MONOGRAFIAS DE FÍSICA

XXII

FIELD THEORETICAL METHODS IN THE THEORY OF METALS

by

Richard E. Prange

Notes prepared by:
Prem P. Srivastava
I. Kímel

INDEX

* * *

I. INTRODUCTION

In this lecture we shall give a sort of preview, of the
rest of the course. We are going to discuss the results   of
the following experiment. Take a piece of quartz and evaporate
a thin strip of some metal, say, lead, on it, of thickness,
say, 10,000 A^O. Allow this to oxidize, to a thickness of, say
30 A^O. Then evaporate a thin strip of the same, or some other
metal, perhaps aluminium, at right angles. Hook up a voltmeter,
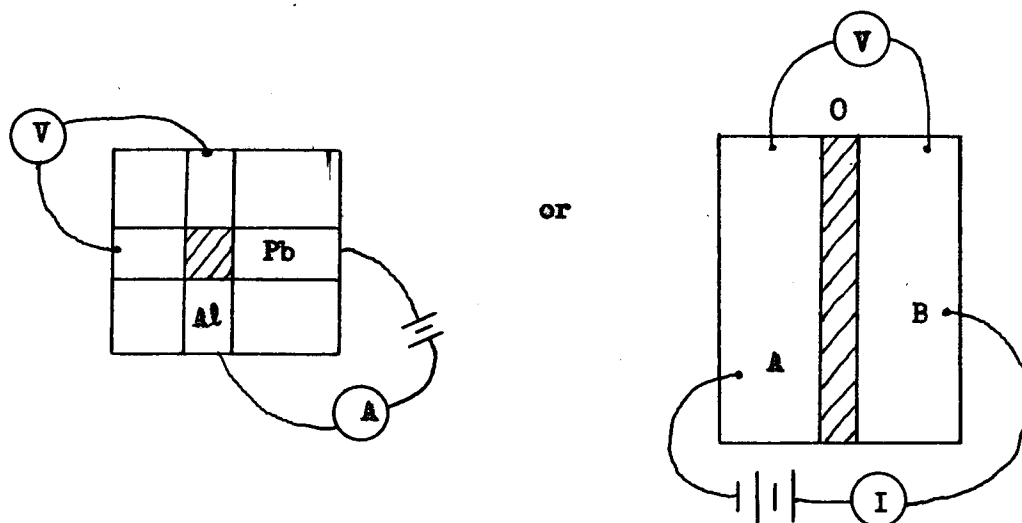ammeter, and battery as in the diagram.

FIG. 1

Keep this at very low temperature, say 1^OK, and observe I vs.
V. What is observed is:

structure here - phonon
induced density of states

structure here

Josephson effect structure here, energy gap
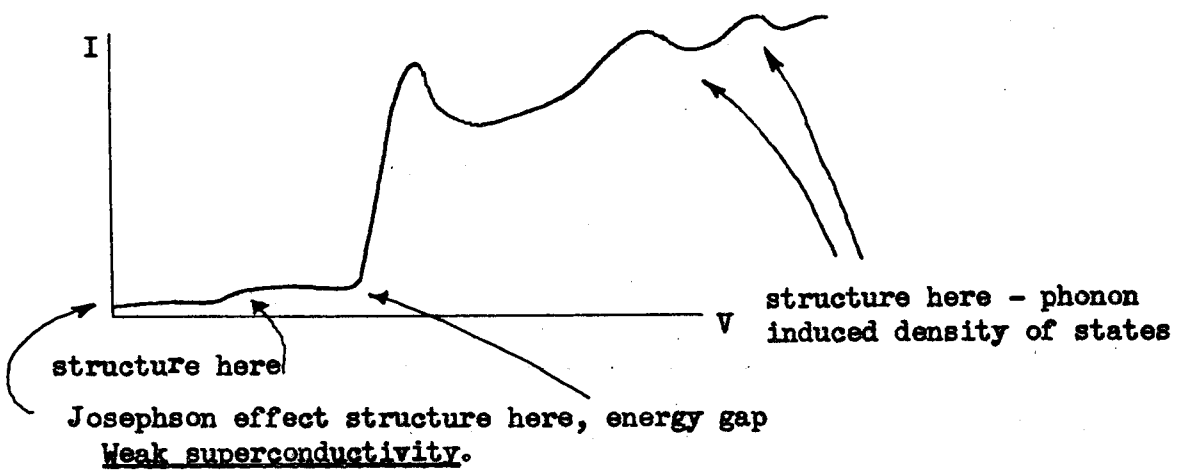Weak superconductivity.

FIG. 2

This phenomenon is remarkable in that it can be studied both theoretically and experimentally to great precision, and will probably become very useful as a tool in the future to map out some of the internal structure of metals.

A very elementary model of this phenomenon is as follows:
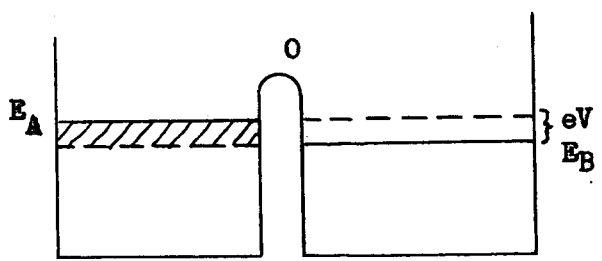
Represent the arrangement of metals by potential wells.

FIG. 3

Electrons fill all the energy states in metal A below E_A, and similarly for B, but $E_A > E_B$ because of the battery. By quantum tunneling, an electron in A can pop over into B, provided a state of the right energy is available to it. Thus only those electrons in the shaded region can tunnel.

But suppose B is a super-conductor. Then, there are no states at the Fermi surface for electrons, there is an energy gap. Thus, one must raise the energy of the electrons by an amount, at least the energy gap. This is the reason for the gap in the I vs. V graph of Fig. 2.

Suppose we raise the voltage still further. Then electrons will tunnel from a state of A into an excited state of B. It can subsequently decay by emission of a photon, i.e., it can give up some energy to distortion of the lattice.

This is a sort of final state interaction which can effect the tunneling rate.

FIG. 4
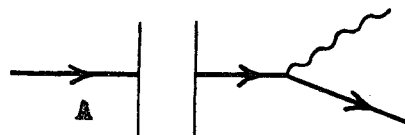
If there are particularly many phonons which can be emitted, that is if the lattice can be easily distorted at this energies, we will obtain a bump (or dip) in I/V.

However, the most naive theory of this is quite misleading, since renormalization effects are very important.

These effects are most naturally and intuitively described by means of the concepts of field theory. We thus have to

4

study the _field theory_ of _electrons_ and _phonons_. It turns out that only when we have _superconductors_ are interesting results obtained. So we have to study _superconductors_.

The _tools_ we use, are 2nd quantization, Green's functions, Feynman graphs, and dispersion relations. All of these we will use heuristically, and not bother much about details and proofs. I will take for granted some intuitive knowledge of the creation and destruction operators, $\psi^+(x)$, $\psi(x')$ which obey the anti-communtation relations:

$$\left\{\psi(x), \psi^+(x')\right\} = \delta^3(x - x')$$

$$\left\{\psi(x), \psi(x')\right\} = 0$$

We will often use these in the Heisenberg representation, so,

$$\psi(x, t) = e^{iHt} \psi(x) e^{-iHt}$$

$$H \equiv H_0 - \mu N \quad (\mu = E_A \text{ of Fig. 3}) \quad (\text{sometimes } (\underline{x}, t) = x)$$

Also, we shall usually expand

$$\psi(x) = \frac{1}{\sqrt{V}} \sum_k c_{\underline{k}} \, e^{i\underline{k}\cdot\underline{x}}$$

$$\left\{c_{\underline{k}'}, c_{\underline{k}'}^+\right\} = \delta_{\underline{k}\underline{k}'} \quad (\text{periodic box normalization})$$

and convert sums to integrals by

$$\frac{1}{V} \sum_k = \int \frac{d^3k}{(2\pi)^3}$$

The _Green's functions_ are defined as

$$G(x - x') = \frac{1}{i} \left\langle T\left(\psi(x)\, \psi^+(x')\right)\right\rangle$$

where

$$T(A(t), B(t')) = A(t) B(t') \qquad t > t'$$
$$= - B(t') A(t) \qquad t \leqslant t'$$

$\langle \quad \rangle$ means thermodynamic expectation value.

In the theory of tunneling this Green's function is important. For most other purposes, the Green's function

$$G_2 = \left(\frac{1}{i}\right)^2 \langle T[\psi(1) \, \psi(2) \, \psi^+(3) \, \psi^+(4)] \rangle \qquad \text{is more important} \qquad \text{since}$$

it contains information such as the density correlations

$$\langle \rho(1) \, \rho(2) \rangle \qquad \text{where} \quad \rho(x) = \psi^+(x) \psi(x)$$

We shall begin therefore, by obtaining some general properties of the Green's function. We shall follow by calculating it in a specific model, which should be very good. (It can be compared with experiment).

We shall follow by extending the theory to supercondutivity and discuss some very important results which are obtained in this way.

Finally we shall discuss the tunneling, and how the phonons are imaged. If we have time, we shall discuss the weak superconductivity which is a spectacular recent development, but for which the full development of the theory is not really needed, yet.

II. MATHEMATICAL PRINCIPLES

The properties of a quantum mechanical system composed of many identical particles are described conveniently in terms of second-quantized Heisenberg representation operators $\psi^+(\underline{x},t)$ and $\psi(\underline{x},t)$. The creation operator $\psi^+(\underline{x},t)$, when acting to the right on a state of the system, adds a particle to the state at the space-time point $(\underline{x},t)$ while $\psi(\underline{x},t)$ is the operator which removes a particle at $(\underline{x},t)$.

The density of particles at the point $(\underline{r},t)$ is

$$\psi^+(\underline{r}\ t)\ \psi(\underline{r}\ t)$$

while the total number of particles is

$$N(t) = \int d^3r\ \psi^+(rt)\ \psi(rt)$$

Similarly, the total energy operator H and in fact any physical operator can be expressed in terms of $\psi(\underline{r},t)$ and $\psi^+(\underline{r},t)$.

The equation of motion of any operator (not depending explicity on time) in the Heisenberg representation is ($\hbar = 1$)

$$\frac{id\ X}{dt} = \Big[X(t),\ H(t) \Big]$$

It follows that H(t) is well as N(t) are independent of time. Then we can integrate the differential equation to obtain

$$X(t) = e^{iHt}\ X(0)\ e^{-iHt}$$

The symmetry requirement on the wave function of any state of a collection of particles is expressed by

$$\psi(\underline{r}t)\,\psi(\underline{r}'t) \mp \psi(\underline{r}'t)\,\psi(\underline{r}t) = 0$$

$$\psi(\underline{r}t)\,\psi^+(\underline{r}'t) \mp \psi^+(\underline{r}'t)\,\psi(\underline{r}t) = \delta(\underline{r} - \underline{r}')$$

where the upper sign refers to Bose-Einstein particles and the lower to Fermi-Dirac particles.

We will be interested in the behaviour of many-particles systems at finite temperature. For a system in thermodynamic equilibrium the thermodynamic average of any operator $\{\ \}$ may be computed by using the grand-canonical ensemble, viz.

$$\langle \{\ \} \rangle = \frac{\text{TR}\left[\{\ \}e^{-\beta \bar{H}}\right]}{\text{Tr}\ e^{-\beta H}}$$

where $H = (H_{usual} - \mu N)$, μ is the chemical potential and $\beta = 1/k_B T$ Zero temperature or $\beta \to \infty$ describes the ground state of the system. In the energy representation the average can be written as

$$\langle \{\ \} \rangle = \sum_s \langle s|\{\ \}|s\rangle\ e^{-\beta E_s} \Big/ \sum_\ell e^{-\beta E_\ell}$$

where

$$H|s\rangle = E_s|s\rangle$$

III. THERMODYNAMIC GREEN'S FUNCTIONS

The application of the methods of quantum field theory to many body problem can be greatly extended, just as in the quantum field theory, if we use Green's functions, which enables us to obtain approximations which differ from the expansions of the perturbation theory, being as a rule the result of the summation of an infinite set of definite terms of the perturbation-theory series.

The one-particle Green's function is defined by *

$$G(1,2) = \frac{1}{i} \langle T | \psi(1) \, \psi^+(2) | \rangle$$

while the two particle Green's function is defined by

$$G_2(1\,2\,3\,4\,) = \frac{1}{i}^2 \langle T \left[\psi(1) \, \psi(2) \, \psi^+(3) \, \psi^+(4) \right] \rangle$$

where T represents the time-ordering operator and 1 stand for $(\underline{r}_1, t_1)$. The operator T is defined by

$$T \left[\psi(1) \, \psi^+(2) \right] = \psi(1) \, \psi^+(2) \qquad t_1 > t_2$$
$$= \pm \, \psi^+(2) \, \psi(1) \qquad t_1 < t_2$$

the upper sign referring to bosons while the lower to fermions.

The $G(1, 2)$ describes the propagation of disturbances in which a single particle is either added to or removed from the many particle equilibrium system. For example, for $t_1 > t_2$ the disturbance produced by the addition of a particle at $(\underline{r}_2 \, t_2)$ propagates to the later time t_1 when a particle is removed at

---

* Factor $(-i)$ is purely conventional.

$\underline{r}_1$ taking back the system to its equilibrium state. For $t_1 < t_2$ the disturbance caused by the removal of a particle at $(r_1 t_1)$ propagates to time t_2 when it is terminated by the addition of a particle at the point r_2. A similar interpretation to many particle Green's function can be easily given.

In our discussion we will only make use of one particle Green's functions, whose mathematical properties we will now discuss. In this connection we will also make use of the definitions *

$$G^{>}(1,2) = \frac{1}{i} \langle \psi(1)\,\psi^{+}(2)\rangle$$

$$G^{<}(1,2) = \pm \frac{1}{i} \langle \psi^{+}(2)\,\psi(1)$$

We will assume that the Hamiltonian is invariant with respect to rotations and translations in space so that $G^{\lessgtr}$ depends only on $|\underline{r}_1 - \underline{r}_2|$ and $(t_1 - t_2)$
viz

$$G^{\lessgtr}(1\,2) \equiv G^{\lessgtr}(1-2) = \underline{G}^{\lessgtr}(|r_1-r_2|,\, t_1 - t_2)$$

We can develop some of the general properties of the Green's functions by expanding out the trace as a sum over states. Thus,

$$i\,G^{>}(1,2) = \sum_{nm} \langle n|\psi(1)m\rangle\langle m|\psi^{+}(2)|n\rangle\, e^{-\beta E_n}/\sum_k e^{-\beta E_k}$$

$$= \sum_{nm} \langle n|\psi(\underline{1})m\rangle\langle m|\psi^{+}(2)|n\rangle\, e^{-iE_{nm}(t_1-t_2)}\, e^{-\beta E_n}/\sum_k e^{-\beta E_k}$$

$$\pm i\,G^{<}(1,2) = \sum_{n,m} e^{iE_{nm}(t_1-t_2)-\beta E_n}\langle n|\psi^{+}(2)|m\rangle\langle m|\psi(1)|n\rangle/\sum_k e^{-\beta E_k}$$

Take the Fourier transform w.r.t. $t_1 - t_2$. It then follows at once, that

$$G^>(r_1 r_2 \omega) = i \int e^{i\omega t_{12}} G^>(r_1 r_2 t_{12}) =$$

$$= 2\pi \sum_{nm} \delta(\omega - E_{nm}) e^{-\beta E_n} \langle n|\psi(1)|m\rangle \langle m|\psi^+(2)|n\rangle$$

etc. (Note the i)

Also the Fourier transform w.r.t. $r_1 - r_2$

$$G^>(k\omega) = 2\pi \sum_{nm} \delta(\omega - E_{nm}) e^{-\beta E_n} |\langle n|C_k|m\rangle|^2$$

$$G^<(k\omega) = 2\pi \sum_{nm} \delta(\omega + E_{nm}) e^{-\beta E_n} |\langle m|C_k|n\rangle|^2$$

$$G^>(k\omega) = e^{-\beta\omega} G^<(k\omega)$$

$G^>(k\omega)$ has the interpretation of density of states of electrons of energy ω, momentum k.

$G^<(k\omega)$ has the interpretation of density of electrons of energy ω, momentum k, or density of states of holes of energy $-\omega$, momentum $-k$.

Consider now the combination $\psi(1)\ \psi^+(2) \mp \psi^+(2)\ \psi(1)$ according as we have Bose or Fermi statistics. Expressing the Fourier transform of this by the G's, we have

$$A(k\omega) = G^>(k\omega) \mp G^<(k\omega)$$

i.e.,

$$G^<(k\omega) = f(\omega)\ A(k\omega)$$

$$G^>(k\omega) = \left[1 \pm f(\omega)\right] A$$

where

$$f(\omega) = \frac{1}{e^{\beta\omega} \mp 1}$$

Note that we have

$$\int \frac{d\omega}{2\pi} A(k\omega) = 1$$

and

$$A(\underline{k}\omega) \geqslant 0 \qquad \omega > 0$$

For free electrons,

$$A(k\omega)_{\text{free}} = 2\pi \,\delta\left(\omega - \frac{k^2}{2m} + \mu\right)$$

In generalm $A(\underline{k}\omega)$ will in favorable cases have some behaviour approximately as a δ-function.

Let us also insert a complete sum over states into G. Let us write (for fermions)

$$T\,\psi(1)\,\psi^+(2) = 0(1-2)\,\psi(1)\,\psi^+(2) - 0(2-1)\,\psi^+(2)\psi(1)$$

Now

$$0(1-2) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{e^{i\omega'(t_1 - t_2)}}{\omega' - i\eta}$$

Therefore, by the Faltung theorem of Fourier analysis,

$$G(\underline{k}\omega) = \int d^3 x_{12} \int dt_{12}\, e^{i\omega t_{12}}\, e^{-ik\,x_{12}}\, G(12)$$

$$= \int \frac{d\omega'}{2\pi}\, \frac{G^>(k\omega')}{\omega - \omega' + i} + \frac{G^<(k\omega')}{\omega - \omega' - i\eta}$$

Thus, $\text{Re } G\,(\underline{k}w) = P\int_{-\infty}^{\infty} \frac{d\omega'}{2\pi}\, \frac{A(k\omega')}{\omega - \omega'}$

Therefore $A(\underline{k}\omega)$, which has simple properties, completely determines G, and is, to first approximation, independent of temperature.

The free electron Green's function at zero temperature is

$$\frac{1}{\omega - \frac{k^2}{2m} + \mu + i\eta(k)}$$

where

$$\eta(k) > 0 \qquad k > k_o$$
$$\eta(k) < 0 \qquad k \leqslant k_o$$

Also,

$$G(kz) = \int_{-\infty}^{\infty} \frac{d\omega'}{2\pi} \frac{A(k\omega')}{z - \omega'} \, , \quad z \text{ complex}$$

Sometimes, $G(\underline{k}\,\omega_N)$ is first defined where

$$\omega_N = (2N+1)T\pi i \qquad \text{(for fermions)}$$

Note $f(\omega_N) = \infty$ i.e. ω_N are the poles of $f(z) = \dfrac{1}{e^{\beta z} + 1}$

$\sum\limits_{N}$ is equivalent to the integration above.

IV. LATTICE VIBRATIONS

We now turn to a discussion of the lattice vibrations in metals. The purpose of this will be to show that the small shakings and distortions can be described by phonons, which are quantized sound waves with properties like bosons. This is a subject which is very simple in principle, but very difficult neumerically. (Actually, there are some difficult points of principle also, which we shall gloss over). We shall obtain the oder of magnitude of the phonon wave lengths and frequencies. We shall also obtain the coupling between phonons and electrons, and discuss the order of magnitude of this coupling. Better estimates and fuller discussions of this problem are to be found in such standard works as Ziman (/), Peierls (5), and Pines (6). It is to be emphasized, however, that the problem is not solved satisfactorily at present, and in fact, one of the uses of the tunneling experiments in the future will be to obtain experimental information on this subject.

Consider that the ions are located near their equilibrium points, the position of the i'th ion being

$$\underline{X}_i = \underline{a}_i + \underline{u}_i$$

where a_i is the position in a perfect lattice, and u_i is small, The kinetic energy of the ions is,

$$\sum_{k=1}^{3} \sum_{i=1}^{N} - \frac{1}{2M} \frac{\partial^2}{\partial u_{i,k}^2}$$

$u_{i,k}$ is the k'th component of the displacement.

and their potential energy is some (poorly known) function,

$V(X_1 \ldots X_N)$

$$V(a_1 \ldots a_N) + \sum_{i,j} \sum_{k\ell} \frac{1}{2} u_{i,k} \, u_{j\ell} \, G_{ik,j\ell}(a_1 \ldots) + \ldots$$

Since $V(a_1 a_2 \ldots a_N)$ is constant, we drop it. There are no linear terms in u since the lattice is in equilibrium at $X_1 = a_1$. The problem is to find what $\underline{G}$ is in a reasonable way, and then diagonalize it.

The result is going to be that the normal modes are harmonic oscillators. We can reduce the diagonalization problem considerably, since $\underline{G}$ can only depend on $a_i - a_j$, if we neglect surface effects. We exploit this, as usual, by bringing in the Fourier transform.

Thus, let us introduce

$$\underline{u}_i = \sum_{\rho=1}^{3} \sum_{f} \frac{e^{if \cdot a_i}}{\sqrt{MN}} \, q_\rho(f) \, \underline{e}_\rho(f)$$

The vector $\underline{f}$ runs over values $\frac{2\pi}{L}(n_1, n_2, n_3)$, if we make the fiction that we have a crystal cube of side L, and impose periodic boundary conditions. We can add to $\underline{f}$ any vector $\underline{G}$ such that $\underline{G} = \underline{a}_i = 2\pi n$. The usual convention is to allow only the shortest inequivalent values of $\underline{f}$. These fill what is called the <u>first Brillioun zone</u>: $\underline{G} \; \underline{a}_i = 2\pi \, m_i$.

It is easy to check that there are exactly N values of $\underline{f}$ in this zone. The orthogonality relation $\frac{1}{N} \sum_{i} e^{i(f-f') \cdot a_i} = \delta_{ff'}$

The <u>polarization</u> subscript (p) runs from one to three, and corresponds to the fact that we may have to mix components of $\underline{u}$ in order to diagonalize $\underline{G}$. The coordinates q play the role of normal coordinates for the phonons.

With this substitution, we find for the potential energy,

$$V = \frac{1}{2} \sum_{f} \sum_{f'} \sum_{pp'=1}^{3} \sum_{i,j=1}^{N} \frac{e^{-i\,f(a_i-a_j)}\,e^{-i(f-f')\cdot a_j}}{N}\,q_p^*(f)q_{p'}(f')$$

$$+ \frac{1}{M} \sum_{k,\ell} e_p^{*k}\ G^{k\ell}(a_i-a_j)\ e_{p'}^{\ell}(f^-)$$

(We have need the fact that $\underline{u}_i$ is real, to replace it by $\underline{u}_i^*$). If we perform the sum over $a_i - a_j$ and a_j, we obtain

$$V = \frac{1}{2} \sum_{\underline{f},p} \omega_p^2(\underline{f})\ q_p^*(\underline{f})\ q_{p'}(\underline{f}')$$

where the polarization vectors e are chosen to make

$$\frac{1}{M} \sum_{k,\ell} e_p^{*h}(f)\ G^{h\ell}(\underline{f})\ e_{p'}^{\ell}(f) = \delta_{pp'}\cdot\omega_p^2(f)$$

and

$$G^{h\ell}(\underline{f}) = \sum_i e^{-if\cdot a_i}\ G^{h\ell}(a_i)$$

It is easily shown that $\omega_p^2(f)\geqslant 0$ and that $\omega_p(f) = \omega_p(-f)$.

We have therefore formally diagonalized the Hamiltonian, so it now reads

16

$$H_\phi = -\frac{1}{2} \sum_{\rho f} \frac{\partial^2}{\partial q_p^*(f)\, \partial q_p(f)} + \frac{1}{2} \omega_p^2(f)\, q_p^*(f)\, q_p(f)$$

Finding the frequencies $\omega(\underline{f})$ is a difficult numerical problem. Having reduced the Hamiltonian to this harmonic oscillator form, we introduce the usual raising and lowering operators to make the vibrations look like particles. Let,

$$a_p(f) = \sqrt{\frac{\omega_p(f)}{2}}\, q_p(f) + \frac{1}{\sqrt{2\omega_p(f)}}\, \frac{\partial}{\partial q_p^*(f)}$$

$$a_p^+(f) = \sqrt{\frac{\omega_p(f)}{2}}\, q_p^*(f) - \frac{1}{\sqrt{2\omega_p(f)}}\, \frac{\partial}{\partial q_p(f)}$$

It turns out that the commutator is

$$\left[a_p(f),\ q_{p'}^+(f') \right] = \delta_{pp'}\ \delta_{ff'}$$

and thus

$$N_p\, a_p^+ = a_p^+\, (N_p + 1)$$

$$N_p(f) = a_p^+(f)\, a_p(f) \qquad\qquad \text{where}$$

$N_p(f)$ is the operator for the <u>number</u> of <u>phonons</u> in the state <u>p.f.</u> The phonons are thus to be regard as a gas of bosons, with wave number $\underline{f}$, polarization p, energy $\omega_p(f)$. The Hamiltonian is, in terms of the a's;

$$H_\phi = \sum \omega_p(f)\, a_p^+\, a_p(f) + \qquad \text{(zero point energy)}$$

We now consider the range of frequencies and wave numbers

of the phonons. The wave vectors $\underline{f}$ are confined to the Brillioun zone, which is a complicated polyhedron. If we replace this by a sphere, we have

$$\sum_{f < f_0} = (2\pi)^{-3} \, V \int_{f < f_0} d^3 f = \frac{V}{6\pi^2} \, f_0^3 = N$$

or $\qquad f_0 \sim \frac{\pi}{a}$ $\qquad\qquad\qquad$ where $a^3 = \frac{V}{N}$

The bulk of the phonons therefore have wave lengths comparable with a few lattice spacing, or, in other words, most lattice vibrations involve only a few neighboring atoms. The very long wave length phonons are important for some special purposes, but do not appreciably influence the tunneling.

An important thing to know is the density of oscillators of a given frequency, i.e.

$$d\omega \, F(\omega) = \frac{1}{V} \sum_{\ell f} \left[\delta\big(\omega + d\omega - \omega_p(f)\big) - \delta\big(\omega - \omega_p(f)\big) \right].$$

This function typically is complicated, and may have a graph, as follows
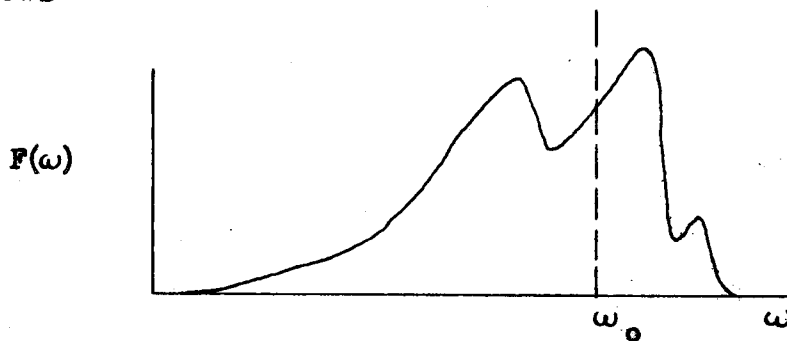

FIG. 5

We want to give a single number, such as ω_0, to describe this distribution in a crude way.

Purely in order to simplify the writing, we are going to assume that all phonons have the same frequency. (Einstein). This is not an anormously bad approximation, and it will save us much notation.

We now consider how the electrons interact with the phonons. The interaction occurs because the presence of an electron tends to distort the lattice, and conversely, a distorted lattice will deflect the electrons. To find the form of this coupling to a good degree of approximation is very difficult, and is an unsolved problem. However the basic idea is very simple.

Let the potential seen by an electron be (in the second quantized notation)

$$\int d^3x \; \psi^+(x) \sum_i V(x - X_i) \; \psi(x)$$

Expand

$$V(x - x_i) = V(x - a_i) - \underline{u}_i \cdot \nabla V(x - a_i)$$

and put in the expansion for $\underline{u}_i$. The first term gives
$\sum_i \int d^3x \; \psi^+(x) \; V(x - a_i) \; \psi(x)$ i.e. a perfectly periodic potential for the electrons. One should solve this part of the problem and obtain Bloch wave functions for the electrons, but to obtain simpler expressions and the order of magnitude, we use plane waves. This is probably not a bad approximation in any case.

Thus, we have,

$$\int \frac{d^3}{V} \sum_{k'} C_k^+ e^{-ik' \cdot x} \sum_{l} \sum_{f} \frac{a(f) + a^+(-f)}{\sqrt{2\omega(f) M N}} e^{if \cdot a_l} \underline{e}(f) \cdot \nabla V(-a_l)$$

$$\times \sum_{k} C_k e^{ik \cdot x}$$

In the i'th term above, make the replacement $x \to x + a_l$. All of the dependence on a_l' then occurs in the exponential,

$$\sum_{l} e^{i(k+f-k') \cdot a_l} = N \delta_{\underline{k}+\underline{f}-\underline{k}'}$$

We should have allowed also value $\underline{f} + \underline{G}$, (Umklapp) but we suppress these for simplicity. We obtain, therefore,

$$H_{e\phi} = \frac{1}{\sqrt{N}} \sum_{kk'f} \alpha(hh'f) C_{k'}^+ C_k (a(f) + a^+(-f)) \delta_{k',k+f}$$

where

$$\alpha(kk'f) = -\frac{N}{V} \int \frac{d^3}{\sqrt{2\omega(f)M}} \underline{e}(f) \cdot \nabla V(x) e^{i(k-k') \cdot x}$$

Since α depends predominantly on $\underline{f}$, in most model approximations, we write it as $\alpha(f)$. What is the order of magnitude of α ? For that purpose, replace

$$\frac{N}{V} \to \frac{1}{a^3} , \quad \omega(f) \to \omega_0 \quad d^3x \to a^3$$

(the range of the potential $\sim a$)

$\nabla \to \frac{1}{a}$ (same reasoning) $V \to \mathcal{E}_0$ (it is the potential of an electron near an ion, therefore some few electronvolts).

Thus

$$|\alpha| \sim \sqrt{\frac{\varepsilon_o^2}{Ma^2\omega_o}} = \sqrt{\frac{m}{M}\frac{\varepsilon_o}{\omega_o}} \sim \sqrt{\varepsilon_o \omega_o}$$

or $\alpha(f) = \lambda(f)\sqrt{\varepsilon_o\omega_o}$ where $\lambda(f)$ is dimensionless, and of the order of magnitude unity. It turns out that the problem can be solved even through λ is not small.

V. COMPUTATION OF THE GREEN'S FUNCTION

We now want to obtain $G(\underline{k},\omega)$ for a normal metal. To do this we want to exploit the facts which we have discovered, namely, $\omega_0/\epsilon_0 \ll 1$ but typical values of f are $1/a$, and typical eletronic wave vectors are also of that order of magnitude.

First, we consider the general structure of $G(\underline{k},\omega)$. We create an electron of momentum k, and later on destroy it returning it to the same state from which we started. What can happen ?
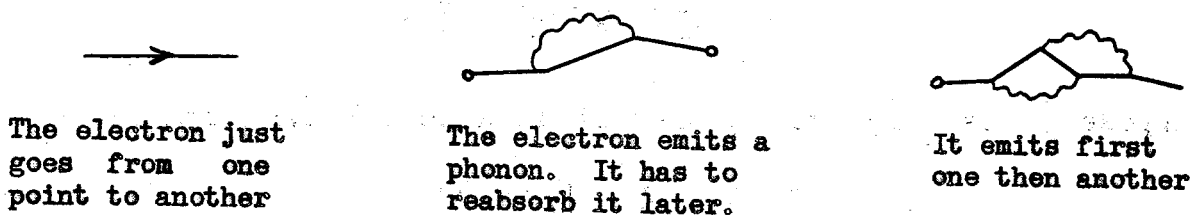
The electron just goes from one point to another

The electron emits a phonon. It has to reabsorb it later.

It emits first one then another

FIG. 6

In general the contributions to G arise from the diagrams.

+

+ ...

It does something complicated

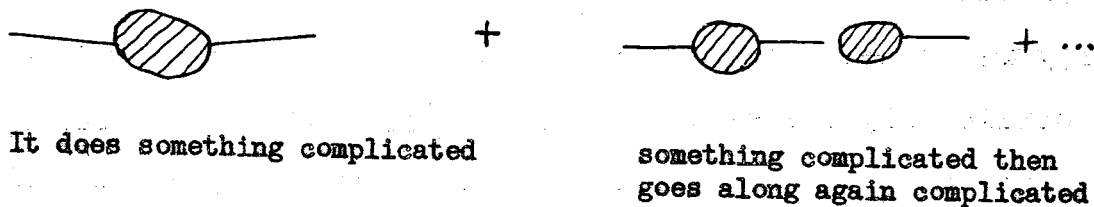something complicated then goes along again complicated

FIG. 7

Write G in the form: $G(kz) = G^0 + G^0 M G^0 + G^0 M G^0 M G^0 + G^0 +$ $+ G^0 M G$. Where M is called the mass operator and $G^0 = \dfrac{1}{z - \epsilon_k}$.

We thus have $G(kz) = \dfrac{G^0}{1 - G^0 M} = \dfrac{1}{z - \epsilon_k - M(kz)}$. Mathematically, it is more convenient to write Z, a complex number, instead

of ω. Then $M(k,z)$ has a dispersion relation, since G does.

$$M(\underline{k},z) = \frac{1}{2\pi} \int d\omega' \frac{\Gamma(k\omega')}{z - \omega'}$$

It follows:

$$M(k,\omega+i\eta) = \sum(k\omega) - \frac{1}{2}\Gamma(k\omega)$$

where

$$\sum(k\omega) = \frac{P}{2\pi} \int d \frac{\Gamma(k\omega')}{\omega - \omega'}$$

Thus, since $A = -2\,\text{Im}\,G(k,\omega+ i\eta)$, we find

$$A(k\omega) = \frac{\Gamma}{\left[\omega - \epsilon_k - \sum\right]^2 + \frac{1}{4}\Gamma^2}$$

Suppose Γ is very small, then it is a well known formula,

$$A(k\omega) \simeq 2\pi\,\delta(\omega - \epsilon_k - \sum(k\omega))$$

(to be compared with $2\pi\delta(\omega - \epsilon_k)$, the <u>free case</u>).

Actually, for given k, A has the interpretation as giving the probability that either C_k or C_k^+ will create a state of energy ω, relative to the "ground state". For the free gas, we can obtain only states of energy ϵk. <u>Now</u>, there is a <u>width</u> to the state of Γ i.e., $A(k, w)$ has the form: (in the case of interacting electrons).
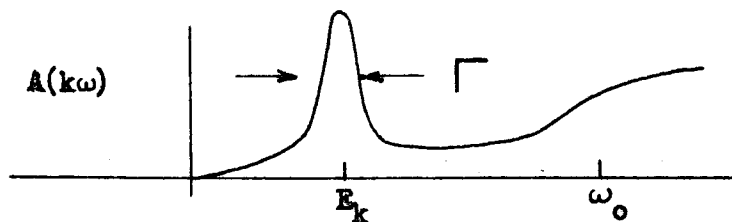

FIG. 9

By the uncertainty principle, Γ^{-1} is regarded as the lifetime of the state. All of this holds if Γ is small (This turns out to be true for $\omega \ll \omega_0$).

We note also that in this case

$$A(k\omega) \simeq 2\pi \, \delta(\omega - \varepsilon_k - \sum(k\omega)) = 2\pi \, z_k \, \delta(\omega - E_k)$$

where $E_k = \sum_k + \sum (k \, E_k)$, i.e. $\sum(k_\omega)$ is a "self-energy" correction.

$$z_k^{-1} = 1 - \left(\frac{\partial \sum}{\partial \omega}\right)_{\omega = E_k}$$

z_k is a renormalization factor. It comes about because we have injected the electron suddenly into the metal. (It is possible to show (Exercise:) that $0 \leqslant z_k \leqslant 1$.

The other electrons have to adjust themselves (in a time $\frac{k}{\varepsilon_0}$; the ions adjust themselves in a time $\frac{k}{\omega_0}$, afterwards, there is left a long lived state, lasting for a time $\frac{\hbar}{\Gamma}$. There is the possibility that the other electrons don't adjust themselves, etc; they do something nasty, or a sound wave is created. Only with a probability z_k will the long lived state be created.

Of course $\int A(\omega) \, d\omega/2\pi = 1$; so the δ-function can't be the whole story. And this is clearly true mathematically, since if $(\partial \sum/\partial \omega)$ is appreciable, $\Gamma(\omega)$ must be appreciable at some frequency. Where ? Clearly near $\omega \sim \omega_0$, and again near $\omega \sim \varepsilon_0$.

We actually expect Γ to be small for $\omega/\omega_0 \ll 1$ and k near k_0. We are going to calculate Γ in a moment, but we can say now the general idea. Γ is the rate at which an electron leaves the state $\underline{k}$, E_k. Consider the rate due to creation of

one phonon. This rate will be, by the golden rule

$$\Gamma = 2\pi \sum_q (\alpha(q))^2 \, \delta(E_{k-q} + \omega_q - \omega) \qquad E_{k-q} > 0$$

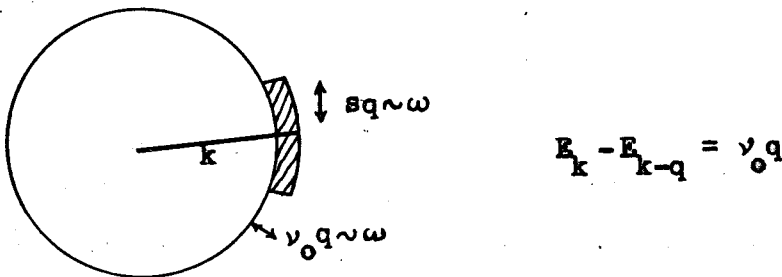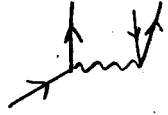Let us look at the volume in k space for which these processes can occur.

$$E_k - E_{k-q} = \nu_o q$$

FIG. 9

Hatched volume is region over which k - q can run.

This volume is proportional to ω^2. The (matrix element)^2 (it turns out) is proportional to q i.e. it is bounded by ω.

Thus $\Gamma \sim \omega^3/\omega_o^2$ since Γ must be an energy. The factor of ω_o^{-2} has to be verified in a more explicit fashion, which we will do later.

In a similar way, we can see that processes like

lead to Γ coul $\sim \omega^2/\varepsilon_o$, which except for a very small region $\omega < \omega_o^2/\varepsilon_o$ is negligible until $\omega \sim E_o$. The plot of $\Gamma(\omega)$ vs. turns out to be:
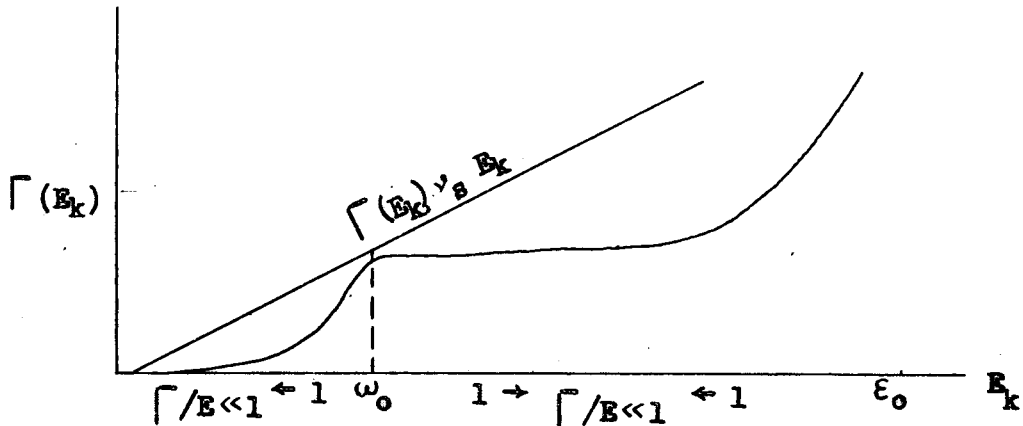
If we are willing to keep $\omega \ll \omega_o$, then Γ is small, A =
$= 2\pi Z_k \delta(\omega - E_k)$ and the whole business looks a great deal like
a free particle system, with altered energy levels. Most pro-
perties such as thermodynamical ones, (tunneling is not one)
depend only on E_k and not on Z_k since the electrons involved
are not <u>actually</u> injected suddenly from the outside so there
are no transient effects to consider.

The Landau theory is based on this fact, and describes
completely all phenomena in this low frequency region in terms
of the function E_k (which Landau does not calculate) i.e. it
essentially behaves as a free particle system, with energy E_k
replacing ε_k. (The change of E_k as a function of the number of
excited quasi-particles must also be taken into account).

The Landau theory is very halpful in describing all the

low energy phenomena. However, it is possible to extend some of the considerations right through the region about ω_0, and to solve for Γ (phenomenaologically) as long as $\omega \ll \varepsilon_0$ (even though $\omega \gtrsim \omega_0$).

The fact that the electron phonon system can be described simply when $\omega \ll E_0$ is based on the idea that although the phonon frequencies are small, their wave-vectors are not. In other words, typical phonons involve only a few neighboring ions, but the disturbance is very slowing moving, since the ions are so heavy.

Consider a quantity such as $\Gamma(\underline{k},\omega)$. Let us examine the scale of energy involved: This is clearly ω_0: if we change ω by ω_0, we obtain an appreciable change in Γ. On the other hand as a function of $\underline{k}$, Γ is slowly varying, i.e. it is necessary to change $\underline{k}$ by something of order $\underline{k}_0$ before Γ is appreciably affected. All this is a sort of dimensional argument based on the idea that since there is only one length introduce into the problem, Γ must depend only on that length. If some other fundamental length appears, we have some new physics (e.g. superconductivity). Since we one always going to consider $\dfrac{k-k_0}{k_0} \ll 1$, we expand

$$\Gamma(k\omega) = \Gamma(\omega) + (k - k_0)\frac{\partial \Gamma}{\partial k} \simeq \Gamma(\omega)$$

$$\Gamma(\omega) = \Gamma(k_0\omega)$$

$$\frac{\partial \Gamma}{\partial k} \sim \frac{\Gamma}{k_0}$$

If the restriction $\omega \ll \omega_0$ is made, we could do the same for ω,

and we would obtain $\Gamma(\omega) \sim 0$. (This is the Landau theory).

The same holds for $\sum(k\omega)$. It is replaced by $\sum(\omega) \equiv \sum(k_0\omega)$. More precisely since

$$\sum(k,\omega) = \sum(k,0) + \frac{\omega}{2\pi} \int \frac{\Gamma(k\omega')}{\omega - \omega'} \frac{d\omega'}{\omega'}$$

we have $\sum(k\omega) \quad \sum(k0) + \sum_1(k_0\omega)$, where $\sum_1$, is the integral, which because of the subtraction, involves only values of $\omega' \lesssim \omega$. $\sum(k0)$ depends on the high frequency absorptions, so to speak. If Coulomb interactions are taken into account, we would have

$$\sum(k,0) \sim -\Delta\mu + \frac{k-k_0}{k_0} k_0^2 \left[\frac{1}{m_c} - \frac{1}{m} \right] \qquad \text{where}$$

m_c is a partial effective mass from the Coulomb interactions and $\Delta\mu$ is a shift of the chemical potential. If phonon interactions only are taken into account, $\sum(k0)$ is a factor ω_0/E_0 smaller, and can be neglected. We suppose, therefore, that $\varepsilon_k = \frac{k^2}{2m} - \mu + \sum(k0)$.
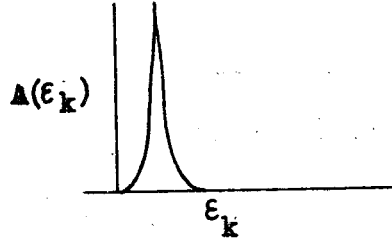
Consider again

$$A(k\omega) = \qquad \Gamma(k\omega) / \left\{ \left[\omega - \varepsilon_k - \sum(\omega) \right]^2 + \frac{1}{4}\Gamma^2 \right\}$$

If we regard this a function of ω, for fixed k, there may be a broad deformed peak near $\omega - \sum(\omega) = \varepsilon_k$ but the width and structure can be comparable with ω itself.

$A(\omega)$ (Fixed k)
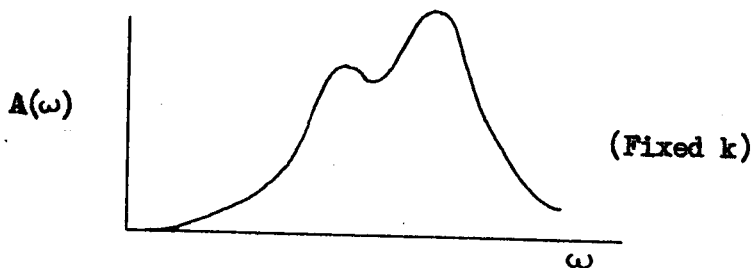
i.e. $A(k)$ is sharply peaked in ε_k, when ε_k is measured on the scale of E_0.

$A(\varepsilon_k)$

In words, this result is: An electron of definite momentum, near the Fermi surface, may have a range of energies which cannot be neglected, but, an electron of definite energy near the Fermi energy, will always be found very near the Fermi surface.

Another way of saying this:

$$\int \frac{d^3k}{(2\pi)^3} \, g(k) \, A(k\omega) = 2\pi N(0) \, g(0)$$

where $g(k)$ does not change unless k is changed by k_0. $N(0)$ is the density of states at the Fermi surface, neglecting the self-mass corrections.

This is true, even though we <u>cannot</u> replace

$$\int d\omega \, A(k\omega) \qquad \text{by} \qquad \int d\omega \, 2\pi \, Z_k \, \delta(\omega - E_k)$$

We use this result to obtain the answer to the simplest tunneling problem. To do this, we must develop a formalism to treat the tunneling.

VI. THE TUNNELING FORMALISM

In this lecture we want to develop a formalism for treating tunneling. We shall follow the simple ideas of Bardeen. PRL6(57) (1961). A somewhat more convincing and formal derivation has been given by the author to be published in P.R. Aug. (1963)). Usually, if we have some barrier we calculate a transmission coefficient by considering an incident wave, and a transmitted wave. The transmission coefficient, I remind you depends most strongly on a factor (squared)

$$e^{-\int_{x_0}^{x_1} K(x)dx}$$

where $K(x)$ is

$$\sqrt{2m\left(V(x)-\frac{k^2}{2m}\right)}$$

(We represent the barrier by a potential $V(x)$, and treat the electrons as independent,   to obtain this approximation).
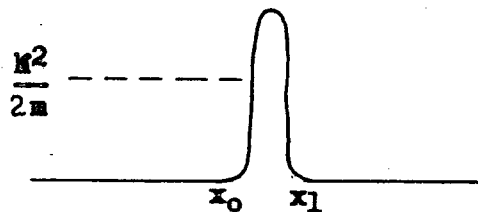
That is, the amplitude of the wave-function drops off exponentially inside the forbidden region.

What was pointed out by Bardeen, was that, since for thick barriers, the transmission coefficient is very small, one can treat the problem as transition between nearly stationary states.

Let ϕ_0 be the many electron state at time $t = 0$. (It could be a state in which the electron is to the left of the barrier). If we don't allow tunneling, the state will evolve in time ac-

acording to

$$\phi_0(t) = e^{-i\varepsilon_0 t} \phi_0$$

Suppose we allow tunneling to take place, then, according to time dependent perturbation theory,

$$\phi = \phi_0 e^{-iE_0 t} + \sum_\nu \phi_\nu e^{-iE_\nu t} a_\nu(t)$$

where the ϕ_ν are states with the electron on the other side of the barrier. We can find the <u>transition</u> <u>rate</u> across the barrier, by the usual golden rule i.e.

$$\frac{d}{dt} \sum_\nu |a_\nu(t)|^2 = W = \frac{2\pi}{\hbar} \sum_\nu |(\phi_\nu, (H-E_0) \phi_0)|^2 \, \delta(E_\nu - E_0)$$

We have to evaluate the matrix element

$$T_\nu = \int \phi_\nu^* (H - E_0) \phi_0$$

Let the coordinate X be perpendicular to the barrier, and let $X = 0$ be in the center of the barrier. When the electron is to the left of the barrier, $H \phi_0 = E_0 \phi_0$ so

$$T_{\nu 0} = \int \cdots \int d\tau_1 \cdots d\tau_N \int dX \; \phi_\nu^* (H - E_0) \phi_0$$

$$= \int \cdots \int d\tau_1 \cdots d I_N \int_0 dx \left[\phi_\nu^* (H-E_0) \phi_0 - \phi_0 (H-E_\nu) \phi_\nu^* \right]$$

Where o indicates that the integral is to be taken over the re‐ gion to the right of the barrier $X > 0$ and we have subtracted a zero, by the same reasoning. Since $E_\nu = E_0$; we have

$$T_{\nu 0} = -\frac{1}{2m} \int \cdots \int d\tau_1 \cdots d\tau_N \int dx \frac{\partial}{\partial x} \left[\phi_\nu^* \frac{\partial}{\partial x} \phi_0 - \left(\frac{\partial}{\partial x} \phi_\nu^* \right) \phi_0 \right] =$$

$$= - \frac{1}{e} \left[J_x(0) \right]_{\nu 0}$$

$J_x(0)$ is the <u>total</u> current operator across the barrier.
In the other words, the small perturbation $(H-E_0)$ is just

$$- \frac{1}{e} J_x(0)$$

The same result can be obtained as follows: Let the Hamilto-
nian of the whole system be

$$H_R + H_L + T$$

where

$$T = \sum_{r \ell} (C_r^+ C_\ell + C_\ell C_r^+) T_{r\ell}$$

with

$$T_{r\ell} = - \frac{1}{\ell} \left[j_x(0) \right]_{r\ell}$$

and Hr is the Hamiltonian of the electrons on the right, and
H_ℓ is that of the electrons on the left. This is plausible
intuitively and has been verified (with certain reservations)
in my paper. We shall therefore accept this result and pro-
ceed.

Let us consider the <u>current</u> across the barrier. We treat
the tunneling operator T by the golden rule. The <u>rate</u>   for
electrons to go from right to left is:

$$2\pi \sum_f | \langle f | \sum T_{r\ell} c_\ell^+ c_r | 0 \rangle |^2 \quad \delta(E_0 - E_f - eV)$$

and similarly for the rate from left to right. To obtain the
<u>current</u>, we multiply this by $-e$, and the left-right rate   by
e .

Therefore

$$J = -2\pi \, e \sum_f |\langle f| \sum T_{r\ell} \, c_\ell^+ \, c_r |0\rangle|^2 \; \delta(E_o - E_f - eV)$$

$$+ \, 2\pi \, e \sum_f |\langle f| \sum T_{r\ell} \, c_r^+ \, c_\ell |0\rangle|^2 \; \delta(E_o - E_f + eV)$$

$$= -2\pi e \left\{ \sum_{f_r f_\ell} |\sum_{r\ell} T_{r\ell} \langle f_r|c_r|0_r\rangle \langle f_\ell |c_\ell^+|0_\ell\rangle|^2 \; \delta(E_o - E_f - eV) \right.$$

$$- \sum_{f_r f_\ell} |\sum_r T_{r\ell} \langle f_r|c_r^+|0_r\rangle \langle f_\ell |c_\ell|0_\ell\rangle|^2 \; \delta(E_o - E_f + eV)$$

$$= -2\pi e \int \frac{d\omega r}{2\pi} \int \frac{d\omega}{2\pi} \sum_{r\ell} |T_{r\ell}|^2 \sum_{fr} |\langle f_r|c_r|0_r\rangle|^2 \; 2\pi \, \delta(\omega_r - E_{or} + E_{fr})$$

$$\sum_{f_\ell} |\langle f_\ell|c_\ell^+|0_\ell\rangle|^2 \; 2\pi \, \delta(\omega_\ell - E_{f_\ell} + E_{o_\ell}) \cdot \delta(\omega_r - \omega_\ell - eV)$$

This follows if we take the states r, ℓ to be wave packets of definite momentum, then $\langle f_r|c_r^+|0_r\rangle \langle 0_r|c_r^+|f_r\rangle =$
$= \delta_{rr'}|\langle f_r|c_r^+|0_r\rangle|^2$ for example.

Thus:

$$J = -2\pi e \sum_{r,\ell} |T_{r\ell}|^2 \int \frac{d\omega_r}{2\pi} \left\{ G_R^<(r, \omega_r) \, G_L^>(\ell \, \omega_\ell) \right.$$

$$\left. - \, G_R^>(r, \omega_r) \, G_L^<(\ell, \omega_\ell) \right\} \delta(\omega_r - \omega_\ell - eV)$$

This has the usual interpretation according to the Golden Rule:

The first term is the <u>rate</u> at which electrons of energy ω_r state r, are transferred across the barrier into a final state of momentum ℓ, energy ω_ℓ. $G^<$ is the density of these final

states, and the total current is obtained by summing over all initial electronic states. $G^<$ is the density of these initial states. We perform the integrals:

$$J = -2\pi e \cdot 4 \int \frac{d^3r}{(2\pi)^3} \int \frac{d^3\ell}{(2\pi)^3} \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} A_R A_L \left[f(\omega_1) - f(\omega_2) \right]$$

$$\delta(\omega_1 - \omega_2 - eV) |T_{r\ell}|^2$$

Doing the integral over d^3r first, then over $d^3\ell$

$$J = -2\pi e \cdot 4 \; N_R(0) \; N_L(0) \langle |T_{r\ell}|^2 \rangle_{angles} \int_{-\infty}^{\infty} d\omega \, |f(\omega) - f(\omega - eV)|$$

$$= 8\pi^2 e^2 V N_R(0) N_L(0) \langle T^2 \rangle$$

The same result can be obtained when $A_R \sim 2\pi \, Z_r \, \delta(\omega - E_r)$ but then it has to be recognized that

$$\frac{dE_r}{dr} = \frac{d\varepsilon_r}{dr} + \frac{\partial\Sigma}{\partial\omega} \frac{\partial E_r}{\partial r} = \frac{d\varepsilon_r}{dr} \frac{1}{1 - \frac{\partial\Sigma}{\partial\omega}} = Z_r \frac{\partial\varepsilon_r}{\partial r}$$

$$N_R(0) \quad \overset{\text{Renorm.}}{\underset{}{Z_o}} = Z_o \frac{P_o^2}{2\pi^2} \frac{\partial P_o}{\partial E_p} = N_R(0)$$

In this case, the wave function renormalization Z_r cancels the mass renormalization. Thus no experimentally interesting results can be expected.

VII. GRAPHICAL ANALYSIS OF THE SELF-ENERGIES

In this lecture we want to analyze the graphs contributing to $M(kz)$. I will give only a heuristic argument. To be correct, one should write down the expressions in perturbation   theory, and examine them.

The graphs can be arranged as follows:

Graphs for $M(kz)$:
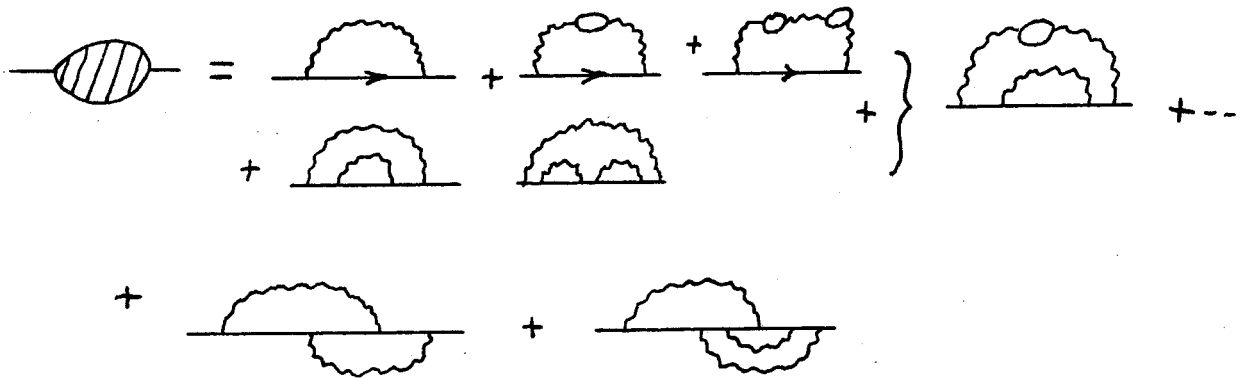
The top line consists of self energy correction to the phonon. The second line consists of self energy corrections to the electron. The third line consists of _vertex_ corrections

We really should have introduced a phonon Green's function, etc. We shall take Migdal's word for it, however. There is an important shift of the phonon energies, but no appreciable width. So, we say that the phonon energies are ω_q, and the coupling is still α_q where these are renormalized, but we keep the same name.

The second line we can include, by replacing it by

Let us estimate the relative order of magnitude of corrections such as
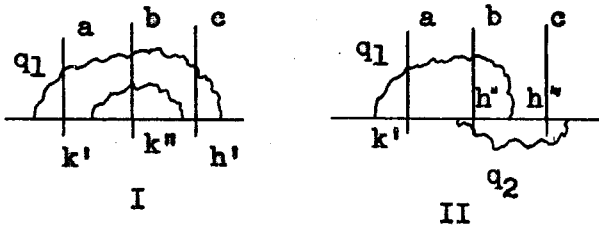
Each will contribute a factor $|\alpha_q|^4 \sim (\omega_o \, E_o)^2$

Then, there will be some energy denominators, for the times a, b, c, where a) we have electron + phonon, b) electron + 2 phonons c) electron + phonon.

These energy denominators will have to be of order ω_o, if there is to be an appreciable contribution. The phonons will always allow a small denominator, but the electron has to be confined near the Fermi surface. In order to do that, we cut down the integral over k' by a factor ω_o/E_o.

The same is true of the integral over k".

In region (c) there are two possibilities. (I) We absorb q_2. We automatically have a small energy denominator. Therefore,
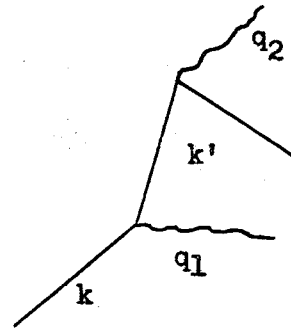
$$(I) \sim \omega_o^2 \, E_o^2 \, \frac{\omega_o^2}{E_o^2} \, \frac{1}{\omega_o^3} \sim \omega_o$$
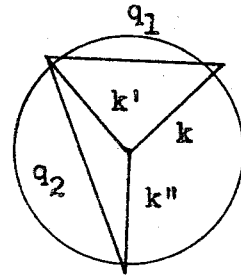
(II) Graph) we absorb q_2 first. In general the electron k'' will be far from the Fermi surface. Its energy denominator will be E_o.

(III) Graph $\sim \omega_o \, \frac{\omega_o}{E_o}$ <u>negligible</u>.

In general, we cannot allow phonon lines to cross. This kind of analysis can be extended, and eliminates a large class of graphs. I invite you to find the graphs "responsible" for superconductivity.

Let us believe the analysis: it is no doubt correct <u>if</u> superconductivity is not present. Then

$$M(k\omega) \equiv \quad \overset{k-k', \, \omega - \omega'}{\underset{k', \, \omega'}{\frown}}$$
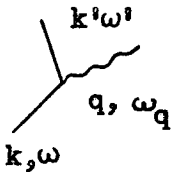
there is <u>no</u> vertex correction.

According to the rules, such a graph is written:

$$M(k\omega) = +i \int \frac{d\omega'}{2\pi} \sum_q \frac{|\alpha_q|^2}{N} G(k'\omega') \left\{ \frac{1}{\omega-\omega'-\omega_q+i} - \frac{1}{\omega-\omega'+\omega_q-i\eta} \right\}$$

The expression in the brackets is the phonon propagator, (at $T = 0$). The factor $+i$ in front is put in to make the answer come out correctly. We show below that the imaginary part of this, Γ, is given by

$$\Gamma(k\omega) = \frac{2\pi}{N} \sum_{k',q} |\alpha(q)|^2 \int \frac{d\omega'}{2\pi} \left[G^>(k',\omega')\delta(\omega-\omega'-\omega_q)\,\delta_{k-k'-q} \right.$$

$$\left. + G^<(k'\omega')\,\delta(\omega'-\omega-\omega_q)\,\delta_{k'-k-q} \right.$$

This expression could have been written down at once if we remember the Golden Rule, and if we believe the interpretation of $G^>$ as the density of states, which are empty of electrons, therefore available to an electron in the final state. $G^<$ is the density of filled electron states, or conversely, $G^<(-k, -\omega)$ is the density of states available for holes. At zero temperature, $\Gamma(k, w)$ is the lifetime of an electron, for $\omega > 0$. Hence the first term.

For $\omega < 0$, $\Gamma(k,\omega)$ is the lifetime of an electron <u>below</u> the "Fermi energy" or the lifetime of a <u>hole</u>, of energy, momentum $-\omega, -k$.

Thus

$$\Gamma(k,\omega) = \frac{1}{N} \sum_{k'} |\alpha_{k'-k}|^2 \; A(k', \omega - \omega_{k-k'})$$

$$\left[1 - f(\omega - \omega_{k-k'}) + f(\omega + \omega_{-k+k'})\right]$$

1st let us suppose $\alpha = \alpha_0$, $\omega_q = \omega_0$ (Einstein's hypothesis).

Then we can do the sum over k' by the formula obtained in lecture V:

$$\Gamma(k,\omega) = 2\pi \frac{N(0)}{p} |\alpha_0|^2 \left[1 - f(\omega - \omega_0) + f(\omega + \omega_0)\right]$$

$$\begin{cases} = 2\pi \dfrac{N(0)}{p} |\alpha_0|^2 & ; \; |\omega| > \omega_0 \\[3mm] = 0 & |\omega| < \omega_0 \end{cases} \quad (T = 0)$$

$$\sum (k\omega) = \frac{N(0)}{\rho} |\alpha_0|^2 \log \left| \frac{\omega - \omega_0}{\omega + \omega_0} \right|$$

$$\frac{\partial \sum}{\partial \omega}\bigg|_{\omega=0} = \frac{3}{4} \lambda$$

The more general case can be solved by noting that $\omega_{k-k'}$ does not depend on $|k'|$ appreciably (since $|k'| = k_o + $ small) but only on the angle. It is a trivial matter to convert the angular integration of $\hat{k}'$ to $|k' - k|^2 = k'^2 + k^2 - 2kk' \cos\theta$

$$d|k-k'|^2 = 2k_o \, d \cos\theta \quad d\Omega_{k'} = 2\pi \frac{d(k-k')^2}{2k_o^2}.$$

Thus in general,

$$\Gamma(\omega) = 2\pi \frac{N(0)}{\rho} \int d\omega_q \, F(\omega_q)|\alpha(\omega_q)|^2 \, 0(|\omega| - \omega_q)$$

where

$$F(\omega_q) = \frac{\pi}{2k_o^2} \frac{dq^2}{d\omega_q} , \qquad \begin{aligned} \theta(x) &= 1 \qquad x > 0 \\ &= 0 \qquad x < 0 \end{aligned}$$

$$\frac{\partial \Gamma(\omega)}{\partial \omega} = \frac{2\pi N(0)}{\rho} F(\omega)|\alpha(\omega)|^2 \qquad \omega > 0$$

$$\Gamma(\omega) = N(\omega)/q(\omega)$$

Insofar as $\Gamma(k,\omega)$ is given by the formula derived in the text even when $\omega \sim E_o$; that is, when $\Gamma(|\omega|) \longrightarrow$ constant, for $\omega \to \infty$ it follows that $\sum(k, 0) = 0$. However, this is not precisely true. In terms of the graphs, it means that the graph makes contributions also
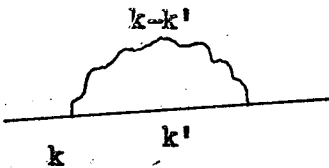
for k' well a ay from the Fermi surface. This contribution is, however, practically constant in both frequency and wave number, and is therefore of no interest.

VIII. <u>SUPERCONDUCTIVITY</u>

In this lecture we begin to study superconductivity. There are new physical entities involved, and corresponding, new dimensions of length and time, which show up in the self energy.

The key idea is the concept of the Cooper pair. This is a <u>bound</u> <u>state</u> of two electrons (which we believe to have total spin zero). It is remarkable that even very weak forces suffice to bind the electrons. The reason is that the "low" energy electron states are near the Fermi surface. There are many more momentum states available to the electrons, of low energy, than there are in the neighborhood of zero momentum. It is an easy calculation to show that the amount of kinetic energy needed to keep a pair of electrons within a distance ξ_0 of one another goes as $1/\xi_0^3$ $\ln \xi_0$ when ξ_0 is large. (Compare with $1/\xi_0^2$ for electrons in free space). If ξ_0 is greater than the range of the forces attracting the electrons, the mean potential energy will drop as ξ_0^{-3}. Hence, by taking ξ_0 large enough, the kinetic energy can always be made less than the potential energy, so the electrons will always bind.

This phenomena, discovered by Cooper, is fundamental to superconductivity. However, we have the identity of the electrons to take into account. If we put two electrons into a Cooper pair, they will immediately exchange with other electrons, losing the effect, <u>unless the other electrons are al-</u>

ready in the same Cooper pair state.

We can rephase this remark as follows: the pairs of electrons are more like Bosons than Fermions. Like Bosons, they prefer company (the operator $a_k^+|N_k\rangle = \sqrt{N_{k+1}}|N_k+1\rangle$). The Bose factor enhancing the material occupation of the same state, makes it possible for the Cooper pair to exist at all. We can't have a state in which one pair of electrons is bound, but in a different state than the others, for example.

How do we describe this mathematically ? Let

$$F(x_1\ x_2) \qquad\qquad \text{be the pair wave function}$$

To create a pair, we operate with

$$\mathbb{F} = \int F(x_1 x_2)\psi_\uparrow^+(x_1)\psi_\downarrow^+(x_2)\,d^3x,\ d^3x_2$$

Then, the ground state is

$$|N\rangle = |\mathbb{F}|^{N/2}|0\rangle \quad \text{where } |0\rangle \text{ is the vacuum.}$$

It is automatically anti-symmetrized. The BCS form of the wave-functions is usually more convenient. Let $F(x_1 x_2) =$
$= \frac{C}{V}\sum_k \frac{\mathcal{V}_k}{\mathcal{U}_k} e^{ik(x_1-x_2)}$ then $\mathbb{F} = C\sum_k \mathcal{V}_k/\mathcal{U}_k\ a_{k\uparrow}^+\ a_{-k\downarrow}^+$.

The BCS wave function is

$$\prod_k (U_k + \mathcal{V}_k\ a_{k\uparrow}^+\ a_{-k\downarrow}^+)|0\rangle$$

where $|N\rangle$ is proportional to the projection of the BCS state into a state of N particles, and $U_k = \sqrt{1-V_k^2}$. The main advantage of the BCS formulation is that the state $|N\rangle$ is difficult to normalize, whereas that of BCS is already normalized.

We shall not use explicit wave functions, however, but we shall exploit the fact that

$$a_{-k\downarrow}\, a_{k\uparrow}|N\rangle \qquad \text{is proportional to } |N-2\rangle \text{ (Except}$$

the pair k, -k is absent).

Why ? Because, whenever an electron is present in state $k\uparrow$ there is also one in state $-k\downarrow$, coming from the same F operator; one F is eliminated by distorting the pair. Since N is very large, it is convenient to identify N, $N \pm 2$, etc, as BCS have done. Then we can say that

$$\langle a_{-k\downarrow}\, a_{k\uparrow} \rangle \neq 0$$

Nambu has introduced a convenient notation for studying this problem. Call $\psi_\uparrow(x) = \psi_1(x)$ $\psi_\downarrow^+(x) = \psi_2(x)$ then

$$\left\{ \psi_i(x), \psi_j^+(y) \right\} = \delta(x-y)\delta_{ij}$$

Let

$$G_{ij}(xy) = \frac{1}{i}\langle T\, \psi_i(x)\, \psi_j^+(y)\rangle$$

$$G_{11} = G_{\uparrow\uparrow}, \quad G_{22} = -\, G_{\downarrow\downarrow}\quad G_{12} = \frac{1}{i}\langle T\, \psi_\uparrow(x)\psi_\downarrow(y)\rangle \neq 0$$

We can also introduce $\underline{G}^{>}$, $\underline{G}^{<}$, $\underline{A}$, $\underline{M}$ etc, which will be __matrices__. It is easy to prove:

$$\underline{G}^{>}, \underline{G}^{<}, \underline{A} \quad \geqslant 0 \qquad \text{(hermiterm, positive)}$$

$$\underline{G}(z)^*_{ij} = \underline{G}(z^*)_{ji} \quad \det \underline{G}(Z) \neq 0 \quad (\text{Im } Z \neq 0)$$

$$\int \frac{d\omega}{2\pi}\, \underline{A}(\omega) = \underline{1} \quad \int \frac{\underline{A}(\omega')}{Z-\omega'}\, \frac{d\omega'}{2\pi} = \underline{G}(Z).$$

In the simplest approximation

$$v_k^2 = \frac{1}{2} - \frac{1}{2} \frac{\varepsilon_k}{\sqrt{\varepsilon_k^2 + \Delta^2}}$$

where Δ is the energy gap parameter.

The spreading of the wave function F, is determined by the range over which $_k$ varies, i.e., for $\varepsilon_k \sim \Delta$ or $\varepsilon_k \sim (k - k_o)v_o$

$$\Delta \sim 10^{-3} \qquad\qquad k - k_o \sim \frac{\Delta}{v_o} \qquad \text{or} \qquad \delta x \sim \frac{v_o}{\Delta}$$

$$\frac{\pi v_o}{\Delta} = \xi_o \sim 10^4 \, A^o$$

The radius of the "bound pair" is therefore enormously greater than the range of the forces binding it (which range is only a few A^o). This fact has very important consequences. It means that impurities do not have a very serious effect on the binding energy of the pair, at least so long as they do not change the phase of the electrons. However, we shall have no need to exploit this fact.

The Green's function formalism in the matrix notation is practically the same as before.

There is one important modification:

Consider, for example, the kinetic energy

$$T = \sum_k \left(\frac{k^2}{2m} - \mu\right) \left[C_{k\uparrow}^+ C_k - C_{-k\downarrow} C_{-k\downarrow}^+ + 1 \right] = \sum_{k,ij} \varepsilon_k (\tau_3)_{ij} C_{ki}^+ C_{kj} +$$

$$+ \text{const.}; \quad \tau_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

In general, we can regard the C_1^+ as creating an electron of spin

$\uparrow$ and C_2^+ creates a <u>hole</u> of spin $\uparrow$. But it is not convenient to keep this too much in mind.

Again, the electron-phonon interaction is

$$\frac{1}{\sqrt{N}} = \sum_{k,q} \alpha(q) \, (a_q + a_{-q}^+)(C_{k+q\uparrow}^+ \, C_{k\uparrow} - C_{-k-q\downarrow} \, C_{-k\downarrow}^+)$$

$$= \frac{1}{\sqrt{N}} \sum_{k,q} \alpha(q) \left[a_q + a_{-q}^+\right] \sum_{i,j} (\tau_3)_{ij} \, C_{k+qi}^+ \, C_{kj}$$

This rule may be summarized as follows: The electron kinetic energies are replaced by $\tau_3 \epsilon_k$, and the electron-phonon interaction replaced by $\tau_3 \, \alpha(h)$.

For example:

$$\underline{G}^0(kz) = \frac{1}{z - \tau_3 \, \epsilon_k} \quad , \quad A^0(k\omega') = 2\pi \, \delta(\omega' - \tau_3 \, \epsilon_k)$$

Suppose we try perturbation theory: Since only the matrices $\underline{1}, \tau_3$ enters into $\underline{G}_0$, or into $\underline{H}$, we shall be able to obtain only the matrices $\underline{1}, \underline{\tau}_3$ in any result, eg. $\underline{G}$ itself will be diagonal. If

$$\underline{G} = \frac{1}{\omega - \underline{\tau}_3 \, \epsilon_k - \underline{M}(k\omega)}$$

then, according to perturbation theory $\underline{M}(k\omega) = M_0 \underline{1} + M_3 \, \underline{\tau}_3$. In the superconductor, this result is wrong. There is turns out that

$$\underline{M} = M_0 \underline{1} + M_3 \, \underline{\tau}_3 + M_1 \, \underline{\tau}_1$$

(There is a certain ambiguity: $\underline{M}$ could have a part with a $\underline{\tau}_2$

equally well, but a gauge transformation can be made to eliminate this term). $\underline{M}$ is a self-energy. There are several ways we can regard it. For example, we can think of it as being due to a self-field of the electrons on this case, a sort of self-consistent fields of all the other electrons. The fact that $\underline{M}$ can contain some off-diagonal terms we may interpret as follows:

a) The electrons can set-up a self-field which does <u>not</u> have the original symmetry $\left[\underline{H}, \underline{\tau}_3\right] = 0$. The original symmetry is broken. This interpretation has been fruitful in speculations about broken symmetries of elementary particles, for example.

b) The off-diagonal M_1, may be regarded as the field generated by the electrons playing their role of Cooper pair.

c) Suppose, $M_0 = M_3 = 0$. Then

$$\underline{G} = \frac{1}{\omega - \underline{\tau}_3\, \varepsilon_k - \underline{\tau}_1\, M_1} = \frac{\omega + \underline{\tau}_3\, \varepsilon_k + \underline{\tau}_1\, M_1}{\omega^2 - \varepsilon_k^2 - M_1^2}$$

The diagonal part of $\underline{G}$ say G_k is

$$\frac{\omega + \varepsilon_k}{\omega^2 + \varepsilon_k^2 - M_1^2} = \frac{1}{\omega - \varepsilon_k - \dfrac{M_1^2}{\omega + \varepsilon_k}}$$

Thus $M_1^2/\omega + \varepsilon_k$ is a contribution to the ordinary mass operator. It means that an extra electron has the possibility of being captured by some Cooper pair of momentum $-k$, a hole propagates, and it is released. Regarded in this way
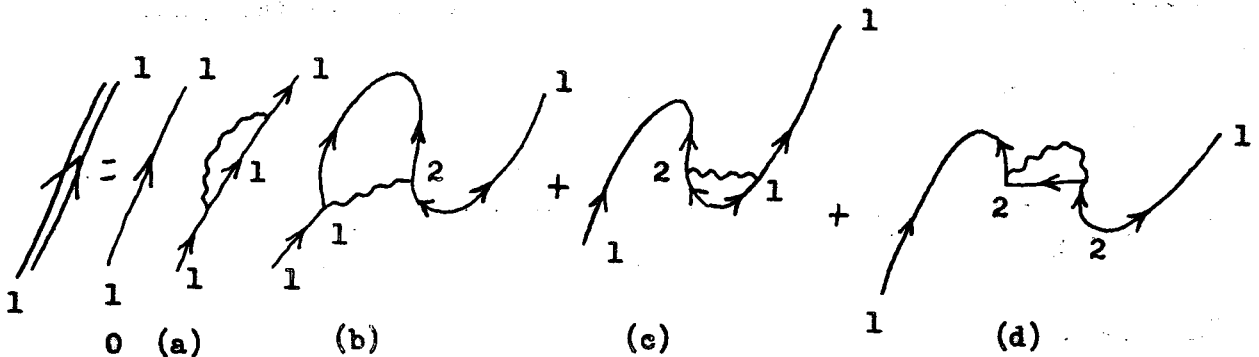
G_{12} G_{21} is a factorization of the two-particle Green's functions.

We now study how a self consistent field can arise. Consider again the process, described by the graph.

Each of the heavy line is a matrix, so this is really a short-hand for graphs. Ist:

0 (a)   (b)   (c)   (d)

(0) is the direct propagation.

(a) is the ordinary self energy part.

(b) a phonon is emitted, it is absorbed by one member of a
     Cooper pair, the other member being in the same state
     as the initial. The two excited electrons then bind
     each other.

(c) (d) similar interpretations apply.

Next
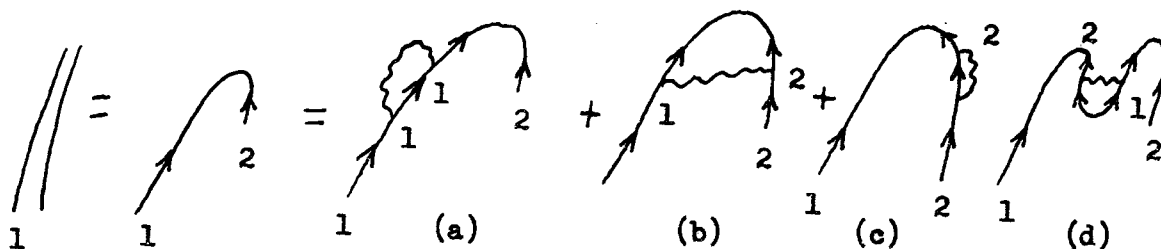
In this case there is no zero <u>th</u> order term. The important feature is a graph like (b). If we iterate this many times we find,

We can regard this as a vertex correction

It is easy to verify that all the energy denominators are <u>small!</u>
It is therefore essential to take into account graph of   arbi-
trarily high order, which describe the exchange of phonons
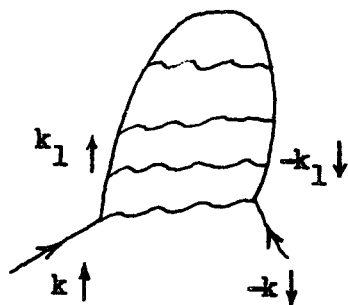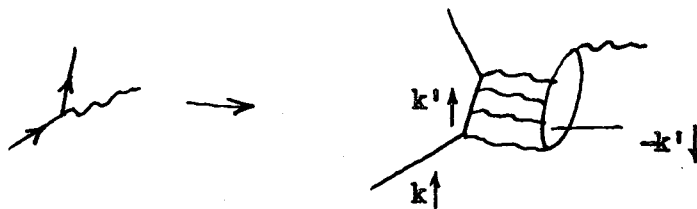between electrons of equal and opposite (or nealy) momentum.

It is tricky to count graphs in the ordinary notation, but
that of Nambu is very elegantly designed to do the hard work for
us.

The generalized mass operator is, therefore

$$\underline{M} = \frac{1}{(2\pi)^4} \int d^3k' \, d\omega' \, \frac{|\alpha(q)|^2}{\rho} \underline{\tau}_3 \, \underline{G} \, (k'\omega') \, \underline{\tau}_3 \, D(\omega-\omega', \, k-k')$$

where D =

$$\frac{1}{\omega-\omega' - \omega_q + i\eta} - \frac{1}{\omega-\omega' + \omega_q - i\eta} \qquad q = k - k'$$

The original method of analyzing this expression was (in effect)
as follows: The exchange of a phonon, described by the   D pro-
pagator, was argued to give rise to an effective attractive po-
tential. Since it is usual to treat potentials as causing   an
instantaneous force, $(\alpha(q)|^2/\rho \, D$ was replaced by some potential
$- V(q)$. It was further argued that this potential acted only on
electrons near the Fermi surface, with in an energy distance $\sim \omega_0$
from it. It was idealized, therefore, to be   constant   within
this small region, and zero without. Thus,

$$\underline{M} = \frac{1}{(2\pi)^4} \int_{|\epsilon_k| < \omega_o} d^3k' \int d\omega' \; \underline{\tau}_3 \; G(k'\omega') \; \underline{\tau}_3 (-V)$$

where V is constant.

It was also desired to keep only those corrections of specific interest to superconductivity. Thus, it was assumed

$$\underline{M} = \underline{\tau}_1 \Delta , \qquad \underline{G} = 1/(\omega - \epsilon_k \underline{\tau}_3 - \underline{\tau}_1 \Delta)$$

In other words, ordinary self energy corrections are neglected $\underline{G}$ is diagonalized by the Bogoliubov transformation

$$\underline{U}_k \; \underline{G}_k \; \underline{U}_k^{-1} = \frac{1}{\omega - \underline{\tau}_3(E_k - i\eta)}$$

$$\underline{U}_k = (v_k \underline{\tau}_1 + u_k \underline{\tau}_3)$$

$$U_k^2 + V_k^2 = 1 \qquad U_k^2 - V_k^2 = 2 \quad \epsilon_k/E_k , \qquad 2U_k V_k = \frac{\Delta}{E_k}$$

$$E_k = \sqrt{\epsilon_k^2 + \Delta^2}$$

$$\underline{\tau}_3 \; G \; \underline{\tau}_3 = (\omega + \epsilon_k \underline{\tau}_3 - \underline{\tau}_1 \Delta)/\left[\omega^2 - E_k^2 + i\eta\right]$$

(the $+ i\eta$ comes by analogy with $G^o = \dfrac{1}{\omega - \underline{\tau}_3 \epsilon_k + i\eta(k)\underline{\tau}_3} =$

$= \dfrac{\omega + \tau_3 \epsilon_k}{\omega^2 - (\epsilon_k - i\eta_k)^2} = (\omega + \tau_3 \epsilon_k)/(\omega^2 - \epsilon_k^2 + i\eta)$

$$\eta > 0 \quad \text{since} \quad \epsilon_k \; \eta_k > 0$$

Then

$$\Delta = - \frac{i}{(2\pi)^4} \int d^3k' \, d\omega' \, \frac{V\Delta}{\omega'^2 - E_{k'}^2 + i\eta}$$

$$I = V \int \frac{d^3k'}{(2\pi)^3} \frac{1}{E_k'} = 2VN(0) = \int_0^{\omega_0} d\varepsilon_{k'} \, \frac{1}{2\sqrt{\varepsilon_k^2 + \Delta^2}}$$

If $V\,N(0) \ll 1$, the approximate solution is

$$1 = V\,N(0)\,\log \frac{\omega_0}{\Delta} \qquad\qquad \Delta = \omega_0 \, e^{-\frac{1}{VN(0)}}$$

which shows the famous exponential dependence. The number $N(0)V$ is treated as an adjustable parameter, and could not be calculated with any reliability. ($VN(0) \sim |\alpha|^2/\omega_0\,\rho \sim E_0/\rho$, so $VN(0)$ is independent of isotopic mass M). The fact that $\Delta \propto \omega_0 \propto M^{-s}$ was regarded as an early triumph of the theory, until experiments showed that not all superconductors followed this simple law.

In this from of the theory, $N(0)V$ is treated as a phenomeno logical parameter [i.e. Δ is measured, not predicted]. A great number of experiments are correlated in this way. However, some important questions are unresolved by these approximations.

A) the dependence of Δ on crystal structure, electronic structure, etc, is not understood (Δ is not predicted).

B) the dependence of Δ on ω_0, or on M is not correct in all cases (isotope effect).

C) the structure of Δ as a function of frequency (measured in the tunneling experiments), is not predicted.

IX. THE RETARDED INTERACTION

The greatest advance in the theory of superconductivity of the last two years, (by Swithart, Morel and Anderson,   and Schrieffer, et al.) is the removal of this simple approximation.

From the present point of view, it is rather amazing that the old set of approximation to $\underline{M}$ was so successful,   since great violence was done to the physics of the electron phonon interaction. We shall tackle the problem in the same way that the normal-state problem was handled, except that here,   we cannot obtain explicit solutions. It does not simplify things appreciably to consider only the width, either. We   introduce the dispersion relation for $\underline{G}$ into $\underline{M}$ and performe the integral over ω'.

Then

$$\underline{M} = (2\pi)^{-4} \int d^3 k' \int d\omega'' \left[\underline{\tau}_3 \, \underline{G}^{>}(k', \omega'') \, \underline{\tau}_3 \, \frac{1}{\omega - \omega'' - \omega_q + i\eta} \right.$$

$$\left. + \underline{\tau}_3 \, \underline{G}^{<}(k', \omega'') \underline{\tau}_3 \, \frac{1}{\omega - \omega'' + \omega_q - i\eta} \right.$$

Notice; $\underline{M} = \underline{M}(\omega)$, by the same arguments presented previously. Suppose $\alpha \to \alpha_0$, $\omega_q \to \omega_0$. Consider that $\underline{M}$ has the form

$$\underline{M}(z) = z(1 - Z(z)) \, \underline{1} + Z(z) \Delta(z) \, \underline{\tau}_1$$

We have dropped the term in $\underline{\tau}_3$ since we will see later that it is small.

Then

$$z(1 - Z(z)) = \frac{1}{(2\pi)^4} \int d^3k' \int d\omega' \frac{|\alpha(0)|^2}{\rho} A_0(k', \omega')$$

$$\left[\frac{1 - f(\omega')}{z - \omega' - \omega_0} + \frac{f(\omega')}{z - \omega' + \omega_0} \right]$$

That is, $z(1-Z(z))$ satisfies a dispersion relation with a non-negative weight function. $A_0 = \frac{1}{2} \operatorname{Tr} \underline{A}$. In the same way,

$$Z(z) \Delta(z) = - \frac{1}{(2\pi)^4} \int d^3k' \int d\omega' \frac{|\alpha(0)|^2}{\rho} [A(k'\omega')]_1$$

$$\left[\frac{1 - f(\omega')}{z - \omega' - \omega_0} - \frac{f(\omega')}{z - \omega' + \omega_0} \right]$$

We know only that $[A]_1 = \frac{1}{2} \operatorname{Tr} \underline{A} \, \underline{\tau}_1$ is real.

Consider now

$$\int \frac{d^3k}{(2\pi)^3} \underline{G}(k,z) = N(0) \int_{-\infty}^{\infty} d\varepsilon \frac{z \, Z(z) + \underline{\tau}_3 \varepsilon + \underline{\tau}_1 Z(z) \Delta(z)}{z^2(z) \, (z^2 - \Delta(z)^2) - \varepsilon^2}$$

$$= - 2\pi i \, N(0) \frac{z \, Z(z) + \underline{\tau}_1 Z(z) \Delta(z)}{2 \, Z(z) \sqrt{z^2 - \Delta(z)^2}}$$

We have to determine later the sign of the square root. Using

$$A(k\omega) = - 2 \operatorname{Im} \underline{G}(k, \omega + i\eta)$$

$$\int d\varepsilon \, \underline{A}(k \,) = 2\pi \operatorname{Re} \frac{\omega + \tau_1 \Delta(\omega+)}{2 \sqrt{(\omega+)^2 - [\Delta(+)]^2}}$$

Since $A_{11} \geqslant 0$, the sign of the root is such that

$$\text{Re } \omega \sqrt{\omega^2 - \Delta(\omega)^2} \geqslant 0$$

For ω small, Δ becomes real. Hence $\text{Re } \sqrt{\omega^2 - \Delta(\omega)^2} = 0 \quad \omega < \Delta_o$ where $\Delta_o = \Delta(\Delta_o)$. That is to say, there are no states of energy less than Δ_o. $A(k\omega) = 0 \quad |\omega| < \Delta_o$. We thus have an energy gap in this formulation also.

We can use the formula derived in the previous line, namely

$$\int \frac{d^3k}{(2\pi)^3} A(k,\omega) = 2\pi N(0) \text{ Re } \frac{\omega + \underset{\sim}{\tau_1} \Delta(\omega)}{\sqrt{\omega^2 - \Delta^2(\omega)}}$$

to simplify the equations for $Z(\omega)$ and $\Delta(\omega)$. We obtain,

$$\omega[1 - Z(\omega)] = \int d\omega' |\alpha_o|^2 \frac{N(0)}{\rho} \text{ Re } \frac{\omega'}{\sqrt{\omega'^2 - \Delta'^2}} \left[\frac{1 - f(\omega')}{\omega - \omega' - \omega_0 + i\eta} + \right.$$

$$\left. + \frac{f(\omega')}{\omega - \omega' + \omega_0 - i\eta} \right]$$

Using the fact that $\text{Re } \frac{\omega'}{\sqrt{\omega'^2 - \Delta'^2}} \geqslant 0$, we can rewrite this

$$\omega(1 - z(\omega)) = \int_{\Delta_o}^{\infty} d\omega' \text{ Re } \frac{\omega'}{\sqrt{\omega'^2 - \Delta'^2}} \frac{\alpha_o^2 N(0)}{\rho} \left[\frac{1}{\omega + \omega' + \omega_0 - i\eta} - \frac{1}{\omega - \omega' + \omega_0 - i\eta} \right]$$

In a similar way

$$\Delta(\omega) = \frac{1}{Z(\omega)} \int_{\Delta_o}^{\infty} d\omega' \text{ Re } \left\{ \frac{\Delta'}{\sqrt{\omega'^2 - \Delta'^2}} \right\} \frac{\alpha_o^2 N(0)}{\rho}$$

$$\circ \left[\frac{1}{\omega + \omega' + \omega_0 - i\eta} + \frac{1}{\omega' - \omega + \omega_0 - i\eta} \right]$$

In a similar way

$$\Delta(\omega) = \frac{1}{Z(\omega)} \int_{\Delta_0}^{\infty} d\omega' \, \text{Re} \left\{ \frac{\Delta'}{\sqrt{\omega'^2 - \Delta'^2}} \right\} \frac{\alpha_0^2 \, N(0)}{\rho}$$

$$\left[\frac{1}{\omega + \omega' + \omega_0 - i\eta} + \frac{1}{\omega' - \omega + \omega_0 - i\eta} \right]$$

since in this case the factor Re $\{ \ \}$ is odd.

We are going to study these equations, but first we must generalize them to include some of the effects of the Coulomb interaction. Although we can't hope to calculate exactly, we do know that only at very high frequencies will there be a contribution to the absorptive parts (Im Z, Im Δ). Since we only need $\Delta(\omega)$ for low frequencies, the detailed structure will be washed out, and its effects can be described in terms of two parameters: The total mass of the distribution, and the position of the center of mass.

In order to get all the signs straight, we can think of the Coulomb interaction as being simulated by the exchange of a "Coulomb" of frequency ω_c, and coupling $- |\alpha_c|^2$. (We need the $-$ sign, since the effect is repulsive, and the exchange of one meson always gives an attractive force. Thus we have

to supply the sign by hand). Thus the phonon propagator and coupling is modified to be

$$\alpha_o^2 \left[\frac{1}{\omega - \omega_o + i\eta} - \frac{1}{\omega + \omega_o - i\eta} \right] - \alpha_o^2 \left[\frac{1}{\omega - \omega_o - i\eta} - \frac{1}{\omega + \omega_o - i\eta} \right]$$

Therefore, we obtain

$$\omega(1-Z(\omega)) = \frac{N(0)}{\rho} \int_{\Delta_o}^{\infty} d\omega' \left(\mathrm{Re} \, \frac{\omega'}{\sqrt{\omega'^2 - \Delta'^2}} \right) \left\{ \alpha_o^2 \left[\frac{1}{\omega + \omega' + \omega_o - i\eta} - \frac{1}{\omega' - \omega + \omega_o - i\eta} \right] \right.$$

$$\left. - \alpha_c^2 \left[\frac{1}{\omega + \omega' + \omega_c - i\eta} - \frac{1}{\omega' - \omega + \omega_c + i\eta} \right] \right\}$$

which is a negligible correction, since $\omega_c \sim E_o \gg \omega_o, \Delta_o, \omega$. However,

$$\Delta(\omega) = \frac{1}{Z(\omega)} \frac{N(0)}{\rho} \int_{\Delta_o}^{\infty} d\omega' \left\{ \mathrm{Re} \, \frac{\Delta'}{\sqrt{\omega'^2 - \Delta'^2}} \right\} \left\{ \alpha_o^2 \left[\frac{1}{\omega + \omega' + \omega_o - i\eta} + \frac{1}{\omega' - \omega + \omega_o + i\eta} \right] \right.$$

$$\left. - \alpha_c^2 \left[\frac{1}{\omega + \omega' + \omega_c} + \frac{1}{\omega' - \omega + \omega_c} \right] \right\}$$

It is convenient to simplify this somewhat, by recognizing that the last term is nearly independent of ω, ω'. Thus, we replace it by $-\alpha_o^2 \frac{U}{\omega_o}$, and cut off the integral at $2\omega_c$. Here $U = \frac{\alpha_o^2}{\alpha_o^2} \frac{\omega_o}{\omega_c}$ (U is a number independent of isotopic mass). We also give up the Einstein approximation in writing down the final result. $F(\omega_q)$ was defined previously.

$$\Delta(\omega) = \frac{1}{Z(\omega)} \int_{\Delta_0}^{2\omega_c} d\omega' \; \mathrm{Re} \; \frac{\Delta'}{\sqrt{\omega'^2 - \Delta'^2}} \int d\omega_q \; F(\omega_q) \; \alpha^2(\omega_q)$$

$$\left[\frac{1}{\omega + \omega' + \omega_q - i\eta} + \frac{1}{\omega' - \omega + \omega_q - i\eta} - \frac{U}{\omega_0} \right]$$

The cutoff is needed only in the term containing U.

We now undertake an analysis of these equations. They have been solved numerically by Schrieffer, using a fairly realistic phonon distribution function. However, the main features can be seen in the following way: We first make the Einstein approximations $\alpha_q \rightarrow \alpha_0$ $\omega_q \rightarrow \omega_0$. We next uncouple the equations by assuming $Z(\omega) = 1$. We have now to solve

$$\Delta(\omega) = \frac{\alpha_0^2 \, N(0)}{\rho} \int_{\Delta_0}^{\infty} \mathrm{Re} \; \frac{\Delta'}{\sqrt{\omega'^2 - \Delta'^2}} \left[\frac{1}{\omega' + \omega + \omega_0 - i\eta} + \frac{1}{\omega' - \omega + \omega_0 - i\eta} - \frac{U}{\omega_0} \right]$$

There are two features of interest: The first is the magnitude of $\Delta(0)$ as a function of the parameters, since $\Delta(0)$ plays a role of the BCS gap parameter of the simpler versions. The transition temperature is proportional to $\Delta(0)$. In particular, the dependence of Δ_0 on ω_0 is of interest (isotope effect). The other feature of interest is the structure of $\Delta(\omega)$ in the neighborhood of $\omega \sim \omega_0$. This structure is reflected in the structure of the tunneling current.

To examine Δ_o we ignore the structure. Only values of $\omega' \lesssim \omega_o$ are important in the phonon terms: We replace $\Delta' = \Delta_o = \Delta(0)$, $\omega_c = \infty$. The integral is readily performed (for $\omega = 0$), and the result is (dropping terms of $\sim \Delta_o/\omega_o$).

$$\Delta(0) \lambda \Delta(0) \ln \frac{2\omega_o}{\Delta_o} - \mu \int_{\Delta_o}^{2\omega_c} \mathrm{Re} \frac{\Delta'}{\omega'^2 - \Delta'^2}$$

where

$$\lambda = 2\alpha_o^2 \frac{N(0)}{\omega_o \rho} , \quad \mu = \frac{U}{2}\lambda$$

Neglect of the Coulomb term yields

$$\Delta_o = 2\omega_o \, e^{-1/\lambda} \quad \text{(the BCS equation)}$$

To treat the Coulomb term we break the integral into

$$\int_{\Delta_o}^{2\omega_o} + \int_{2\omega_o}^{2\omega_c}$$

In the first, we again put $\Delta' = \Delta_o$ and obtain $-\mu\,\Delta(0) \ln \left(2\frac{\omega_o}{\Delta_o} \right)$. In the second, we drop the in the square root.

$$\Delta(0) = (\lambda - \mu) \Delta(0) \ln\left(\frac{2\omega_o}{\Delta_o}\right) - \mu \int_{2\omega_o}^{\omega_c} \frac{\Delta'}{\omega'} d\omega'$$

We now replace Δ' by some average Δ_1. Next, we need to calculate Δ_1. For values of ω of the order of $\frac{1}{2}\omega_c$, $\Delta(\omega) \sim \Delta_1$.

The first terms drop completely, so

$$\Delta_1 = -\mu\,\Delta(0) \ln\left(\frac{2\omega_o}{\Delta_o}\right) - \mu\,\Delta_1 \ln \frac{\omega_c}{\omega_o}$$

These equation are solved at once for Δ_o, and yield

$$\ell n \; \frac{2\omega_o}{\Delta_o} = \left[\lambda - \frac{\mu}{1+\mu \; \ell n \; \frac{\omega_c}{\omega_o}} \right]^{-1} = \left[\lambda - \mu * \right]^{-1}$$

This is, the effective couping constant λ is reduced by the Coulomb repulsions, but the Coulomb repulsion itself is reduced because it acts over such a large frequency interval that the can adjust to it, i.e. it is less effective because it acts over very short times.

The problem of the prediction of transition temperatures, and the isotope effect, is the problem of putting numbers into this formula (or somewhat better versions of this formula). λ can be estimated quite reliably, to say, 10% or better. It is usually about 0.4 μ is less reliable, but the formula is less sensitive to it. ω_c is poorly known, but the formula does not depend strongly on it. However, no doubt $\ell n \; \frac{\omega_c}{\omega_o} \sim 2 - 8$ is known to perhaps 10%. μ^* usually is about 0.1.

According to the most recent work, (of James Garvin (unpublished thesis)) the formula is not in disagreement with the data, and certainly follows the general trends.

The isotope effect: i.e., the value of

$$\delta_I = \frac{\partial \ell n \; \Delta}{\partial \ell n \; \omega_o} = 1 - \mu^{*2}/(\lambda - \mu^*)$$
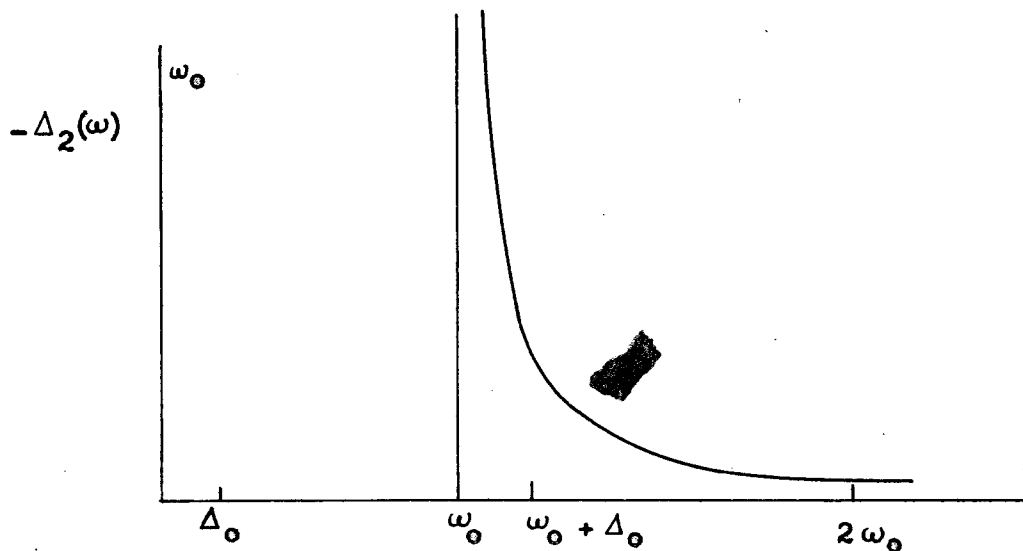
is also not in disagreement with experiment. For metals such

as lead, when $\ln \omega_c/\omega_o \sim$ $\mu^* \lesssim 0.1$, and $\delta_I \sim 1$ as observed. For the transition metals, where there are both d- and s- bands, the effective value of the ω_c is much reduced, $\mu^* \sim .2$ and $\delta_I \sim 0$. ($\ln \omega_c/\omega_o$ is much smaller for the transition metals).

We next take up the variation of Δ with frequency. The only frequency variation of interest occurs for $\omega \ll \omega_c$. We again replace $Z(\omega) \simeq 1$, and put $\Delta = \Delta_o$ inside the integral. Then $\Delta_2 = \ln \Delta$ is given by

$$\Delta_2(\omega) = -\frac{\pi \alpha_o^2 \, N(0)}{\rho} \frac{\Delta_o}{\sqrt{(|\omega| - \omega_o)^2 - \Delta_o^2}} \qquad |\omega| > \omega_o + \Delta_o$$
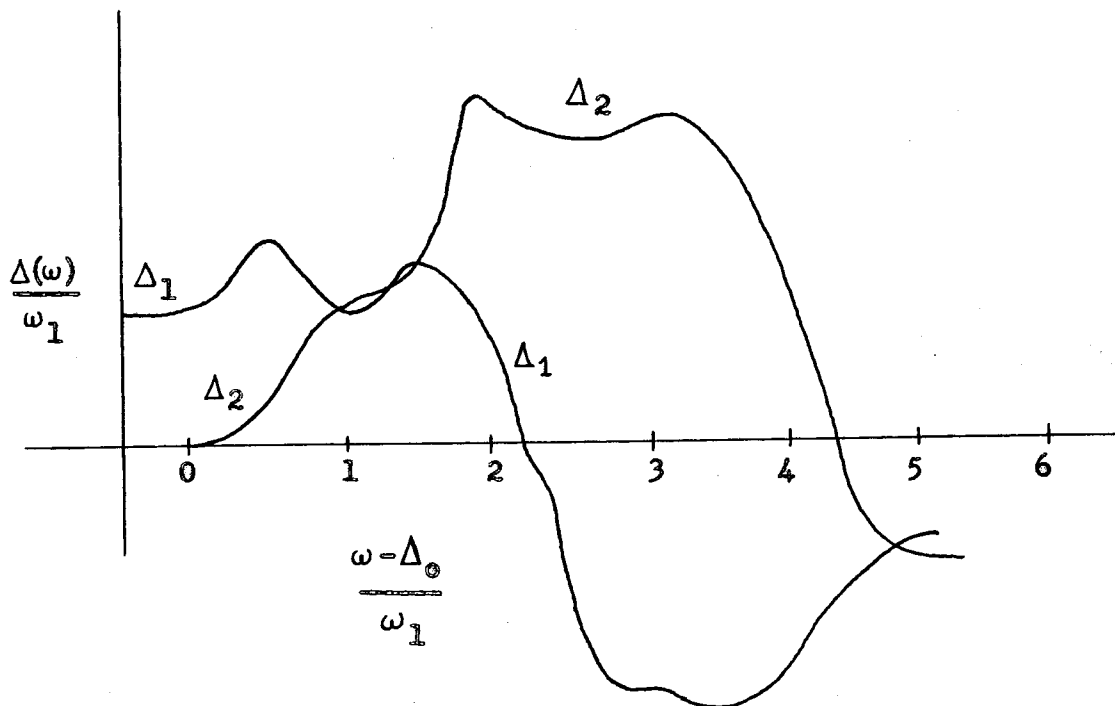
$$= 0 \quad |\omega| < \omega_o + \Delta_o$$

If we take into account the spectrum of phonons,

$$\Delta_2(\omega) = \frac{\pi N(0)}{\rho} \int d\omega_q \, F(\omega_q)|\alpha(\omega_q)|^2 \frac{\Delta_o}{\sqrt{|\omega - \omega_q|^2 - \Delta_o^2}}$$

That is, the shape of the function $F(\omega_q)|\alpha(\omega_q)|^2$ is nearly re-produced, but is somewhat spread out. In frequencies $\omega \sim 2\omega_o$, $3\omega_o$ etc. there will be additional structure, which arises if this first approximations is used in an iterative procedure.

Scalapino and Wilkins (PRL 10 336 (63)). The result of Schrieffer et al. for Pb. The approximations discussed before in linearizing the equation are worst for this metal.

The shape of Δ_1 is related to that of Δ_2 by a dispersion relation. We reproduce below the results of Schrieffer for lead. He has used a simplified description of the phonon distribution. Lead and mercury are the metals in which the electron-phonon coupling is strongest and the approximation ω_0/Δ_0 is worst. The crude approximations made previously are quite bad in this case. There are two peaks in the phonon spectrum of lead, the transverse at about 4.4×10^{-3} eV and the longitudinal at twice that value. Bumps in Δ_2 can clearly be observed at the value $n\omega_1 + \Delta_0$, $n = 1, 2, 3, 4$.

We are finally equipped to study the tunneling. As before, the current is

$$ I = 2\pi e \sum_{k,\ell} |T_{k\ell}|^2 \int \frac{d\omega_1}{2\pi} \int \frac{d\omega_2}{2\pi} \left[G_R^>(k\omega_1)\, G_2^<(\ell\omega_2) \right. $$

$$ \left. - G_R^<(k\omega_1)\, G_L^>(\ell\omega_2)\, \delta(\omega_1 - \omega_2) \right) $$

$$ = \sum |T_{k\ell}|^2 \int \frac{d\omega_1}{2\pi} A_R(k\omega_1)\, A_L(\ell\omega_1 - eV) \left[f(\omega_1 - eV) - f(\omega') \right] $$

These G's are the ordinary ones. (diagonal elements of the matrix functions). Suppose the A_R is for a superconductor, and A_L for a normal metal: Then

$$I(V) = 2\pi e \int \langle |T_{k\ell}|^2 \rangle\, 2\, N_L(0)\, 2\, N_R(0) \left| \mathrm{Re}\, \frac{\omega_1}{\sqrt{\omega_1^2 - \Delta(\omega_1)^2}} \right|$$

$$\left[f(\omega_1 - eV) - f(\omega_1) \right]\, d\omega_1$$

$$\frac{\partial I}{\partial V} = 2\pi e^2 \langle |T_{k\ell}|^2 \rangle\, 4\, N_R\, N_L\, \mathrm{Re}\, \frac{eV}{\sqrt{(eV)^2 - \Delta(eV)^2}}$$

The gross features can be understood as follows: Treat $\Delta < eV$. Then

$$\frac{\partial I}{\partial V} \sim \text{const.} + \frac{1 + \Delta_1^2 - \Delta_2^2}{2eV}$$

as $eV \to \omega_0$, Δ_2 shoots up, and Δ_1 comes down, so there is a <u>dip</u> in the neighborhood of those points. The effective density of states in reduced by the possibility of phonon emissions.

As we reach a frequency at which a great number of phonons can be emitted, Δ_2 increases, and Δ_1 decreases, by the dispersion relation. Hence there is a <u>dip</u> at these frequencies.

Experimentally, it is more interesting to tunnel between superconductors, because the sharp peak in the effective density of states of one superconductor can be used as a probe to pick out details of the density of states of the other one. The van Hove singularities (discontinuities in the slope of the <u>phonon</u> density of states function $F(\omega_q)$ can be seen in this way, although detailed shapes are clearly harder to analyse.

In sum, we have seen that the electron-phonon problem can be studied by means of Green's function techniques, and that because the speed of sound is so slow in comparison with that of the electrons, a very good approximate solution can be obtained. The tunneling functions acts as an injector of electrons, consequently the tunneling is described in terms of the one particle Green's function. In the case of a superconductor, the phonon spectrum is imaged in the energy gap function which is in tern reflected in the tunneling current.

* * *

64

REFERENCES

1. J. R. Schrieffer, Superconductivity, (To be published).

2. Bardeen, Cooper, Schrieffer, Phys. Rev. 108 1175 (1957).

3. J. Bardeen, J. R. Schrieffer, Prog. in Low Temp. Physics (North Holland) 1961.

4. L. P. Kadanoff and G. Baym, Benjamin, Quantum Statistical Mechanics, 1963.

5. A. A. Abrikosov, L. P. Gorko, I. E. Dzyaloshinski, Prentice-Hall, Quantum Field Theory in Statistical Physics, 1961.

6. D. Pines, The Many Body Problem, Benjamin (1961) (contains many reprints) Field Theory Methods.

7. A. B. Migdal, Sov. Physics, JETP 1 996, (1958).

8. Y. Nambu, Phys. Rev. 117 648 (1960).

9. G. M. Eliashberg, Sov. Physics JETP 11 696 (1960).

10. P. Morel and P. W. Anderson, Phys. Rev. 125 1263 (1962).

11. J. R. Schrieffer, D. J. Scalapino, J. W. Wilkins, Phys. Rev. Lett. 10 336 (1963).

12. I. Giaever, Phys. Rev. Letters, 5 147, 464 (1960).

13. J. Bardeen, Phys. Rev. Letters, 6 57 (1961) 9 147, (1962).

* * *

A ESCOLA LATINO AMERICANA DE FÍSICA de 1963 foi patrocinada pelas seguintes instituições:

CONSELHO NACIONAL DE PESQUISAS (BRASIL);

COMISSÃO COORDENADORA DOS CURSOS DE PÓS-GRADUAÇÃO DA UNIVERSIDADE DO BRASIL;

CENTRO LATINO-AMERICANO DE FÍSICA (BRASIL);

DEPARTAMENTO CIENTÍFICO DA UNIÃO PAN-AMERICANA.

* * *