater or less than zero. Equation (61) can be written as

$$\frac{\tan^2\theta_{cr}\cos^2\theta^{\mp}_{cr}}{m_{\perp}{}^2}\,(\tan^2\theta_{cr} - \tan^2\theta^{\mp}_{cr}) \qquad (62)$$

For $\theta < \theta_{cr}$ the sign of (69) is positive and $I^{-}(q,\theta,z)$ is the logarithmic function since

$$\int \frac{dx}{(ax^2+bx+c)^{\frac{1}{2}}} = \frac{1}{a^{\frac{1}{2}}} \ln \left| 2\left[a(ax^2+bx+c)\right]^{\frac{1}{2}} + 2ax+b \right|$$

for $a > 0$ (see for example Dwight 1961).

But for $\theta > \theta_{cr}$ $I^{+}(q,\theta,z)$ is a function of arc sin type because the value of the above standard integral is

$$\frac{-1}{(-a)^{\frac{1}{2}}} \sin^{-1} \frac{2ax+b}{(b^2-4ac)^{\frac{1}{2}}} \quad , \quad a < 0,\ b^2 > 4ac \quad |2ax+b| < (b^2-4ac)^{\frac{1}{2}}$$

Since $I^{+}(q,\theta,z)$ is of the arc-sin type for $\theta > \theta_{cr}$ the Migdal-Kohn singularities vanish. Whence in rupture of the connecting neck the Migdal-Kohn singularities may be observed only in the case when the angle between the phonon wave-vector of the incident sound and the axis of the neck is less than θ_{cr}.

According to the results of Davydov and Kaganov (1974) the absorption coefficient Γ has an appreciable anisotropy upon the rupture of a connecting neck. In certain cases $\theta < \theta_{cr}$ Γ undergoes a jump as in the formation of new cavity in others $\theta > \theta_{cr}$ it possesses a logarithmic singularity.

The results of this section of the thesis for the phonon shift in frequency $\Delta\omega$ and that of the absorption coefficient Γ as acquired by Davydov and Kaganov (1974) are in agreement with the recent results of Kaganov and Lisovskaya (1981). According to the last result the singularities in Γ and $\Delta\omega$ are interdependent which is also in line with the prediction using the Kramer's and Kronig relations (see for example Landau and Lifshitz, 1958).

Γ : Jump in the derivative $\Delta \ \ell n|\Delta|$

$\Delta\omega$: $\Delta \ \ell n|\Delta|$ jump in the derivative

These relations indicate that the singularities in the absorption coefficient manifest themselves in the phonon spectrum.

CONCLUDING REMARKS

In general it is found out in this thesis that the anomalies in the sound absorption coefficient Γ and the shift of the phonon frequency $\Delta\omega$ depend on the topology of the phase transitions of order $2\frac{1}{2}$ and on the local geometry of the Fermi surface.

During the formation or disappearance of a new spherical cavity Γ undergoes a jump (equation 42) and $\Delta\omega$ has singularity of type $x \ \ln x$ (equation 43) for any direction of the phonon wave vector.

In the case of appearance or disappearance of ellipsoidal cavity at phase transition of $2\frac{1}{2}$ order the jump in the absorption coefficient was found out to be anisotropic (equation 47) because of the θ and ϕ dependence of the equation. The singularity in the phonon spectrum for this phase transition is also anisotropic and of the $x \ \ln|x|$ type. Besides this $\Delta\omega$ has undergone a change which is directly proportional to $\sqrt{|z|}$ (the second term of equation 48).

Upon the rupture of the connecting neck three cases were considered.

<u>Case 1a</u>: $\vec{q} = (0,0,q)$ and $z > 0$. $\Delta\omega$ has unobservable singularity of type $\ln x$ (equation 51).

Case 1b: $\vec{q} = (0,0,q)$ and $z < 0$. $\Delta\omega$ has a jump of logarithmic function as compared to case 1a. The singularity is stronger than the previous ones. The group velocity has hyperbolic singularity since $\Delta\omega$ is of type $\ell n|x|$.

Case 2: $\vec{q} = (q,0,0)$. $\Delta\omega$ has a constant value for fixed $|\vec{q}|$ and $z > 0$, and a jump of arc sin type for $z < 0$ (54). So the Migdal-Kohn singularities vanish for this case.

Finally, I would like to stress the fact that every analysis discussed in this thesis on the Migdal-Kohn singularities is upon the assumption that the temperature T is equal to zero. If T increases from zero gradual smearing off of the singularities takes place and experimental observation of the image of the Fermi surface becomes more difficult. Also $\hbar\omega$ is ignored compared with the Fermi Energy ε_F or $z = \varepsilon_F - \varepsilon_c$, in this thesis. It is now an established result that fine structure of the singularities (ie. two closely located kinks) should appear on the absorption coefficient and change in phonon frequency curves.

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