INVESTIGATIONS

TOWARDS AN UNDERSTANDING OF SUPERCONDUCTIVITY

R. M. MAY

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By

Robert McCredie MAY

SUMMARY

of the Thesis

entitled

"INVESTIGATIONS TOWARDS AN UNDERSTANDING OF SUPERCONDUCTIVITY"

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This thesis describes an investigation of three distinct topics, each of which is related to the problem or providing a microscopic theory of superconductivity.

Firstly, the magnetic behaviour of a charged, ideal, 2-dimensional Bose gas is discussed (Chapter I). In contrast to the 3-dimensional case, the 2-dimensional gas does not exhibit any condensation phenomenon : it is, nevertheless, shown to undergo a transition (which is nearly sharp) in the presence of a magnetic field. The Bose gas model of superconductivity may then be reconciled with the experimental fact that superconductivity is not destroyed by taking thin ("2-dimensional") films. The most interesting feature of this model is, however, that it demonstrates the occurrence of an essentially perfect Meissner effect, without any irregularity in the thermodynamic properties such as the specific heat.

Secondly, the Meissner effect in the Bogoljubov theory is considered. Such a consideration is complicated by the fact that the Bogoljubov approximation scheme violates requirements of gauge-invariance. This difficulty is circumvented by first setting up a new method for finding the magnetic response of a system which is described by a non gauge-covariant hamiltonian (Chapter II). This technique is then employed to demonstrate the occurrence of a Meissner effect in the Bogoljubov theory (Chapter III).

Thirdly, the eigenvalue spectrum of the so-called "quenched pair-correlation matrix", $\widetilde{U}_2$, is considered, for electrons in metals. A knowledge of this spectrum is necessary before any quantitative theory of superconductivity can be attempted along the lines of the quasi-chemical equilibrium approach. It is found (Chapter IV) that the present method of evaluating $\widetilde{U}_2$ is unsatisfactory : what is needed is a self-consistent method, which at no stage refers explicitly to electrons which are not "quenched" by the Fermi statistics of the assembly.

PREFACE

Thesis

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PREFACE

The work embodied in this thesis falls into three distinct parts :- the magnetic behaviour of a charged 2-dimensional Bose gas; the Meissner-Ochsenfeld effect in the Bogoljubov theory; and a study of pair correlations in the quasi-chemical equilibrium approach to superconductivity.

The Preamble contains a very brief survey of the main developments which have taken place towards a fundamental theory of superconductivity, placing particular emphasis on my own work in relation to the field as a whole.

Chapter I contains an account of the magnetic behaviour of the mathematical model of a charged ideal 2-dimensional Bose gas : the model is related to the case of thin superconducting films in section 1.6. I am indebted to Prof. M.R. Schafroth for some pertinent criticisms on the writing-up of this work.

A technique for evaluating the magnetic response of a system when using an approximate Hamiltonian which is not gauge-covariant is set forth in Chapter II. This work was carried out jointly by Profs. J.M. Blatt, T. Matsubara

and myself : discussions with Profs. S.T. Butler and M.R. Schafroth are also acknowledged. The method is then applied to the (original) Bogoljubov theory in Chapter III. The problem of investigating the Meissner-Ochsenfeld effect in the Bogoljubov theory was suggested to me by Prof. M.R. Schafroth, and my thanks are due to him for many illuminating suggestions and comments with regard to subsequent work on the problem.

A study of the eigenvalue spectrum of the "quenched pair-correlation matrix" of the quasichemical equilibrium theory is carried out in Chapter IV. This project was also suggested and supervised by Prof. M.R. Schafroth : acknowledgement is due to Prof. J.M. Blatt who drew to my attention the "separable potential" employed in section 4.3.

The preparation of this thesis was facilitated by suggestions from Dr. M.J. Buckingham, who has been my supervisor since Prof. Schafroth's death.

* * *

In general, my thanks are due to Prof. H. Messel for his constant interest and encouragement, and to General Motors Holden Ltd. for their grant of a Research Fellowship.

Finally, I wish to take this opportunity to pay tribute to the late Prof. M.R. Schafroth. His qualities - not only as a physicist - have been an inspiration to me. I shall always consider myself highly privileged to have undertaken my Ph.D. under his supervision.

CONTENTS

P R E A M B L E

Super conductivity was discovered by Kamerlingh Onnes in 1911. For many years afterwards it was thought to consist simply of the vanishing of electrical resistance below the critical temperature. A major advance in the subject was the discovery in 1933 of the Meissner - Ochsenfeld (M-O) effect - i.e. the expulsion of a magnetic field from the interior of a superconductor. Phenomenological theories of both the thermodynamic and electrodynamic properties followed. However, the problem of providing a microscopic theory of superconductivity is one which has defied solution until very recently.

The basic task of such a fundamental theory is to provide an explanation of the M-O effect : this effect is characteristic of superconductors (in contrast to, say, the existance of a thermodynamic transition, which may occur for a variety of other reasons). It is, moreover, an equilibrium property (in contrast to the vanishing of electrical resistance), a feature which enables one in principle to determine uniquely whether a given model displays a M-O effect, by the use of Equilibrium Statistical Mechanics.

A useful quantitative criterion for the occurrence of a M-O effect is the following : - We write the relation between the magnetization $\underset{\sim}{M}$ and the magnetic induction $\underset{\sim}{B}$, in Fourier space, as

$$\underset{\sim}{M}(q) = K(q)\ \underset{\sim}{B}(q) \qquad (1)$$

and consider K(q) in the limit as $q \to 0$. Then a $1/q^2$ singularity characterizes a perfect or London (1935, 1950) M-O effect, in which the superconducting particles have infinite correlation length in momentum space; a weaker singularity corresponds to an imperfect M-O effect, with finite correlation length; while if K(q) is regular in q the system is simply diamagnetic.

The most significant of the earlier attempts towards providing a fundamental theory was made by Frohlich (1950) when he suggested that the mechanism responsible for superconductivity was the interaction between electrons, due to their coupling with the lattice vibrations or "phonons" - this interaction is attractive when the energy-difference between the electron states involved is less than the phonon energy. Although qualitative arguments left little doubt that this was indeed the correct mechanism, mathematical difficulties have hindered the development of the theory.

Over the past few years it has become increasingly plain that to derive the superconducting behaviour of metals from the Frohlich Hamiltonian, one must use an approximation technique which takes explicit account of the pair correlations between electrons. Two main lines of approach to this problem may be distinguished : - the Quasichemical Equilibrium approach (Schafroth, Butler and Blatt, 1956) and the theories of Bardeen-Cooper-Schrieffer (1958) and Bogoljubov (1958 (a); (b); (c); 1959; Bogoljubov, Tolmachov, Shirkov 1958)

A: The Quasichemical Equilibrium Approach

This approach is based on the remark (Schafroth 1955) that a charged ideal Bose gas exhibits a London type M-O effect below its condensation temperature. Thus a theory of superconductivity is established if charge-carrying bosons can be shown to occur in a metal at low temperatures: this is the case if the interaction between electrons is such that it produces resonant states of electron pairs.

We now pause to make the following remark about such a Bose gas model of superconductivity : - Unlike the 3-dimensional gas, the 2-dimensional Bose gas does not condense, and no transition occurs in its thermodynamic behaviour. It might thus be expected that a 2-dimenional

charged Bose gas will not display a M-O effect, which would be in contradiction to the experimental fact that thin films of superconducting material do indeed exhibit the effect. For this reason, I have investigated the 2-dimensional Bose gas (Chapter I), and have shown that in a magnetic field it undergoes a transition which is nearly sharp. Below this transition point it displays on imperfect M-O effect, which is experimentally indistinguishable from the London one. Also a critical field quite analogous to the 3-dimensional case is found. Probably the main interest of this model is, however, that it gives an (essentially perfect) M-O effect without any irregularity in the thermodynamic properties.

In order to make a more detailed consideration of the possibility of "resonant pairs" of electrons in metals, the Quasichemical Equilibrium approach was developed. This takes statistical correlations into account exactly, but neglects dynamical correlations between more than two particles. The thermodynamic behaviour of the system is now given in terms of an equilibrium between the fermions ("atoms") and diatomic "pseudomolecules" , the latter obeying a kind of Bose statistics. Under certain conditions there is a singularity in the partition function - that is to say the system undergoes a form of Bose-Einstein condensation, producing a superconducting state.

Any attempt to derive a quantitative theory of superconductivity from this approach requires a knowledge of the pair correlations : that is, using the customary terminology, a knowledge of the eigenvalue spectrum of the "quenched 2-particle correlation matrix". To this end, I have employed various model interactions to study the eigenvalue spectrum (Chapter IV). The prescription given for calculating the matrix elements, which involves first calculating the correlation matrix for unquenched electrons and subsequently introducing the statistical Fermi quenching-factors

$$q(k) = \left[e^{\alpha(\mu - E_k)} + 1 \right]^{-1} \qquad (2)$$

is found to be inadequate, leading to unphysical results.

It is concluded that before a quantitative theory of superconductivity can be deduced from the Quasichemical Equilibrium approach we require a self-consistent method of calculating the "quenched pair-correlation matrix" , which at no stage refers to unquenched electrons. Attempts to provide such a self-consistent method have to date not proved amenable to solution.

B: The BCS and Bogoljubov Theories

Starting from an approximate Fröhlich Hamiltonian, BCS use a self-consistent method to set up wave functions

describing a number of coherent electron pairs. First, wave functions are constructed containing independent pairs of opposite momentum and spin, and the best of these wave functions is chosen by means of a variation principle. This theory has been very successful in accounting for energetic quantities: however, it cannot be unambiguously extended to the case when a magnetic field is present because the approximate Hamiltonian used is not gauge-covariant. [BCS investigate the magnetic behaviour of their model by assuming a particular gauge (the London gauge, div $\underset{\sim}{A} = 0$). This choice is in fact a new and independent assumption of the theory, equivalent to assuming the M-O effect itself.]

Recently, Bogoljubov (1958 (a)) has developed a new method which combines the main features of the BCS theory with greater mathematical transparency. This method (in its original form) shares both the successes of the BCS theory and the defect that the approximate Hamiltonian violates gauge-covariance.

Bogoljubov's early papers contain no attempt at a derivation of the M-O effect. An attempt by Rickayzen (1958) again assumes the London gauge, thus remaining inconclusive. On the other hand, Wentzel (1958), realizing the gauge difficulty, follows a course which amounts to

treating the magnetic terms by a perturbation expansion in powers of the electron-phonon coupling constant, when for the non-magnetic terms such an expansion is not permissible. The consequent results differ from the later calculations described below.

As a first step towards a study of the M-O effect in the Bogoljubov theory, Blatt, Matsubara and myself (1959) developed a technique for extracting unambiguous results from non gauge-covariant approximations to gauge-covariant Hamiltonians (Chapter II). I was then able to apply this method to the Bogoljubov model, and show that it indeed exhibits a M-O effect (Chapter III). The resulting kernel function K(q) differs from the London kernel at large q, in the manner anticipated by Pippard (1953).

In a later version of his theory, Bogoljubov introduced a concept of collective excitations by taking a selective summation over the most singular terms in each order of perturbation theory. These excitations have been used by Blatt and Matsubara (1958 (b)) to make a calculation of K(q) which fulfils gauge identities. Their result was derived at the same time as my own: the two are in agreement.

Finally, Bogoljubov (1958 (c); 1959) has developed a new and more general formalism which is explicitly gauge-invariant (the so-called "method of the self-consistent field"). The subsequent derivation of the M-O effect is, in

principle, a more sophisticated and rigorous version of the Blatt-Matsubara calculation. In both these calculations $K(q)$ is found only in the limiting case of $q \rightarrow 0$: deviations from the London kernel at larger q (which relate to the details of magnetic field penetration in the superconductor) are not considered.

C H A P T E R I.

MAGNETIC BEHAVIOUR OF A CHARGED IDEAL 2 - DIMENSIONAL BOSE GAS.

1.1 INTRODUCTION

At a certain temperature , T_c , a 3-dimensional ideal gas of charged particles obeying Bose-Einstein statistics undergoes a sharp thermodynamic transition (Einstein 1924, London 1938) : for $T<T_c$, a macroscopic number of particles condenses into the ground state of the system. It has been shown (Ginzberg 1952, Schafroth 1955, which we refer to as (I)) that these condensed bosons then give rise to a perfect M-O effect.

However, if one considers, as a mathematical model, the 2-dimensional Bose gas, one finds that it does not condense and no transition whatsoever appears in its thermodynamic behaviour. The specific heat is a regular function of temperature, proportional to T near absolute zero. It might thence be expected (e.g. Feynman 1957) that a 2-dimensional charged Bose gas will <u>not</u> display a M-O effect. If this were the case it would be a discrepency in any Bose gas model of superconductivity (Schafroth 1954, Schafroth et al 1956, Bogoljubov et al 1958), because the 2-dimensional gas is relevant to very thin films of superconducting material, which do indeed exhibit the M-O phenomenon.

In this chapter, we show that (contingent upon the fulfilment of a mathematical restriction which is valid for all practical applications to thin films) the 2-dimensional charged Bose gas in a magnetic field under-

-goes a transition which is nearly sharp. Below this transition point it displays an imperfect M-O effect which, although K(q) is regular in q, is practically indistinguishable from a perfect one: above the transition temperature there is only a slight dismagnetism.

Also the 2-dimensional gas has a critical field quite analogous to the 3-dimensional case.

The noteworthy feature of the 2-dimensional model is that it exhibits these superconducting properties, while the thermodynamic functions remain analytic in the temperature, with no sign of any discontinuity.

In section 2, the thermodynamics of the 2-dimensional Bose gas are briefly set forth for subsequent use, and contrasted with the 3-dimensional case. By considering a weak, inhomogeneous magnetic field as a perturbation on the field-free system, the kernel function K(q) is derived in section 3 : the consequent magnetic behaviour is investigated in section 4. The B-H curve, which gives the critical field, is found in section 5, by calculating the partition function in the presence of a homogeneous field.

Finally, in section 6, the mathematical abstraction of a 2-dimensional gas is related to the case of very thin films.

1.2 THERMODYNAMICS

The grand canonical partition function, $e^{-\alpha\Omega}$, for the ideal Bose gas (with an arbitrary number of dimensions) is given by

$$\Omega = kT \sum_{\underset{\sim}{k}} \ln \left[1 - \exp\alpha\left(\mu - \frac{\hbar^2 k^2}{2m}\right) \right] \tag{2.1}$$

where $\alpha = 1/kT$, and μ is the chemical potential. The number of bosons, N, is given in terms of μ by

$$N = -\left(\frac{\partial\Omega}{\partial\mu}\right)_T \tag{2.2}$$

$$= \sum_{\underset{\sim}{k}} \frac{1}{\exp\left[\alpha\left(\frac{\hbar^2 k^2}{2m} - \mu\right)\right] - 1} \tag{2.3}$$

To avoid negative occupation numbers, we require

$$\eta \equiv -\alpha\mu \quad > 0 \tag{2.4}$$

(a) 3 dimensions:

If we simply replace sums by 3-dimensional integrals in Eq (2.3), we get

$$n \equiv \frac{N}{V} = \frac{1}{\lambda^3 \Gamma\left(\frac{3}{2}\right)} \int_0^\infty \frac{x^{1/2}}{e^{x+\eta} - 1}\, dx \tag{2.5}$$

with the thermal wavelength λ defined by

$$\lambda^2 = \frac{4\pi\alpha\hbar^2}{2m} \tag{2.6}$$

The integral in Eq (2.5) is a regular function of η (in the range allowed by Eq (2.4)), <u>having a finite upper bound</u> at $\eta = 0$. Thus below some critical temperature T_c,

$$\frac{N}{V} = \left(\frac{2mkT_c}{4\pi\hbar^2}\right)^{3/2} 2.612 \ldots \qquad (2.7)$$

the expression (2.5) for N is inadequate, and the singular ground state must be considered separately.

The consequent specific heat at constant volume, $C_V(T)$, for the 3-dimensional gas is as shown in figure 1 - its slope has a sharp discontinuity at T_c.

<u>(b) 2 dimensions:</u>

The 2-dimensional counterpart of Eq (2.5) is

$$n \equiv \frac{N}{V} = \frac{1}{\lambda^2} \int_0^\infty \frac{dx}{e^{x+\eta}-1} \qquad (2.8)$$

i.e. $$n = -\frac{1}{\lambda^2} \ln (1-e^{-\eta}) \qquad (2.9)$$

where λ is given by Eq (2.6), and V is the 2-dimensional "volume".

The integral in this case diverges as η tends to zero : there is no upper bound. Thus the need to consider the ground state separately, and the consequent transition phenomena, no longer arise.

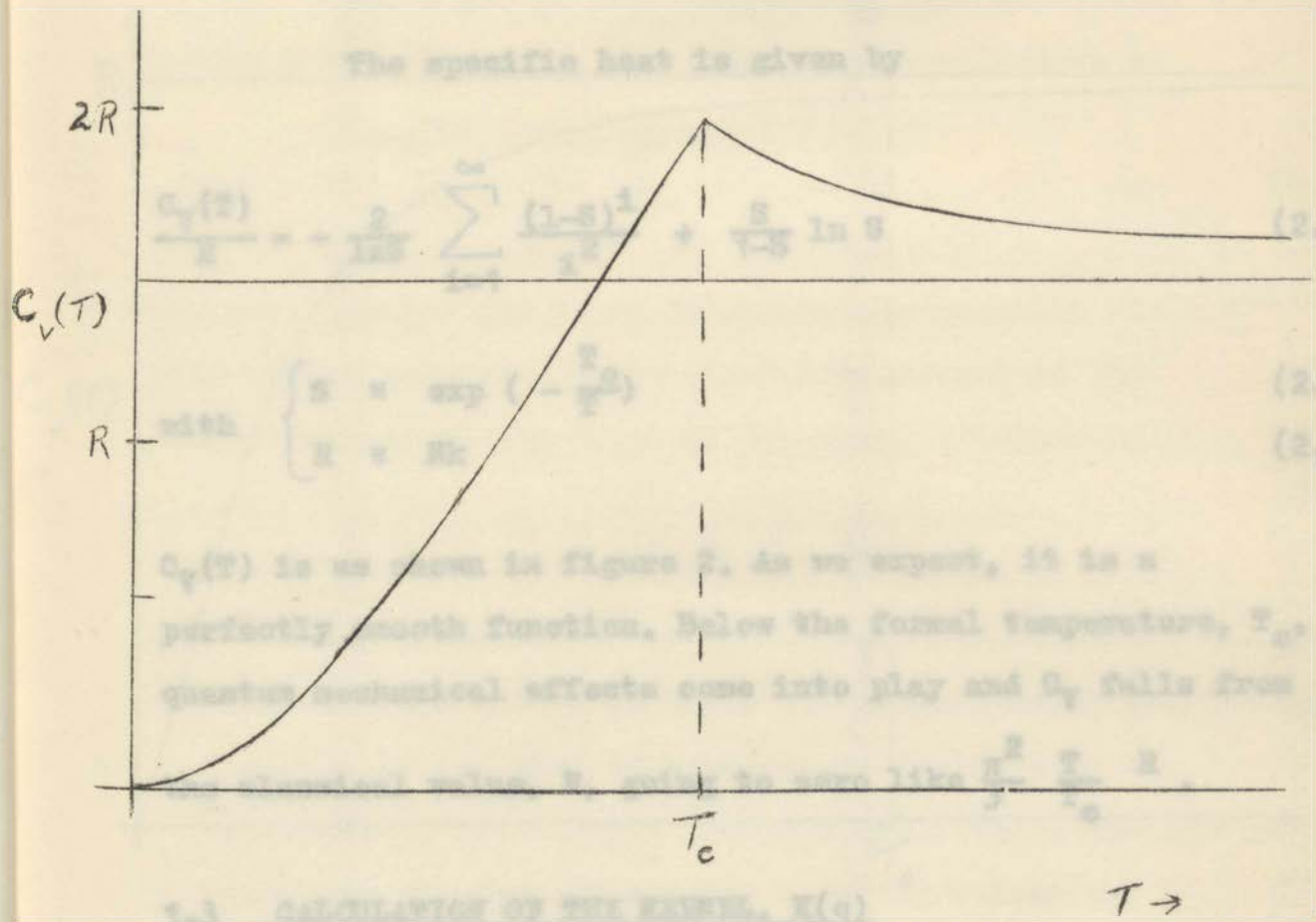

Fig. 1

For convenience, we introduce a "formal temperature", T_o (*), by

$$n = \frac{1}{\lambda_o^2} \tag{2.10}$$

i.e. $$\exp(-\frac{T_o}{T}) = 1 - e^{-\eta} \tag{2.11}$$

The specific heat is given by

$$\frac{C_V(T)}{R} = -\frac{2}{\ln S} \sum_{i=1}^{\infty} \frac{(1-S)^i}{i^2} + \frac{S}{1-S} \ln S \tag{2.12}$$

with
$$\begin{cases} S \equiv \exp\left(-\frac{T_o}{T}\right) & (2.13) \\ R \equiv Nk & (2.14) \end{cases}$$

$C_V(T)$ is as shown in figure 2. As we expect, it is a perfectly smooth function. Below the formal temperature, T_o, quantum mechanical effects come into play and C_V falls from the classical value, R, going to zero like $\frac{\pi^2}{3} \frac{T}{T_o} R$.

1.3 CALCULATION OF THE KERNEL, K(q)

We first find the current density induced in a 2-dimensional charged Bose gas by a weak, inhomogeneous magnetic field, by enclosing the system in a square box with

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(*) We note that in 3 dimensions, the formal temperature, T_o, and the transition temperature, T_c, are one and the same thing: this is not the case in 2 dimensions.

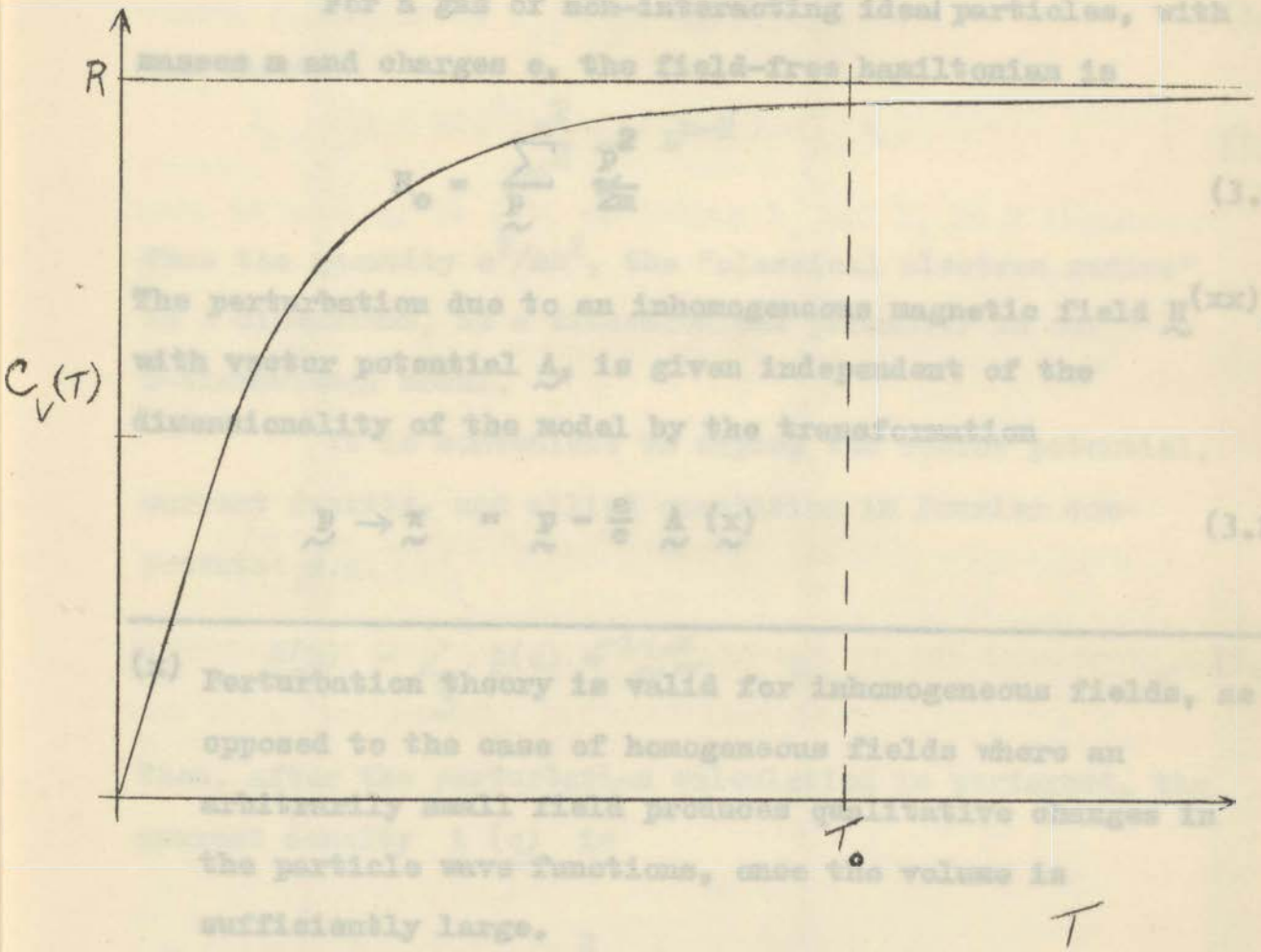


Fig 2

periodic boundary conditions, and then applying perturbation theory[x] (in the form developed by Schafroth (1951)) to the distribution function. This perturbation theory avoids difficulties arising from energy denominators in the case of complete or near degeneracies.

For a gas of non-interacting ideal particles, with masses m and charges e, the field-free hamiltonian is

$$H_o = \sum_{\underset{\sim}{p}} \frac{p^2}{2m} \tag{3.1}$$

The perturbation due to an inhomogeneous magnetic field $\underset{\sim}{H}$[xx], with vector potential $\underset{\sim}{A}$, is given independent of the dimensionality of the model by the transformation

$$\underset{\sim}{p} \rightarrow \underset{\sim}{\pi} = \underset{\sim}{p} - \frac{e}{c} \underset{\sim}{A}(\underset{\sim}{x}) \tag{3.2}$$

(x) Perturbation theory is valid for inhomogeneous fields, as opposed to the case of homogeneous fields where an arbitrarily small field produces qualitative changes in the particle wave functions, once the volume is sufficiently large.

(xx) In a 2-dimensional problem, the magnetic field, $\underset{\sim}{H}$, is a pseudoscalar quantity. It may be represented by a vector perpendicular to the model, in a 3-dimensional realization thereof.

Before proceeding, we note the following point:- from dimensional considerations based on the Lorentz invariant transformation (3.2) and Maxwell's equation, one finds that the charge, e, on a particle in n-dimensional space has dimensions

$$e^2 \sim ML^{n_T-2} \tag{3.3}$$

and thence

$$\frac{e^2}{mc^2} \sim L^{n-2} \tag{3.4}$$

Thus the quantity e^2/mc^2, the "classical electron radius" in 3 dimensions, is a dimensionless parameter in our 2-dimensional model.

It is convenient to expand the vector potential, current density, and allied quantities in Fourier components: e.g.

$$\underset{\sim}{A}(\underset{\sim}{x}) = \sum_{\underset{\sim}{q}} \underset{\sim}{A}(\underset{\sim}{q})\, e^{-i\underset{\sim}{q}.\underset{\sim}{x}} \tag{3.5}$$

Then, after the perturbation calculation is performed, the current density $\underset{\sim}{i}(\underset{\sim}{q})$ is

$$i_\mu(\underset{\sim}{q}) = -\frac{e^2}{mc} \cdot \frac{1}{V} \sum_{\nu=1}^{2} (I_{\mu\nu} + N\delta_{\mu\nu})\, A_\nu(\underset{\sim}{q}) \tag{3.6}$$

$$I_{\mu\nu}(\underset{\sim}{q}) = \sum_{\underset{\sim}{p}} \frac{p_\mu p_\nu}{\underset{\sim}{p}.\underset{\sim}{q}} \left\{ F_o\left(\frac{(\underset{\sim}{p}+\underset{\sim}{q})^2}{2m}\right) - F_o\left(\frac{(\underset{\sim}{p}-\underset{\sim}{q})^2}{2m}\right) \right\} \tag{3.7}$$

$F_0(E)$ is the distribution function of the field-free Bose gas (see Eq (2.3)). The above result is derived in ref. (I) (with, of course, the sum over ν going from 1 to 3): alternatively it may be read off from Eq (1.14) of Chapter II.

Making use of the fact that $\underset{\sim}{q}$ is the only vector contained in $I_{\mu\nu}(\underset{\sim}{q})$, we write

$$I_{\mu\nu}(\underset{\sim}{q}) = a(q^2)\, q_\mu q_\nu + b(q^2)\, q^2\, \delta_{\mu\nu} \tag{3.8}$$

and, in analogy to (I), we define I_0 and I_1 in 2 dimensions by

$$I_0 \equiv \sum_{\mu=1}^{2} I_{\mu\mu} = (a+2b)\, q^2 \tag{3.9}$$

$$I_1 \equiv \sum_{\mu=1}^{2} I_{\mu\nu}\, q_\mu q_\nu = (a+b)\, q^4 \tag{3.10}$$

Substituting from Eqs (3.8), (3.9) and (3.10) into Eq (3.6), and using the readily verified fact that

$$I_1 = -q^2 N \tag{3.11}$$

we get

$$i_\mu(\underset{\sim}{q}) = -\frac{e^2}{mc}\,\frac{1}{V}\,(I_0+2N)\left(\delta_{\mu\nu} - \frac{q_\mu q_\nu}{q^2}\right) A_\nu(\underset{\sim}{q}) \tag{3.12}$$

This expression is explicitly gauge covariant : rewriting in terms of the magnetic induction $\underset{\sim}{B}$ ($\underset{\sim}{B}$ = curl $\underset{\sim}{A}$) and the magnetization $\underset{\sim}{M}$ ($\underset{\sim}{i}$ = c curl $\underset{\sim}{M}$), one gets

$$\underset{\sim}{M}(\underset{\sim}{q}) = K(q)\, \underset{\sim}{B}(\underset{\sim}{q}) \tag{3.13}$$

$$K(q) = -\frac{e^2}{mc^2}\cdot\frac{1}{q^2}\cdot\frac{1}{V}\sum_{\underset{\sim}{p}}\left\{\frac{\underset{\sim}{p}^2}{\underset{\sim}{p}\cdot\underset{\sim}{q}} - \frac{2\underset{\sim}{p}\cdot\underset{\sim}{q}}{\underset{\sim}{q}^2}\right\} x$$

$$x\left\{F_o\left[\frac{(\underset{\sim}{p}+\frac{\underset{\sim}{q}}{2})^2}{2m}\right] - F_o\left[\frac{(\underset{\sim}{p}-\frac{\underset{\sim}{q}}{2})^2}{2m}\right]\right\} \qquad (3.14)$$

We proceed to simplify this expression for the kernel. Replacing sums by integrals

$$K(q) = -\frac{2e^2}{mc^2}\cdot\frac{1}{q^2}\cdot\frac{1}{(2\pi)^2}\int_0^\infty p\,dp F_o\left(\frac{p^2}{2m}\right) P\int_0^{2\pi}\frac{(p^2-\frac{q^2}{4})}{\underset{\sim}{q}\cdot(\underset{\sim}{p}-\frac{\underset{\sim}{q}}{2})}\,d\theta \qquad (3.15)$$

There is no question as to the validity of taking principal values in the angular integration, since the integrand has been obtained by rewriting the summand of Eq (3.14), which is perfectly regular. Performing this angular integration one gets

$$\left.\begin{aligned} \frac{1}{2\pi} P\int_0^{2\pi}\frac{(p^2-\frac{q^2}{4})}{\underset{\sim}{q}\cdot(\underset{\sim}{p}-\frac{\underset{\sim}{q}}{2})}\,d\theta &= 0 \quad \text{for} \quad p > \frac{q}{2} \\ &= \frac{1}{2}\sqrt{1-\left(\frac{2p}{q}\right)^2} \quad \text{for } p < \frac{q}{2} \end{aligned}\right\} \qquad (3.16)$$

Making the change in variable $x = \alpha\hbar^2 p^2/2m$, and using the notation defined in section 2, Eq(3.15) becomes

$$K(q) = -\frac{e^2}{mc^2}\,\frac{1}{\lambda^2 q^2}\int_0^{x_o}\frac{\left(1-\frac{x}{x_o}\right)^{1/2}\,dx}{e^{x+\eta}-1} \qquad (3.17)$$

with

$$x_o \equiv \frac{\lambda^2 q^2}{16\pi} \qquad (3.18)$$

Of particular interest is the limiting case of $x_o \to 0$:

$$\lim_{q\to 0} K(q) = -\frac{e^2}{16\pi mc^2} \times \frac{1}{e^{\eta}-1} \times \int_0^1 (1-t)^{1/2}\,dt \qquad (3.19)$$

Using Eq (2.11), this becomes

$$K(0) = -\frac{1}{24\pi}\,\frac{e^2}{mc^2}\,e^{T_o/T}\left(1-e^{-T_o/T}\right) \qquad (3.20)$$

For larger values of x_o (i.e. for $x_o > \eta$ with $\eta < 1$, or else $x_o > 1$ with $\eta > 1$), the kernel may be written as

$$K(q) = -\frac{e^2 n}{mc^2}\cdot\frac{1}{q^2}\cdot F(q) \qquad (3.21)$$

where the leading term in the function F(q) depends on q either logarithmically or not at all. In the limit as q tends to infinity, F(q) becomes unity.

1.4 PENETRATION OF MAGNETIC FIELD.

We now investigate our model further, imposing the requirement that the dimensionless parameter

$$\frac{e^2}{12mc^2} \ll 1 \tag{4.1}$$

That is, if we define a temperature T_c by

$$\frac{e^2}{12mc^2} = e^{-T_o/T_c} \tag{4.2}$$

we require that T_o/T_c shall be appreciably greater than unity.

From now on, our attention is confined to temperatures below T_o, since temperatures $> T_o$ are found to be of no interest once the above assumption is made. That is, ignoring terms of order $\exp(-T_o/T)$ compared to unity, Eq. (2.10) is simplified to read

$$\eta = e^{-T_o/T} \tag{4.3}$$

Using Eqs (4.2) and (4.3), the kernel in the limit of zero q, Eq (3.20), may be written

$$K(0) = -\frac{1}{2\pi} \exp\left(\frac{T_o}{T} - \frac{T_o}{T_c}\right) \tag{4.4}$$

The kernel for the 2-dimensional Bose gas remains finite as q tends to zero: however, we see that it becomes very large as T decreases below T_c. Above T_c, the exponent

i.e. the customary factor 4π of the 3-dimensional world is replaced throughout by 2π.

The London kernel gives an exponential penetration law,

$$\frac{B(x)}{B_o} = e^{-x/d} \tag{4.6}$$

We now consider the 2-dimensional Bose gas kernel, Eq (3.17). Employing the asymptotic form of Eq (4.5)

$$\frac{B(x)}{B_o} \xrightarrow{x\to\infty} \frac{1}{1-2\pi K(0)} \tag{4.7}$$

we find that the field at large distances within the gas becomes a finite constant

$$\frac{B(x)}{B_o} \longrightarrow \frac{1}{1+\exp\left(\frac{T_o}{T} - \frac{T_o}{T_c}\right)} \tag{4.8}$$

For temperatures below T_c, such that $T_o/T(1-T/T_c) > 1$, a detailed calculation gives

$$\left.\begin{aligned} \frac{B(x)}{B_o} &= e^{-x/d_o}, \quad \frac{x}{d_o} \ll \frac{T_o}{T}\left(1 - \frac{T}{T_c}\right) \\ \frac{B(x)}{B_o} &= \frac{1}{1+\exp\left(\frac{T_o}{T} - \frac{T_o}{T_c}\right)}, \quad \frac{x}{d_o} \gg \frac{T_o}{T}\left(1 - \frac{T}{T_c}\right) \end{aligned}\right\} \tag{4.9}$$

where d_o is quite analogous to the penetration depth for the 3-dimensional Bose gas:

$$d_o = \left\{\frac{2\pi e^2 n}{mc^2}\,(1-T/T_c)\right\}^{-1/2} \left\{1+0\,\frac{\ln\left[\frac{T_o}{T}(1-T/T_c)\right]}{\left[\frac{T_o}{T}(1-\frac{T}{T_c})\right]}\right\} \qquad (4.10)$$

Above T_c, the result (4.8) is adequate for all $x > d_1$, where

$$d_1^2 = \left(\frac{2\pi e^2 n}{mc^2}\right)^{-1} \exp\left[-\frac{T_o}{T_c}\,(1-\frac{T_c}{T})\right] \qquad (4.11)$$

$$\ll d_o^2 \qquad (4.12)$$

This penetration law is now as depicted in figure 3.

A qualitative understanding of these results is given by considering the "modified diamagnet" kernel of (II)

$$K_1(q) = -\frac{1}{2\pi}\,\frac{1}{d^2(q^2+\mu^2)} \qquad (4.13)$$

whose behaviour is similar to that of (3.17), with its limiting forms (3.21) and (4.4). μ^{-1} can be interpreted as the "correlation length" between particles. Substitution of this kernel in Eq (4.5) readily gives the penetration law

$$\frac{B(x)}{B_o} = \frac{(\mu d)^2+e^{-\sigma x}}{1+(\mu d)^2}\,,\quad \sigma = d^{-1}\,(1+(\mu d)^2)^{1/2} \qquad (4.14)$$

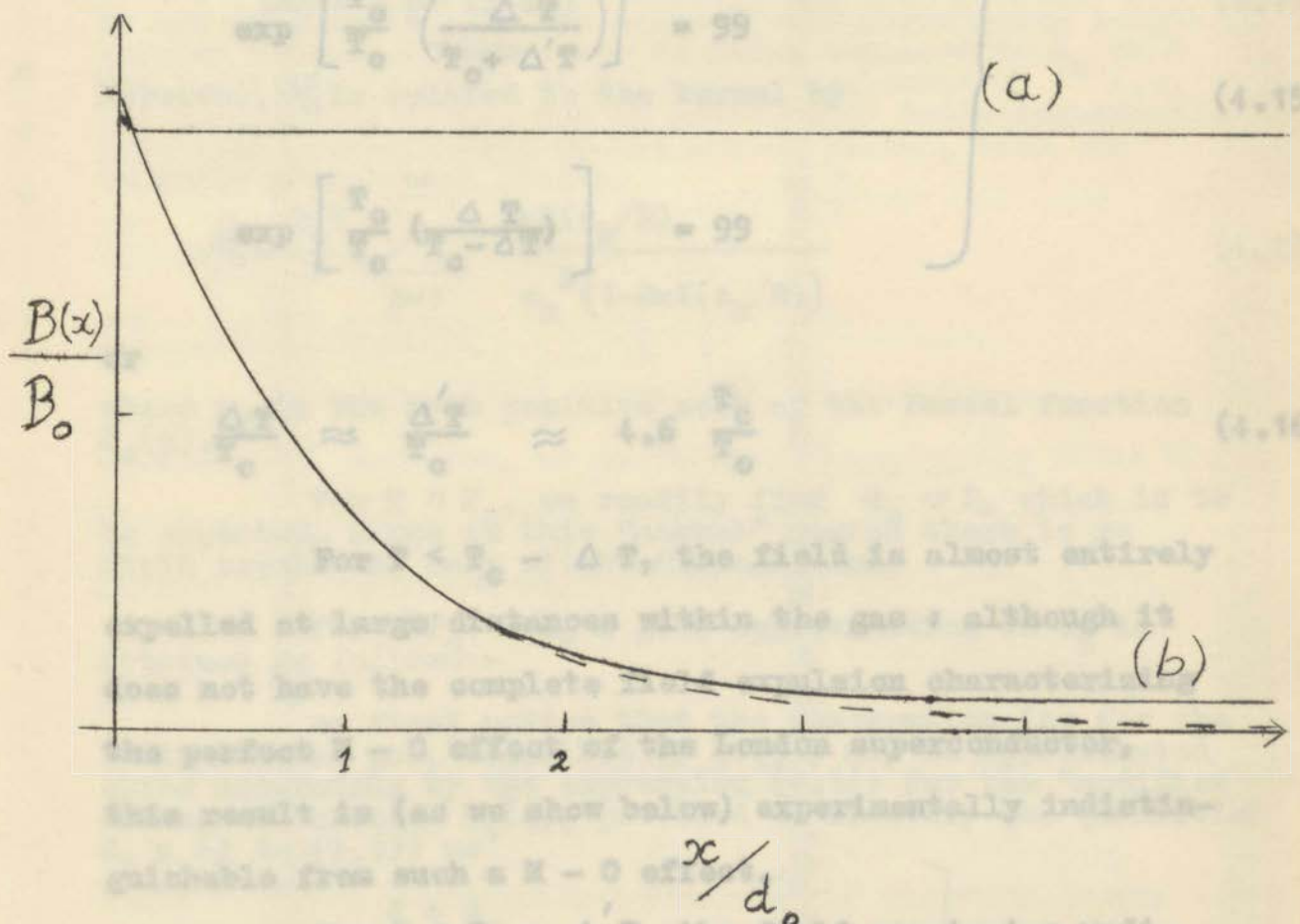


Figure 3: The law of field penetration for an inhomogeneous magnetic field applied to a 2-dimensional charged Bose gas : (a) $T > T_c$, (b) $T < T_c$. The broken line is the "perfect" London exponential law.

We define a temperature width, $\Delta T + \Delta' T$, such that as the temperature decreases from $(T_c + \Delta' T)$ to $(T_c - \Delta T)$, the field at great distances within the Bose gas decreases from 99°/o to 1°/o of the external field. Then

$$\left.\begin{aligned} \exp\left[\frac{T_o}{T_c}\left(\frac{\Delta' T}{T_c + \Delta' T}\right)\right] &= 99 \\ \exp\left[\frac{T_o}{T_c}\left(\frac{\Delta T}{T_c - \Delta T}\right)\right] &= 99 \end{aligned}\right\} \qquad (4.15)$$

or

$$\frac{\Delta T}{T_c} \approx \frac{\Delta' T}{T_c} \approx 4.6\ \frac{T_c}{T_o} \qquad (4.16)$$

For $T < T_c - \Delta T$, the field is almost entirely expelled at large distances within the gas : although it does not have the complete field expulsion characterizing the perfect M - O effect of the London superconductor, this result is (as we show below) experimentally indistinguishable from such a M - O effect.

For $T > T_c + \Delta' T$, the field penetrates undiminished except for a slight diamagnetism.

Thus we may interpret T_c as a transition temperature, from a normal to a superconducting state. The width of this transition is given by Eq (4.16)

* * * * *

Since the actual penetration law, as such, has never been measured for a superconductor, it remains to calculate an experimentally measurable quantity which is determined by the nature of the M-O effect. Such a quantity is the "static penetration depth", d_s. For a circular disk, radius R, of superconducting material, d_s is defined in terms of the total magnetic moment, $\mathcal{M}$, induced by an applied field:

$$\mathcal{M} \equiv -\frac{B_o}{4}(R-d_s)^2 \tag{4.17}$$

Moreover, $\mathcal{M}$ is related to the kernel by

$$\mathcal{M} = \frac{B_o V}{\pi}\sum_{k=1}^{\infty}\frac{2\pi K(z_k/R)}{z_k^2\left(1-2\pi K(z_k/R)\right)} \tag{4.18}$$

where z_k is the k-th positive zero of the Bessel function $J_o(z)$.

For $T > T_c$, we readily find $d_s \approx R$, which is to be expected, since in this "normal" region there is no field expulsion, only slight diamagnetism.

For $T<T_c - \Delta T$, a good approximation to d_s is obtained as follows:-

we first notice that the penetration law for the 2-dimensional gas, described by (4.9), may be approximated quite accurately by the expression (4.14) for the "modified diamagnet" kernel, $K_1(q)$, provided we identify the quantities d, μ of Eq (4.13) as

$$\left.\begin{aligned} d &= d_o \\ (\mu d)^2 &= \exp\left[-\frac{T_o}{T}+\frac{T_o}{T_c}\right] \ll 1 \end{aligned}\right\} \tag{4.19}$$

For $K_1(q)$ we find (cf. (II))

$$d_s = d\left(1+\frac{R}{2d}(\mu d)^2\right)\left(1+\mathcal{O}(\mu d)^2+\mathcal{O}\left(\frac{d}{R}\right)\right) \tag{4.20}$$

Hence for our model, with $R \gg d_o$ (the usual experimental case),

$$d_s \approx d_o \left\{ 1 + \frac{R}{2d_o} \exp\left[-\frac{T_o}{T}\left(1 - \frac{T}{T_c}\right)\right]\right\} \qquad (4.21)$$

Even for large values of the disk radius, R, we see that as T decreases below T_c the correlation length between bosons, μ^{-1}, becomes so large compared to d_o that the R dependence in Eq (4.21) may be neglected - i.e. the penetration depth, d_s, is practically indistinguishable from that corresponding to the London kernel, with its infinite correlation length.

1.5 CRITICAL FIELD

We consider a plane disk, containing a 2-dimenional Bose gas, in an "acting" homogeneous field H'. The grand canonical partition function, $e^{-\alpha\Omega}$, may be derived in a standard way (cf. Pauli 1930)

$$\Omega = kT \frac{eH'}{\hbar c} \frac{V}{2\pi} \sum_{\nu=0}^{\infty} \ln\left(1 - \exp\left\{-\alpha\left[\mu_o H'(2\nu+1) - \mu\right]\right\}\right) \qquad (5.1)$$

where V is the 2-dimensional "volume" of the disk, μ the chemical potential, and $\mu_o = e\hbar/2mc$ the Bohr magneton. The limitation (2.4) on μ is now relaxed somewhat : instead of $\mu<0$ we require $\mu < \mu_o H'$.

The expression (5.1) may be rewritten in a more convenient form by expanding the logarithm, and performing the summation over ν, to get

$$\omega \equiv \frac{\Omega}{V} = -\frac{kT}{\lambda^2} \sum_{i=1}^{\infty} \frac{e^{i\alpha\mu}}{i^2} \frac{i\alpha\mu_o H'}{\sinh(i\alpha\mu_o H')} \tag{5.2}$$

$$n \equiv \frac{N}{V} = \frac{1}{\lambda^2} \sum_{i=1}^{\infty} \frac{e^{i\alpha\mu}}{i} \frac{i\alpha\mu_o H'}{\sinh(i\alpha\mu_o H')} \tag{5.3}$$

with λ defined by Eq (2.6).

The magnetization, M, is derived from $\Omega(H')$ by use of the thermodynamic relation

$$M = -\frac{1}{V} \left(\frac{\partial \Omega(H')}{\partial H'} \right)_{\mu} \tag{5.4}$$

Before proceeding, it is necessary to determine the precise nature of the "acting" field, H'. By a slight modification of the argument presented in appendix II of (I), it is found that for all values of H' which need be considered, the diameter of the boson's orbits is much larger than the mean particle separation, provided that:

$$\frac{e^2}{mc^2} \ll 1 \tag{5.5}$$

This is, however, just the condition imposed on the model earlier (i.e. Eq. (4.1)). The field produced by any one such large orbit is negligible compared to the average field, and therefore the "acting" field H' is to be identified with the average microscopic field, B.

$$H' = B = H + 2\pi M \tag{5.6}$$

To derive the magnetization from Eqs. (5.2), (5.3) and (5.4), we first note that, for all fields of any interest,

$$\varepsilon \equiv \frac{\mu_o B}{kT_o} << 1 \tag{5.7}$$

where T_o is given by (2.10). We introduce x,

$$x \equiv \alpha\mu_o B \tag{5.8}$$

Then in calculating M, two regions of temperature are treated separately : (a) absolute zero, $x>>1$ and (b) finite temperatures, $x<<1$.

(a) Absolute zero : $\mu_o B >> kT$

Here the equations for ω and n are easily reduced to

$$\omega = \frac{2kTx}{\lambda^2} \ln\left(1-\exp\left[-(x-\alpha\mu)\right]\right) \tag{5.9}$$

$$n = \frac{2x}{\lambda^2} \frac{1}{e^{x-\alpha\mu}-1} \tag{5.10}$$

Whence

$$M = -\frac{2\mu_o}{\lambda^2}\left\{\frac{x}{e^{x-\alpha\mu}-1} + \ln\left(1-e^{-(x-\alpha\mu)}\right)\right\} \tag{5.11}$$

i.e. $$M = -n\mu_o\left\{1 - \frac{2T}{T_o}\ln\left(\frac{1+2\varepsilon}{2\varepsilon}\right)\right\} \tag{5.12}$$

In the region under consideration, $T/T_o \ll \varepsilon$, the second term in the brackets is a negligible correction term.

Substituting (5.12) into Eq (5.6), the B-H curve is seen to be the same as for the 3-dimensional Bose gas at absolute zero (except that $4\pi \longrightarrow 2\pi$) :

$$\left.\begin{aligned} B(H) &= 0 \quad , H<H_c \\ &= H-H_c \quad , H>H_c \end{aligned}\right\} \tag{5.13}$$

with $$H_c = 2\pi n \mu_o \tag{5.14}$$

(b) Finite temperatures : $\mu_o B \ll kT$

For $x \ll 1$, the sums (5.2) may, after some manipulation, be approximated by (convergent) integrals. Having done this, M(B) is calculated : all this is done in an Appendix. Purely for reasons of formal convenience, we define a field, B_1, by Eq (I.10), i.e.

$$B_1 = \frac{2\pi}{6}\,\mu_o n \frac{T}{T_o} \exp\left[\frac{T_o}{T_c} - \frac{T_o}{T}\right] \tag{5.15}$$

We find, for $B \leq B_1$,

$$2\pi M = -B \exp\left[\frac{T_o}{T} - \frac{T_o}{T_c}\right]\left\{1 - \frac{3}{40}\left(\frac{B}{B_1}\right)^2 + \ldots\right\} \tag{5.16}$$

To a good approximation, this leads to

$$B = \chi H \tag{5.17}$$

$$\chi = \left[1 + \exp\left(\frac{T_o}{T} - \frac{T_o}{T_c}\right)\right]^{-1} \tag{5.18}$$

For $T > T_c$, χ is almost unity, corresponding to normal diamagnetism : for $T < T_c$, χ becomes very small. This result provides an independent check of the results in section 4, as follows:- For a strip of our Bose gas in the limiting case of infinite area, the ratio of the field at large distances inside (B_∞) to the (small) external field (B_o) may be found in two ways.

(a) We first observe that in this limiting case the inhomogeneities are negligible, and then apply the homogeneous theory above, to get the expression (5.18) for B_∞ / B_o .

(b) Alternatively we may start from the inhomogeneous theory of sections 3 and 4, and then use the asymptotic expression (4.8) to get B_∞ / B_o when the size of the strip becomes infinite. The resulting two equations are identical.

For $T > T_c$, the result (5.17) is valid for all fields which are of any interest — on the other hand, for $T < T_c - \Delta T$ we must also consider the case of $B \gg B_1$. In this region,

$$2\pi M = -\frac{2\pi\mu_o}{\lambda^2} \ln\left(\frac{B}{B_1}\right)\left[1 + \mathcal{O}\left(\frac{\ln(\ln B/B_1)}{\ln B/B_1}\right)\right] \tag{5.19}$$

We now introduce a quantity H_c, which is subsequently identified with the critical field for a superconductor,

$$H_c = \frac{2\pi\mu_o}{\lambda^2} \ln \frac{2\pi\mu_o}{6\lambda^2 B_1} \tag{5.20}$$

i.e. $$\boxed{H_c = 2\pi\mu_o n \left(1 - \frac{T}{T_c} \right)} \tag{5.21}$$

Then Eq (5.19) becomes (neglecting the correction term in the brackets)

$$2\pi M = - H \left\{ 1 + \frac{\ln\left(\frac{6\ aB}{H_c}\right)}{a} \right\} \tag{5.22}$$

where $a \equiv \frac{T_o}{T} \left(1 - \frac{T}{T_c} \right)$, ($>> 1$ by Eq (4.12)) (5.23)

So for $T < T_c - \Delta T$, and $B >> B_1$, the B - H curve is described by

$$H - H_c = B \left\{ 1 + \frac{\ln\left(\frac{6aB}{H}\right)}{\left(\frac{aB}{H}\right)} \right\} \tag{5.24}$$

Finally we notice that as H increases above H_c, the second term in the brackets in Eq (5.24) becomes a small correction term, and

$$B \approx H - H_c \tag{5.25}$$

Combining (5.17) and (5.24), the B–H curve at finite temperatures less that T_c looks as shown in figure 4.

This is quite analogous to the 3-dimensional Bose gas, where

$$\left.\begin{aligned} B &= 0 \quad , \quad H < H_c' \\ &= H - H_c' \quad , \quad H > H_c' \end{aligned}\right\} \tag{5.26}$$

$$H_c' = 4\pi n \mu_o \left(1 - \left(\frac{T}{T_c}\right)^{3/2}\right) \tag{5.27}$$

To summarize, we see that for temperatures above T_c the model exhibits only a slight diamagnetism. Below T_c, if a small homogeneous magnetic field is applied to the surface of the 2-dimensional Bose gas, only a very small fraction (given by (5.17)) of this field penetrates : as the temperature decreases to zero, the expulsion becomes complete. (Any consideration of penetration effects at the surface is, of course, outside the scope of this section).

Once the applied field exceeds some value, H_c, it penetrates the Bose gas as a homogeneous field, with an induction $B \approx H - H_c$. Thus there is a critical field, H_c, given by Eq. (5.21), such that application of a field greater than H_c destroys the superconducting properties of the model.

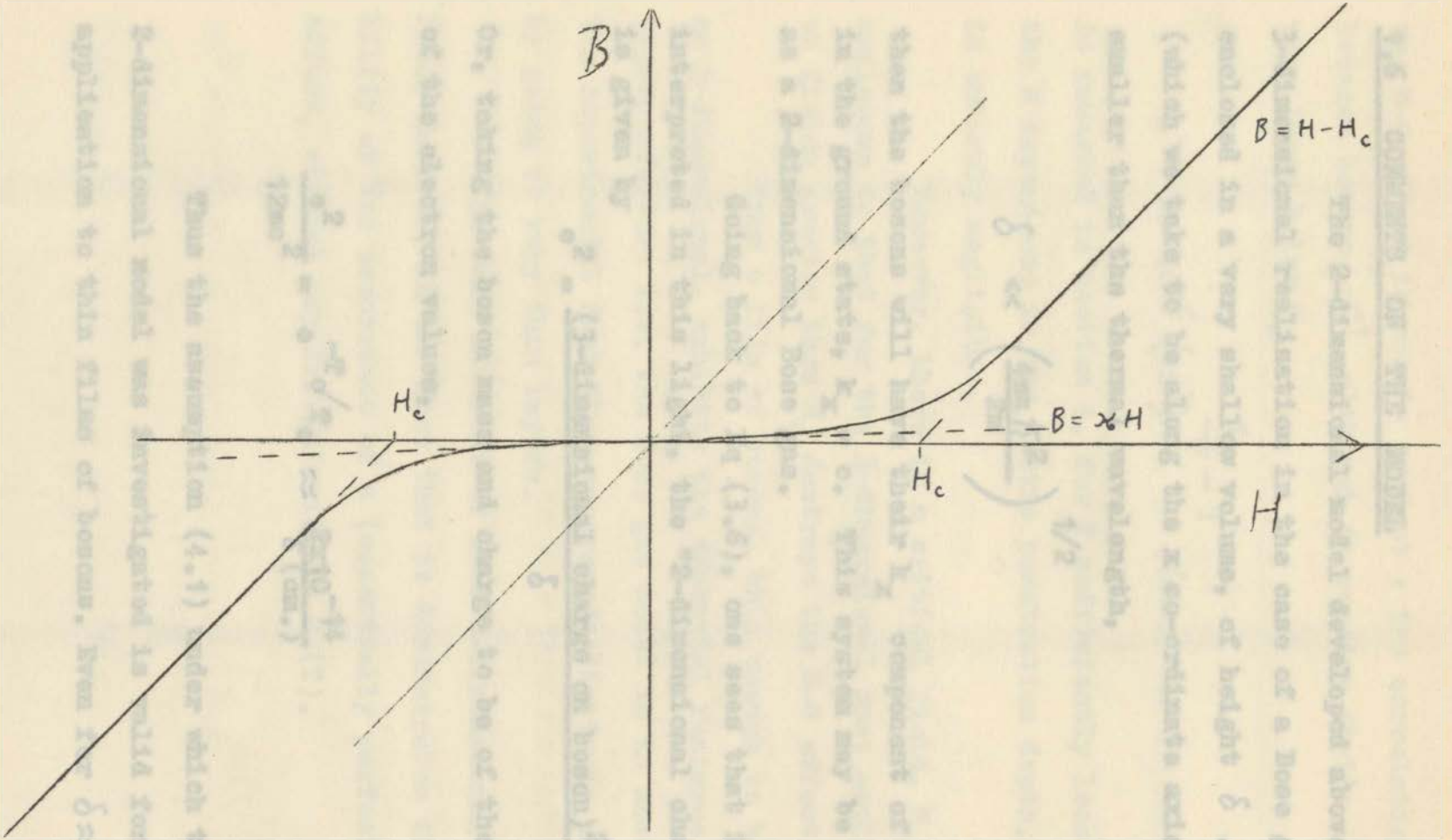


Fig. 4

1.6 COMMENTS ON THE MODEL

The 2-dimensional model developed above has a 3-dimensional realization in the case of a Bose gas enclosed in a very shallow volume, of height δ . If δ (which we take to be along the x co-ordinate axis) is smaller than the thermal wavelength,

$$\delta \ll \left(\frac{4\pi a \hbar^2}{2m}\right)^{1/2} \tag{6.1}$$

then the bosons will have their k_x component of momentum in the ground state, $k_x = 0$. This system may be considered as a 2-dimensional Bose gas.

Going back to Eq (3.6), one sees that if it is interpreted in this light, the "2-dimensional charge", e, is given by

$$e^2 = \frac{(\text{3-dimensional charge on boson})^2}{\delta} \tag{6.2}$$

Or, taking the boson mass and charge to be of the order of the electron values,

$$\frac{e^2}{12mc^2} = e^{-T_0/T_c} \approx \frac{2\times10^{-14}}{\delta\,(\text{cm.})} \tag{6.3}$$

Thus the assumption (4.1) under which the 2-dimensional model was investigated is valid for any application to thin films of bosons. Even for $\delta \approx 10^{-8}$ cm.,

the M-O effect is nearly perfect : the correlation length between bosons, μ^{-1}, although it remains finite, becomes very large below T_c

$$\mu^{-1} \approx 10^{-6} \left(10^{3}\right)^{\frac{T_c}{T} - 1} \quad (cm.) \tag{6.4}$$

As remarked in section 4, for T sufficiently less than T_c the R dependence in the static penetration depth, Eq (4.16), is entirely negligible.

Moreover, there is a critical field, H_c, analogous to that for the 3-dimensional gas; application of fields greater than H_c destroys the M-O effect.

Thus a film of bosons, thin enough to be considered as 2-dimensional, exhibits the essential features of a superconductor: i.e. the Bose gas model is in accord with the experimental fact that superconductivity is not destroyed by going to very thin layers.

The main interest of this 2-dimensional model lies, however, in the fact that it demonstrates the possibility of the occurrence of a (essentially perfect) M-O effect, without any irregularity in $C_V(T)$.

APPENDIX TO 1.5

CALCULATION OF M (B) FOR FINITE TEMPERATURES

In this Appendix, we derive the expressions (5.16) and (5.19) for M in the limit $x \ll 1$.

Introducing σ,

$$\sigma \equiv \frac{\mu}{\mu_o B} \quad (<1) \tag{I.1}$$

equation (5.3) can be rewritten as

$$n\lambda^2 = \sum_{i=1}^{\infty} \frac{e^{ix\sigma}}{i} \left(\frac{ix}{\sinh(ix)} - e^{-ix} \right) + \sum_{i=1}^{\infty} \frac{e^{-ix(1-\sigma)}}{i} \tag{I.2}$$

The expression has been put in this form for mathematical convenience - since $x \ll 1$, we can replace sums over i by integrals, provided they converge at the lower limit. Such is the case for the first term in (I.2), while the second term is easily summed.

$$n\lambda^2 = \int_0^{\infty} \frac{di}{i} e^{ix\sigma} \left\{ \frac{ix}{\sinh(ix)} - e^{-ix} \right\} - \ln \left[1 - e^{-x(1-\sigma)} \right] \tag{I.3}$$

Defining z,

$$z \equiv \frac{1}{2}(1-\sigma) \tag{I.4}$$

we simplify the logarithmic term, and change the variable of integration, to get

$$n\lambda^2 = \int_0^\infty dt\, e^{-zt}\left(\frac{1}{1-e^{-t}} - \frac{1}{t}\right) - \ln 2zx \qquad (I.5)$$

Making use of the facts (see e.g. Whittaker and Watson 1946)

$$\int_0^\infty \frac{dt}{t}\left(e^{-t} - e^{-zt}\right) = \ln z \qquad (I.6)$$

$$\int_0^\infty dt\left(\frac{e^{-t}}{t} - \frac{e^{-zt}}{1-e^{-t}}\right) = \psi(z) \qquad (I.7)$$

where $\psi(z)$ is the logarithmic derivative of the gamma function $\Gamma(z)$, we have

$$n\lambda^2 = -\psi(z) - \ln 2x \qquad (I.8)$$

Finally, noting that $n\lambda^2 = T_o/T$ (Eq (2.10)), we get z in terms of the field B by

$$\ln \frac{B}{B_1} = -\psi(z) \qquad (I.9)$$

where B_1 is introduced for formal convenience :

$$2\alpha\mu_o B_1 = e^{-T_o/T} \qquad (I.10)$$

We now return to Eq (5.2) for ω , and reduce it in a similar manner.

$$-a\lambda^2\omega - \sum_{i=1}^{\infty} \frac{e^{-i2xz}}{i^2} (1+ix)$$

$$= \sum_{i=1}^{\infty} \frac{e^{ix\sigma}}{i^2} \left(\frac{ix}{\sinh ix} - e^{-ix} [1+ix] \right) \qquad (I.11)$$

$$= 2x \int_0^{\infty} \frac{dt}{t} e^{-zt} \left(\frac{1}{e^t - 1} - \frac{1}{t} + \frac{1}{2} \right) \qquad (I.12)$$

This integral is Binets[9] first expression for $\Phi(z)$, the correction to the Stirling approximation to $\ln \Gamma(z)$: i.e.

$$-a\lambda^2\omega = \sum_{i=1}^{\infty} \frac{e^{-i2xz}}{i^2} (1+ix) + 2x\,\Phi(z) \qquad (I.13)$$

with

$$\Phi(z) = \ln \Gamma(z) - \left[(z-\tfrac{1}{2}) \ln z - z + \tfrac{1}{2} \ln 2\pi \right] \qquad (I.14)$$

The magnetization, M, is given by Eq (5.4). Bearing in mind that we have $\omega(x,z)$ rather than $\omega(B)$, we use the definitions of x and z, (5.8) and (I.4), to get

$$M = -\frac{x}{B} \left[\left(\frac{\partial}{\partial x} \right)_z + \frac{1-2z}{2x} \left(\frac{\partial}{\partial z} \right)_x \right] \omega(x,z) \qquad (I.15)$$

Carrying out this operation,

$$\left(\frac{\alpha\lambda^2 B}{x}\right) M = -\sum_{i=1}^{\infty} xe^{-i2xz} + 2\Phi(z)+(1-2z)\Phi'(z) \qquad (I.16)$$

where $\Phi'(z)$ is the derivative of $\Phi(z)$. Performing the summation in (I.16), and simplifying the result,

$$-\frac{\lambda^2}{\mu_o} M = f(z) \qquad (I.17)$$

$$f(z) = \frac{1}{2z} - 2\Phi(z) - (1-2z)\Phi'(z) \qquad (I.18)$$

Thus M is given as a function of z, and thence of B, by Eqs (I.17) and (I.9). It remains to eliminate z between these equations. We do this separately for (i) $z > 1$ and (ii) $z < 1$, to get Eqs (5.16) and (5.19) respectively.

(i) $z > 1$

An asymptotic expansion for $\Phi(z)$, and thence for $\Phi'(z)$ and $\psi(z)$, is given in terms of the Bernoulli numbers by Binets second expression for $\Phi(z)$. This leads to

$z>1$

$$f(z) = \frac{1}{6z}\left(1+\frac{1}{2z}+\frac{2}{15z^2}+\ldots\right) \qquad (I.19)$$

$$-\psi(z) = -\ln z + \frac{1}{2z}\left(1+\frac{1}{6z}+\ldots\right) \qquad (I.20)$$

From (I.9) and (I.20) we see that for $B \leq B_1$, $z>1$. Expanding z as a power series in (B/B_1), and then substituting into (I.19), we get

$$-\frac{\lambda^2 M}{\mu_o} = \frac{1}{6}\,\frac{B}{B_1}\left(1 - \frac{3}{40}\,\left(\frac{B}{B_1}\right)^2 + \ldots\right) \qquad \text{(I.21)}$$

which leads to (5.16) for $B \leq B_1$.

(ii) $z < 1$

Using an expansion for $\ln \Gamma(z)$ in powers of z, we can find

$z < 1$

$$f(z) = \frac{1}{z} + 2\ln z + (C - 1 + \ln 2\pi) + \mathcal{O}(z) \qquad \text{(I.22)}$$

$$-\psi(z) = \frac{1}{z} + C + \mathcal{O}(z) \qquad \text{(I.23)}$$

where C is the Euler-Mascheroni constant. This region of z is seen to be pertinent to $B >> B_1$, where we derive

$$-\frac{\lambda^2 M}{\mu_o} = \ln\frac{B}{B_1}\left\{1 - \frac{2\ln\left[\left(\frac{e}{2\pi}\right)^{1/2}\left(\ln\frac{B}{B_1} - C\right)\right]}{\ln\frac{B}{B_1}} + \ldots\right\} \qquad \text{(I.24)}$$

and thence Eq (5.19).

CHAPTER II

NON GAUGE-INVARIANT APPROXIMATIONS IN A MAGNETIC SYSTEM.

2.1 : A TECHNIQUE FOR NON GAUGE-INVARIANT APPROXIMATIONS.

The Meissner-Ochsenfeld effect is a particular form of linear response of a system to an applied inhomogeneous magnetic field. A general procedure for calculating such a response is outlined in this section. An identity, derived from the requirement of gauge-invariance, is then mentioned and a new technique for dealing with approximations which violate this identity is given.

Consider a system of N particles with masses m_i and charges e_i, which in the absence of magnetic fields is described by the hamiltonian

$$H = \sum_{i=1}^{N} \frac{(\underset{\sim}{p}_i)^2}{2m_i} + V(\underset{\sim}{x}_1, \underset{\sim}{x}_2, \ldots\ldots\ldots, \underset{\sim}{x}_N) \qquad (1.1)$$

Such a system includes, in principle, a very accurate model of a solid : namely a system of N_1 nuclei and N_2 electrons ($N_1 + N_2 = N$) interacting with each other via Coulomb forces.

A magnetic field, with vector potential $\underset{\sim}{A}$, is now introduced into the hamiltonian(*) by means of the transformation

---

*) This accounts for the orbital motion of charges; other possible terms, depending explicitly on the field strength $\underset{\sim}{B}$, would describe magnetic moment of spins, etc., and will not be considered.

$$\underset{\sim}{p}_i \longrightarrow \underset{\sim}{p}_i - \frac{e_i}{c} \underset{\sim}{A}(\underset{\sim}{x}_i) \tag{1.2}$$

$\underset{\sim}{A}(\underset{\sim}{x})$ may be expanded in Fourier components:

$$\underset{\sim}{A}(\underset{\sim}{x}) = \sum_{\underset{\sim}{q}} \underset{\sim}{A}(\underset{\sim}{q}) \; e^{i\underset{\sim}{q}.\underset{\sim}{x}} \tag{1.3}$$

where there is a reality condition giving $\underset{\sim}{A}^{*}(\underset{\sim}{q})$ as

$$\underset{\sim}{A}^{*}(\underset{\sim}{q}) = \underset{\sim}{A}(-\underset{\sim}{q}) \tag{1.4}$$

We shall restrict ourselves to one Fourier component; this is permissible for calculating the linear response. The associated magnetic field is

$$\underset{\sim}{B}(\underset{\sim}{q}) = i \, \underset{\sim}{q} \times \underset{\sim}{A}(\underset{\sim}{q}) \tag{1.5}$$

The current density operator, $\underset{\sim}{j}$, is given by the variational derivative of the transformed hamiltonian H(A).

$$\underset{\sim}{j} = - c \; \frac{\partial H(A)}{\partial \underset{\sim}{A}} \tag{1.6}$$

The operator is thus

$$\underset{\sim}{j}(\underset{\sim}{q}) = \underset{\sim}{j}^{0}(\underset{\sim}{q}) + \underset{\sim}{j}^{1}(\underset{\sim}{q}) \tag{1.7}$$

with the definitions

$$\underset{\sim}{j}^{o}(\underset{\sim}{q}) = \sum_i \frac{e_i}{2m_i}\left(\underset{\sim}{p}_i e^{-i\underset{\sim}{q}.\underset{\sim}{x}_i} + e^{-i\underset{\sim}{q}.\underset{\sim}{x}_i}\underset{\sim}{p}_i\right)$$

$$\underset{\sim}{j}^{1}(\underset{\sim}{q}) = \sum_i \frac{e_i^2}{m_i c}\,\underset{\sim}{A}(\underset{\sim}{q}) \qquad (1.8)$$

The total current density, $\underset{\sim}{i}(\underset{\sim}{q})$, is then found from the distribution function, F(H(A)) of the system :

$$\underset{\sim}{i} = \text{Trace}\left\{\underset{\sim}{j}\ F\right\} \qquad (1.9)$$

The following analogue of the Taylor expansion, for matrix functions, (Schafroth 1951) is now used. In the representation in which the operator Λ_o is diagonal

$$\Lambda_o\,|n\rangle = \lambda_n\,|n\rangle \qquad (1.10)$$

the matrix elements of a function $F_o(\Lambda_o+\varepsilon\Lambda_1)$ of a perturbed operator are given by

$$\langle n|F_o(\Lambda_o+\varepsilon\Lambda_1)|n'\rangle = \langle n|n'\rangle F_o(\lambda_n) + \varepsilon\langle n|\Lambda_1|n'\rangle F_1(\lambda_n,\lambda_{n'})$$
$$+ \varepsilon^2 \sum_{n''} \langle n|\Lambda_1|n''\rangle\cdot\langle n''|\Lambda_1|n'\rangle F_2(\lambda_n,\lambda_{n'},\lambda_{n''})$$
$$+ \mathcal{O}(\varepsilon^3) \qquad (1.11)$$

Here $F_r(x_0, \ldots, x_r)$ are the difference quotients of $F_0(x_0)$ given by

$$F_r(x_0, \ldots, x_r) = \sum_{i=0}^{r} \frac{F_0(x_i)}{\prod_{i \neq j} (x_i - x_j)} \tag{1.12}$$

This theorem may now be applied to Eq (1.9) to get an expression for the total current density in terms of the field-free eigenvectors and eigenvalues of the field-free hamiltonian (1.1):

$$H \; | k > \; = \; E_k \; | k > \tag{1.13}$$

The current density, up to terms linear in $\underset{\sim}{A}$, is

$$i_\mu(\underset{\sim}{q}) = c \sum_{\nu=1}^{3} J_{\mu\nu}(\underset{\sim}{q}) A_\nu(\underset{\sim}{q}) \tag{1.14}$$

with the quantity $J_{\mu\nu}$ given by

$$J_{\mu\nu} = S_{\mu\nu} - L \delta_{\mu\nu} \tag{1.15}$$

$$L = \sum_i \frac{e_i^2}{m_i c^2} \tag{1.16}$$

$$S_{\mu\nu} = -\frac{1}{c^2} \sum_{\underset{\sim}{k}, \underset{\sim}{k}'} \langle k | j_\mu^{\,o}(\underset{\sim}{q}) | k' \rangle \langle k' | j_\nu^{\,o}(-\underset{\sim}{q}) | k \rangle F_1(E_k, E_{k'}) \tag{1.17}$$

At this stage we remark that the vector potential $\underset{\sim}{A}(\underset{\sim}{x})$ is not uniquely determined by $\underset{\sim}{B}(\underset{\sim}{x})$, but only up to a gauge transformation G_Λ :

$$G_\Lambda\,(\underset{\sim}{A}(\underset{\sim}{x})) = \underset{\sim}{A}(\underset{\sim}{x}) + \text{grad}\ \Lambda\,(\underset{\sim}{x}) \qquad (1.18)$$

with $\Lambda(\underset{\sim}{x})$ an arbitrary scalar function. Since the choice of gauge has no physical meaning, our theory has to obey the requirement that all physical results are <u>invariant</u> under the gauge transformation G_Λ . This corresponds to demanding that physical quantities be represented by gauge-covariant operators: such an operator ($O(\underset{\sim}{A})$ say) is defined by the requirement that for any scalar function Λ there exists a unitary transformation U_Λ such that

$$U_\Lambda^{\dagger}\ O(\underset{\sim}{A})\ U_\Lambda = O(\underset{\sim}{A} + \text{grad}\ \Lambda) \qquad (1.19)$$

The requirement of gauge-invariance is now seen to impose on Eq(1.14) the condition that (for an isotropic medium)

$$\sum_\mu q_\mu J_{\mu\nu} = 0\ ;\ \sum_\nu J_{\mu\nu}\, q_\nu = 0 \qquad (1.20)$$

That is to say L and $S_{\mu\nu}$ are related by the gauge identity

$$G \equiv \sum_{\mu,\nu} \frac{q_\mu q_\nu}{q^2}\ S_{\mu\nu} - L = 0 \qquad (1.21)$$

This identity was first derived by Buckingham (1951).

It is often desirable to eliminate the vector potential $\underset{\sim}{A}$ from Eq (1.14) in favour of the physical quantity $\underset{\sim}{B}$. Introducing the magnetization, $\underset{\sim}{M}$ ($\underset{\sim}{i}$ = c curl $\underset{\sim}{M}$), and using equations (1.5), (1.14), (1.15) and (1.21), we get directly

$$M_\mu(\underset{\sim}{q}) = \frac{1}{2q^2}\left\{\sum_\mu S_{\mu\mu} - 3L\right\} B_\mu(\underset{\sim}{q}) \qquad (1.22)$$

The linear magnetic response may thus be characterized by a "kernel" function, K(q), such that

$$M_\mu(\underset{\sim}{q}) = K(q)\, B_\mu(\underset{\sim}{q}) \qquad (1.23)$$

A number of alternative expressions for K(q) may be given by use of the identity (1.21); in particular, if one uses (1.21) to eliminate L from (1.22), one gets the "normal form"

$$K_B(q) = \frac{1}{q^2} \sum_{\mu,\nu}\left(\frac{1}{2}\,\delta_{\mu\nu} - \frac{3}{2}\,\frac{q_\mu q_\nu}{q^2}\right) S_{\mu\nu} \qquad (1.24)$$

In general, (1.21) generates a set of alternative expressions for K(q), which can be written in terms of a parameter α as

$$K(q) = K_B(q) + \alpha\,\frac{G(q)}{q^2} \qquad (1.25)$$

(For example the London gauge, div $\underset{\sim}{A}$ = 0, corresponds to the choice α = 1).

If $S_{\mu\nu}(q)$ and $G(q)$ are calculated from a gauge-covariant hamiltonian H, then of course $G \equiv 0$, and all the forms (1.25) are identical. However, if one evaluates $S_{\mu\nu}$ by using the eigenfunctions of an approximate (field-free) hamiltonian $\hat{H}$, thereby losing gauge-covariance, then in general the resulting approximate $\hat{S}_{\mu\nu}$ violates the identity (1.21). That is $\hat{G} \neq 0$, and one gets an indeterminate result $\hat{K}$ for (1.25), depending linearly on the parameter α

$$\hat{K}(\alpha) = \hat{K}_B + \alpha \frac{\hat{G}}{q^2} \tag{1.26}$$

However, there is still one well-defined value of α, α_1 say, for which $\hat{K}(\alpha_1)$ is <u>closest</u> to the exact value K.

If the difference between true and approximate hamiltonians be characterized by an expansion parameter ε

$$H = \hat{H} + \varepsilon H' \tag{1.27}$$

then the exact K may be expanded around $\hat{K}(\alpha)$ in powers of ε

$$K = \hat{K}(\alpha) + \varepsilon \hat{K}'(\alpha) + \varepsilon^2 \hat{K}''(\alpha) + \ldots \tag{1.28}$$

We now choose $\alpha = \alpha_1$ by demanding that

$$\hat{K}'(\alpha_1) = 0 \tag{1.29}$$

Thus we have

$$\hat{K}(\alpha_1) - K = \mathcal{O}(\varepsilon^2) \tag{1.30}$$

i.e. the approximate kernel is as good as any other physical quantity in the same degree of approximation in H'. The ambiguity due to lack of gauge-covariance has entirely disappeared.

This technique is illustrated in section 2.2 by a simple example (electrons moving in a weak periodic potential). It is then applied to the more difficult task of evaluating the M-O effect in the Bogoljubov theory in Chapter III.

It must be noted that the above method cannot be used with a non gauge-covariant hamiltonian $\hat{H}$, unless $\hat{H}$ is itself defined as an approximation to an exact, gauge-covariant hamiltonian. This is the case in the Bogoljubov scheme.

2.2 : A SIMPLE APPLICATION: PEIERLS DIAMAGNETISM.

In this section, we consider the magnetic behaviour of electrons moving in a periodic lattice. The field-free hamiltonian for these electrons is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{r})\right)\Psi_{\underset{\sim}{k}}(\underset{\sim}{r}) = E(\underset{\sim}{k})\Psi_{\underset{\sim}{k}}(\underset{\sim}{r}) \qquad (2.1)$$

where the potential $V(\underset{\sim}{r})$ has the translational symetry of the lattice : i.e.

$$V(\underset{\sim}{r} + \underset{\sim}{\rho}_n) = V(\underset{\sim}{r}) \qquad (2.2)$$

$\underset{\sim}{\rho}_n$ being any one of the lattice vectors.

The electron wave-functions then have the form (Bloch 1928)

$$\Psi_{\underset{\sim}{k}}(\underset{\sim}{r}) = e^{i\underset{\sim}{k}.\underset{\sim}{r}}\, u_{\underset{\sim}{k}}(\underset{\sim}{r}) \qquad (2.3)$$

with the function $u_{\underset{\sim}{k}}(\underset{\sim}{r})$ having the same periodicity as the lattice.

In the theory of metals, approximate wave functions

$$\Psi^{(o)}_{\underset{\sim}{k}}(\underset{\sim}{r}) = e^{i\underset{\sim}{k}.\underset{\sim}{r}}\, u_o(\underset{\sim}{r}) \qquad (2.4)$$

are frequently employed when dealing with a weak potential. The energy values in the approximation are

$$E^{(o)}(k) = \frac{\hbar^2 k^2}{2m} + E_o \qquad (2.5)$$

and E_o, $u_o(\underset{\sim}{r})$ are determined from the equation

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + V(\underset{\sim}{r})\right) u_o(\underset{\sim}{r}) = E_o\, u_o(\underset{\sim}{r}) \qquad (2.6)$$

The expansion parameter ε in this scheme is defined by

$$H = H^{(o)} + \varepsilon H^{(1)} \qquad (2.7)$$

where H is the gauge-covariant hamiltonian (2.1), and $H^{(o)}$ the approximate hamiltonian corresponding to the above eigenvectors and eigenvalues.

This approximation scheme is an improvement on the free electron one, in that the factor $u_o(\underset{\sim}{r})$ in Eq(2.4) contains the essential features due to the lattice. Quantities such as the cohesive forces in metals due to conduction electrons may be calculated satisfactorarily by use of the method. However, since the approximation is better for small wave numbers $\underset{\sim}{k}$ than for large ones, it may be expected to lead to non gauge-invariant results for magnetic quantities : this is found to be the case. The difficulty is then overcome by applying the technique described in the preceeding section.

* * * * *

We begin the calculation of the zeroth order kernel, $K^{(o)}(q)$, for this example, by writing down the expression for the matrix elements of $\underset{\sim}{j}^{(o)}(\underset{\sim}{q})$:

$$\langle k | j_\mu^{\,o}(\underset{\sim}{q}) | k' \rangle = \frac{e}{2m} (k+k')_\mu \int d\underset{\sim}{r} \, |u_o(\underset{\sim}{r})|^2 \, e^{i(\underset{\sim}{k}'-\underset{\sim}{k}-\underset{\sim}{q}).\underset{\sim}{r}} \qquad (2.8)$$

$$\equiv \frac{e}{2m} (k+k')_\mu \, \chi(\underset{\sim}{k}'-\underset{\sim}{k}-\underset{\sim}{q}) \qquad (2.9)$$

(Use has been made of the fact that $u_o(\underset{\sim}{r})$ must be either even or odd in $\underset{\sim}{r}$.)

Then, after the substitution $\underset{\sim}{k} \rightarrow \underset{\sim}{k} - \frac{\underset{\sim}{k}'+\underset{\sim}{q}}{2}$, $\underset{\sim}{k}' \rightarrow \underset{\sim}{k} + \frac{\underset{\sim}{k}'+\underset{\sim}{q}}{2}$, Eq (1.17) gives $S_{\mu\nu}^{(o)}$ as

$$S_{\mu\nu}^{(o)} = -\frac{e^2}{m^2c^2} \sum_{\underset{\sim}{k}\,\underset{\sim}{k}'} k_\mu k_\nu \left|\chi(\underset{\sim}{k}')\right|^2 F_1 \left\{ \frac{(\underset{\sim}{k}+\frac{\underset{\sim}{k}'+\underset{\sim}{q}}{2})^2}{2m}, \frac{(\underset{\sim}{k}-\frac{\underset{\sim}{k}'+\underset{\sim}{q}}{2})^2}{2m} \right\} \qquad (2.10)$$

with $F_o(E)$ the Fermi distribution function.

At this stage, some simplifying assumptions are made as to the nature of $|u_o(\underset{\sim}{r})|^2$: since this calculation is done to illustrate the technique developed in section 2.1, such mathematical simplifications are quite justified. We put

$$|u_o(\underset{\sim}{r})|^2 = C \left\{ 1+\beta \sum_{\underset{\sim}{\rho}_n} e^{-(\underset{\sim}{r}-\underset{\sim}{\rho}_n)^2/b^2} \right\} \qquad (2.11)$$

This function provides a two-parameter fit (in terms of a strength parameter β, and a range b) to the solution of Eq. (2.6) for any specific $V(\underset{\sim}{r})$: the free electron case corresponds to the limit $\beta \to 0$. We also assume $b \ll a$, a being the lattice spacing. The normalization constant C is given by

$$C \int |u_o(\underset{\sim}{r})|^2 \, d\underset{\sim}{r} = CV \left(1+\beta \left[\frac{\sqrt{\pi}\, b}{a}\right]^3\right) = 1 \qquad (2.12)$$

Substitution of Eq. (2.11) into (2.8) leads, in the limit of infinite volume, to the result

$$\chi(\underset{\sim}{k}) = CV\left\{\delta(\underset{\sim}{k}) + \beta\left(\frac{\sqrt{\pi}\, b}{a}\right)^3 \sum_{\underset{\sim}{\kappa}_n} \delta(\underset{\sim}{k}-\underset{\sim}{\kappa}_n)\, e^{-\frac{k^2 b^2}{4}}\right\} \qquad (2.13)$$

and

$$\left|\chi(\underset{\sim}{k})\right|^2 = \delta(\underset{\sim}{k}) + \left[CV\beta\left(\frac{\sqrt{\pi}\, b}{a}\right)^3\right]^2 \sum_{\underset{\sim}{\kappa}_n \neq 0} \delta(\underset{\sim}{k}-\underset{\sim}{\kappa}_n) e^{-\frac{k^2 b^2}{2}} \qquad (2.14)$$

The sum over $\underset{\sim}{\kappa}_n$ extends over all vectors of the reciprocal lattice : $\delta(\underset{\sim}{k})$ is defined to be 1 if $\underset{\sim}{k} = 0$, zero otherwise.

Comparison of Eqs (2.10) and (2.14) now shows that $S_{\mu\nu}^{(o)}$ can be separated into two parts, the first $\left(S_{\mu\nu}^{(o)}(1)\right)$ corresponding to free electrons and the second $\left(S_{\mu\nu}^{(o)}(2)\right)$ containing perturbation effects due to the lattice

$$S_{\mu\nu}^{(o)}(1) = -\frac{e^2}{m^2c^2}\sum_{\underset{\sim}{k}} k_\mu k_\nu \; F_1\left\{\frac{(\underset{\sim}{k}+\frac{\underset{\sim}{q}}{2})^2}{2m}, \frac{(\underset{\sim}{k}-\frac{\underset{\sim}{q}}{2})^2}{2m}\right\} \qquad (2.15)$$

$$S_{\mu\nu}^{(o)}(2) = -\frac{e^2}{m^2c^2}\left\{\frac{\beta(\frac{\pi b}{a})^3}{1+\beta(\frac{\pi b}{a})^3}\right\}^2 \sum_{\underset{\sim}{k}}\sum_{\underset{\sim}{\chi}_n\neq 0} k_\mu k_\nu \, e^{-\frac{\chi_n^2 b^2}{2}} \times$$

$$\times F_1\left\{\frac{(\underset{\sim}{k}+\frac{\underset{\sim}{\chi}_n+\underset{\sim}{q}}{2})^2}{2m}, \frac{(\underset{\sim}{k}-\frac{\underset{\sim}{\chi}_n+\underset{\sim}{q}}{2})^2}{2m}\right\} \qquad (2.16)$$

The expression for $L^{(o)}$, Eq (1.16), is independent of the approximation used

$$L^{(o)} = L = \frac{e^2}{mc^2} N \qquad (2.17)$$

Eqs (2.15) and (2.17) now describe the Landau (1930) diamagnetism of a free electron gas. It is easy to verify that

$$\sum_{\mu,\nu} \frac{q_\mu q_\nu}{q^2} S_{\mu\nu}^{(o)}(1) - L^{(o)} \equiv 0 \qquad (2.18)$$

$$\lim_{q\to o} \frac{1}{2q^2} \sum_{\mu\nu}\left(\delta_{\mu\nu} - \frac{3q_\mu q_\nu}{q^2}\right) S_{\mu\nu}^{(o)}(1) = -\frac{e^2N}{4mc^2}\cdot\frac{1}{k_F^2} \qquad (2.19)$$

(We have introduced the Fermi wave number, k_F, which is related to the number of electrons by $N = Vk_F^3/3\pi^2$.)

Corresponding equations with $S_{\mu\nu}^{(o)}(2)$ may be obtained by :- (a) assuming $2k_F \lesssim \varkappa_1$, i.e. $k_F a \lesssim \pi$ (if there are $\mathcal{N}$ conduction electrons per lattice ion, this corresponds to the assumption $\mathcal{N} \lesssim \pi/3$), and (b) replacing the sum over reciprocal lattice vectors $\varkappa_n$ by $(\frac{a}{2\pi})^3 \int d\varkappa$

(this is permissible for $b/a \ll 1$, which has already been assumed). The consequent results are

$$\lim_{q \to o} \sum_{\mu\nu} \frac{q_\mu q_\nu}{q^2} S_{\mu\nu}^{(o)}(2) = \frac{\pi\sqrt{2\pi}}{12} \cdot \frac{e^2 N}{mc^2} \cdot \frac{\beta^2 (\frac{b}{a})^3}{\left[1+\beta(\frac{\sqrt{\pi}b}{a})^3\right]^2} \times \left\{1 + O(\tfrac{b}{a})^2\right\} \qquad (2.20)$$

$$\lim_{q \to o} \frac{1}{q^2} \sum_{\mu\nu} (\tfrac{1}{2}\delta_{\mu\nu} - \tfrac{3}{2}\frac{q_\mu q_\nu}{q^2}) S_{\mu\nu}^{(o)}(2)$$

$$= \frac{\pi\sqrt{2\pi}}{20} \cdot \frac{e^2 N}{mc^2} \cdot b^2 \cdot \frac{\beta^2 (\frac{b}{a})^3}{\left(1+\beta(\frac{\sqrt{\pi}b}{a})^3\right)^2} \left\{1 + O(\tfrac{b}{a})\right\} \qquad (2.21)$$

Collecting all these results, and neglecting terms of relative order $(b/a)^2$ and $\beta^2 (b/a)^3$,

$$\lim_{q \to o} \frac{G^{(o)}}{q^2} = \sigma_1 \beta^2 \left(\frac{b}{a}\right)^3 \times \frac{L}{q^2} \tag{2.22}$$

$$\lim_{q \to o} K_B^{(o)} = - \frac{L}{4k_F^2} \left\{ 1 - \sigma_2 \beta^2 \left(\frac{b}{a}\right)^3 (bk_F)^2 \right\} \tag{2.23}$$

with numerical factors $\sigma_1 = \pi \sqrt{2\pi} / 12$, $\sigma_2 = \pi \sqrt{2\pi} / 5$.

Thus the approximate eigenfunctions have led to a result which violates the gauge identity $G \equiv 0$. Referring back to Eq (1.26) we see that $K^{(o)}$ will now depend on a parameter α :

$$K^{(o)}(\alpha) = K_B^{(o)} + \alpha \frac{G^{(o)}}{q^2} \tag{2.24}$$

For instance the London gauge, $\alpha = 1$, would imply that the system is an anti-superconductor!

The technique described in section 2.1 is now applied to choose a best approximate kernel from the set (2.24) : $\alpha = \alpha_1$ is selected according to the criterion that $K^{(1)}(\alpha_1)$ shall vanish.

The function $S_{\mu\nu}^{(1)}$, and thence $K^{(1)}(\alpha)$, is found by extending Eq (1.11) to get

$$S_{\mu\nu}^{(1)}(q) = - \frac{1}{c^2} \sum_{\underset{\sim}{k}, \underset{\sim}{k}', \underset{\sim}{k}''} \langle k | j_\mu^{\,o}(\underset{\sim}{q}) | k' \rangle \Big(\langle k' | H^{(1)} | k'' \rangle \times k'' | j_\nu^{\,o}(-\underset{\sim}{q}) | k \rangle + \langle k' | j_\nu^{\,o}(-\underset{\sim}{q}) | k'' \rangle \times k'' | H^{(1)} | k \rangle \Big) \times F_2\big(E(k), E(k'), E(k'')\big) \tag{2.25}$$

The matrix elements of $H^{(1)}$ are readily found from Eq (2.7):

$$\langle k|H^{(1)}|k'\rangle = \frac{i\hbar}{4m}\int \underset{\sim}{dr}\; e^{-i(\underset{\sim}{k}-\underset{\sim}{k}')\cdot\underset{\sim}{r}}\,(\underset{\sim}{k}-\underset{\sim}{k}')\cdot\underset{\sim}{\nabla}\,\left|u_o(\underset{\sim}{r})\right|^2 \qquad (2.26)$$

or, using the particular form (2.11),

$$\langle k|H^{(1)}|k'\rangle = -\frac{\pi^{3/2}\hbar^2}{4m}\,\beta\,\frac{b}{a^3}\,VC\sum_{\underset{\sim}{\varkappa}_n}(\varkappa_n b)^2\, e^{-\frac{\varkappa_n^2 b^2}{4}}\,\delta(\underset{\sim}{k}-\underset{\sim}{k}'-\underset{\sim}{\varkappa}_n) \qquad (2.27)$$

Thus, substituting from Eqs (2.9), (2.13) and (2.27) into (2.25), we get

$$S_{\mu\nu}^{(1)}(q) = 2\left(\frac{e}{2mc}\right)^2\sum_{\underset{\sim}{k}\underset{\sim}{k}'\underset{\sim}{k}''}\sum_{\underset{\sim}{\varkappa}_n\underset{\sim}{\varkappa}_{n'}}\frac{\pi^3}{4m}\,\beta^2\left(\frac{b}{a}\right)^4\frac{(CV)^3}{a^2}(\varkappa_n b)^2\, e^{-(\varkappa_n^2+\varkappa_{n'}^2)\frac{b^2}{4}}\times$$

$$\times\,(k+k')_\mu(k+k'')_\nu\left\{\begin{array}{l}\delta(\underset{\sim}{k}-\underset{\sim}{k}'+\underset{\sim}{q})\,\delta(\underset{\sim}{k}'-\underset{\sim}{k}''+\underset{\sim}{\varkappa}_n)\;\delta(\underset{\sim}{\varkappa}_n-\underset{\sim}{\varkappa}_{n'})\\ +\,\delta(\underset{\sim}{k}-\underset{\sim}{k}''+\underset{\sim}{q})\,\delta(\underset{\sim}{k}'-\underset{\sim}{k}''-\underset{\sim}{\varkappa}_n)\,\delta(\underset{\sim}{\varkappa}_n-\underset{\sim}{\varkappa}_{n'})\end{array}\right\}F_2\left(\frac{k^2}{2m},\frac{k'^2}{2m},\frac{k''^2}{2m}\right) \qquad (2.28)$$

Making use of the fact that $S_{\mu\nu}$ is a symmetric tensor, this may be reduced, after some manipulation, to

$$S_{\mu\nu}^{(1)} = A \sum_{\underset{\sim}{\chi}_n} (\chi_n b)^2 \, e^{-\frac{\chi_n^2 b^2}{2}} \sum_{\underset{\sim}{k}} (k+\tfrac{q}{2})_\mu \, (k+\tfrac{\chi_n+q}{2})_\nu \times$$

$$\times F_2\left\{\frac{k^2}{2m}, \frac{(k+q)}{2m}, \frac{(k+\chi_n)^2}{2m}\right\} \qquad (2.29)$$

A is a constant,

$$A \equiv \frac{e^2}{mc^2} \cdot \frac{\pi^3}{m^2} \cdot \beta^2 \left(\frac{b}{a}\right)^4 \frac{(CV)^3}{a^2} \qquad (2.30)$$

We now proceed to evaluate $G^{(1)}/q^2$ and $K_B^{(1)}$ in the limiting case of $q \ll k_F$. First $G^{(1)}$ is found from

$$\lim_{q\to 0} \sum_{\mu\nu} S_{\mu\nu}^{(1)} \frac{q_\mu q_\nu}{q^2} = mA \sum_{\underset{\sim}{\chi}_n} (\chi_n b)^2 \, e^{-\frac{(\chi_n b)^2}{2}} \sum_{\underset{\sim}{k}} \times$$

$$\times \frac{(\underset{\sim}{k}\cdot\underset{\sim}{q})\left(\left[\underset{\sim}{k}-\frac{\underset{\sim}{\chi}_n}{2}\right]\cdot\underset{\sim}{q}\right)}{q^2 \, \underset{\sim}{\chi}_n \cdot \left(\underset{\sim}{k}-\frac{\underset{\sim}{\chi}_n}{2}\right)} \left[F_o'\left(\frac{k^2}{2m}\right) - F_1\left\{\frac{k^2}{2m}, \frac{(\underset{\sim}{k}-\underset{\sim}{\chi}_n)^2}{2m}\right\}\right] \qquad (2.31)$$

$$\approx m^2 A \sum_{\underset{\sim}{\chi}_n} (\chi_n b)^2 \, e^{-\frac{(\chi_n b)^2}{2}} \cdot \frac{2N}{\chi_n^2} \qquad (2.32)$$

A partial integration has been performed to reduce $F_o'(k^2/2m)$ to $F_o(k^2/2m)$. Replacing the sum over χ_n by an integral,

$$\lim_{q\to 0} \sum_{\mu\nu} S_{\mu\nu}^{(1)} \frac{q_\mu q_\nu}{q^2} \approx \frac{2}{(2\pi)^{3/2}} \, Nm^2 b^2 \left(\frac{a}{b}\right)^3 \qquad (2.33)$$

That is (since $L^{(1)} = 0$, $L^{(o)}$ being exact)

$$\lim_{q\to o} G^{(1)}/q^2 = \frac{\pi^2}{\sqrt{2\pi}} \beta^2 \left(\frac{b}{a}\right)^3 \times \frac{L}{q^2} \tag{2.34}$$

A similar, but more complicated, calculation gives

$$\lim_{q\to o} \sum_{\mu\nu} \left(\frac{1}{2}\delta_{\mu\nu} - \frac{3}{2}\frac{q_\mu q_\nu}{q^2}\right) S^{(1)}_{\mu\nu} \approx m^2 A \sum_{\underset{\sim}{\chi}_n} (\chi_n b)^2 \, e^{-\frac{(\chi_n b)^2}{2}} \times$$

$$\times \left\{\frac{N}{\chi_n^2} \cdot \frac{q^2}{k_F^2}\right\}\left\{-1 + \frac{2(\underset{\sim}{\chi}_n \cdot \underset{\sim}{q})^2}{\chi_n^2 q^2}\right\} \tag{2.35}$$

(The complications arise from the fact that we now have to consider terms up to order q^2/k_F^2.) Simplifying this expression, we get

$$\lim_{q\to o} K_B^{(1)} = -\frac{\pi^2}{6\sqrt{2\pi}} \beta^2 \left(\frac{b}{a}\right)^3 \times \frac{L}{k_F^2} \tag{2.36}$$

α_1 is now found from the condition

$$K^{(1)}(\alpha_1) = K_B^{(1)} + \alpha_1 \frac{G^{(1)}}{q^2} = 0 \tag{2.37}$$

Thence, for small q,

$$\alpha_1 = \frac{1}{6} \frac{q^2}{k_F^2} \tag{2.38}$$

Hence the above approximation scheme for electrons moving in a (weak) periodic potential finally gives a slightly modified Landau diamagnetism, with a kernel

$$K(q) = K^{(o)}(q, \alpha_1) \tag{2.39}$$

$$= -\frac{e^2 N}{4mc^2} \cdot \frac{1}{k_F^2} \left\{ 1 - \tau\beta^2 \left(\frac{b}{a}\right)^3 \left(1 + \mathcal{O}\left(\frac{b}{a}\right)^2\right) \right\} \tag{2.40}$$

(τ is a numerical constant, $\pi\sqrt{2\pi}/18$).

This is in qualitative agreement with the result first derived for a periodic lattice by Peierls (1933). If the assumed $u_o(\underset{\sim}{r})$ given by Eq (2.11) is fitted to the actual ground state Bloch function for sodium, as given by Wigner and Seitz (1934), the ensuing values of the parameters β and b imply a diminution of the Landau diamagnetism for sodium by about 0.09°/o. This compares favourably with a more detailed calculation recently made by Tani (1959), (using the sound wave formalism to describe the lattice), who gets a correction of 0.06°/o.

C H A P T E R III

MEISSNER - OCHSENFELD EFFECT

IN

THE BOGOLJUBOV THEORY

3.1: INTRODUCTION.

Several attempts have so far been made to derive the Meissner-Ochsenfeld effect (at absolute zero) from the Bogoljubov theory of superconductivity, with conflicting results.

(i) Rickayzen's (1958) calculation consists of a straightforward extension of the Bogoljubov transformation to the case of a hamiltonian with magnetic field. Such a study is complicated by the fact that while the Bogoljubov hamiltonian as such is gauge covariant, a perturbation treatment (such as that used to derive the thermodynamic properties) to any finite order of perturbation theory violates gauge covariance. As we have seen, the ensuing difficulty is that indeterminate answers are obtained for magnetic quantities. Since Rickayzen ignores this difficulty, and makes an a priori choice of the 'London gauge' ($\nabla' \underset{\sim}{A} = 0$), his calculation is not conclusive.

(ii) Wentzel (1958), realizing the gauge difficulty, follows a course different from ours. Commencing with the Frohlich hamiltonian, by successive canonical transformations he eliminates the magnetic field from it, up to order A^2. Such an elimination can only be performed in perturbation series in the coupling constant g - this is done to order g^3. Wentzel then gets an hamiltonian with magnetic field, which is tractable: A Bogoljubov transformation may be

applied, and the calculation performed in a fully gauge covariant manner. The result is a London type M-O effect, but with a coefficient which differs from that obtained from later calculations. This evaluation treats the magnetic terms by a perturbation theory first (expanding them in powers of g), when for the non-magnetic terms such an expansion is not permissible. It would appear that Wentzel's result is due to some lack in cancellation between a function of g, and its formal power-series expansion.

(iii) Very recently, Blatt and Matsubara (1958 (b)), using a concept of collective excitations as introduced by Bogoljubov (Bogoljubov et al 1958) have made a calculation which fulfils gauge identities. They derive the London kernel (in the limit of small wave number, i.e. $q \to o$). This collective excitation formalism may be interpreted as an alternative method of treating the higher order terms in a perturbation calculation : the derivation contains a selective summation over the most singular terms in each order.

This calculation lacks rigour (for example, certain terms in the transformed current density operator are ignored, for simplicity), but it allows a simple physical interpretation of the Bogoljubov theory.

(iv) Subsequently, Bogoljubov (1958 (c); 1959) has developed a new and powerful formalism - the "method of the self-consistent field" - which avoids gauge difficulties. In this method the parameters u and v involved in the transformation of the Fröhlich hamiltonian are so chosen that the approximate hamiltonian remains gauge-covariant. The consequent investigation of the M-O phenomena is, in effect, a more rigorous and sophisticated version of the Blatt - Matsubara calculation.

In this chapter the M-O effect is derived directly from the original Bogoljubov theory, without having recourse to the collective excitations. [This calculation was contemporaneous with that of Blatt and Matsubara : the later calculation of Bogoljubov,(iv), supersedes both.]

We have seen above that such a treatment is complicated by its violation of gauge-covariance, giving rise to indeterminate answers. However, it has been shown in Chapter II that there is an unambiguous way of determining a best approximation from those available. We thus use the Bogoljubov perturbation scheme to define approximate eigenfunctions of the problem, and then apply the technique of Chapter II to derive the magnetic response of the model.

For the case of small q, any finite order of perturbation theory gives a diamagnetic kernel, corresponding

to a finite correlation length (cf. the discussion following Eq (1) in the Preamble). This correlation length becomes larger and larger as the calculation is extended to higher orders, finally giving the singular London kernel in the limit of infinite order. This is illustrated by figure 10 (page 86a). The essential point is that to get the long-range correlations required for a London-type M-O effect it is necessary to go to very high order in the original Bogoljubov perturbation scheme. The result is in accord with the calculations (iii) and (iv) described above (both of which only give K(q) for small q).

In the limit of large q, our K(q) differs from the London one: it agrees with the kernel obtained by BCS, which is understandable since in this limit the ambiguity, due to gauge difficulties, arises only in terms of second order of smallness.

Wentzel's result differs from ours in both limits (Wentzel 1958, Gupta and Mathur 1959) by a factor proportional to ρ , where ρ is, in a sense, the expansion parameter of the Bogoljubov theory. Rickayzen's calculation corresponds to an ad hoc choice of the parameter $\alpha(q) \equiv 1$ (cf. Eq (1.25) of Chapter II). In fact, we find : (a) for small q, $\alpha \ll 1$ to the order of perturbation theory used by Rickayzen, although $\alpha \to 1$ as the calculation is extended to higher order; and (b) for large q, $\alpha \not\to 1$. (However, as remarked above, the choice of gauge parameter α is relatively

unimportant in this region).

* * * * *

In section 2 the main features of the Bogoljubov theory are summarized. The task of evaluating K(q) to second order in this theory is carried out in sections 3 and 4, for the cases of small and large q respectively. This calculation is then extended (for small q) to higher orders in section 5. (Mathematical details associated with sections 3, 4 and 5 are presented in a series of four appendices). Finally, the results are summarized, and their phenomenological implications discussed briefly, in section 6.

3.2 : THE BOGOLJUBOV THEORY.

In this section, we summarize, for subsequent use, the main formulae of the Bogoljubov theory. The treatment outlined here is a refinement of the original theory (1958 (a)) in that it involves renormalization of both electron and phonon energies, thus greatly facilitating the use of perturbation theory. Bogoljubov (1958 (b)) starts from a modified Frohlich hamiltonian.

$$H = \sum_{\underset{\sim}{ks}} (E(\underset{\sim}{k})-\lambda) a^{\dagger}_{ks}\, a_{ks} + \sum_{\underset{\sim}{p}} \omega(\underset{\sim}{p}) b^{\dagger}_{p}\, b_{p}$$

$$+ \sum_{\substack{\underset{\sim}{k}\underset{\sim}{k}'\underset{\sim}{p}s \\ (\underset{\sim}{k}'-\underset{\sim}{k}=\underset{\sim}{p})}} \left\{ g(\underset{\sim}{p}) \left(\frac{\omega(\underset{\sim}{p})}{2V}\right)^{1/2} a^{\dagger}_{ks}\, a_{k's}\, b_{p} + \text{c.c.} \right\} \qquad (2.1)$$

(where λ is a Lagrange parameter associated with the restraint

$$\sum_{\underset{\sim}{k},s} a^{\dagger}_{ks}\, a_{ks} = N$$

and subsequently determined by the condition $\bar{N} = N$.)

A canonical transformation is then made from the electron and phonon operators, $a^{\dagger}$, a and b, to new 'fermion' and phonon operators $\alpha^{\dagger}$, α and β

$$\left.\begin{aligned} a_{k\uparrow} &= u_k\, \alpha_{ko} + v_k\, \alpha^{\dagger}_{kl} \\ a_{-k\downarrow} &= u_k\, \alpha_{kl} - v_k\, \alpha^{\dagger}_{ko} \end{aligned}\right\} \qquad (2.2)$$

$$b_p = \lambda_p\, \beta_p + \mu_p\, \beta^{\dagger}_{-p} \qquad (2.3)$$

where $\alpha^{\dagger}$, α and β obey their respective fermi and bose type commutation rules, provided

$$u_k^2 + v_k^2 = 1, \quad \lambda_p^2 - \mu_p^2 = 1 \tag{2.4}$$

The hamiltonian (2.1) is now written

$$H = H_0 + H_1' + H_2' + H_1'' + H_2'' + H_R + U \tag{2.5}$$

where H_0 is the 'zero-order' hamiltonian, with renormalized fermion and phonon energies,

$$H_0 = \sum_{\underset{\sim}{k}} \tilde{\mathcal{E}}(\underset{\sim}{k})\left(\alpha_{k0}^{\dagger}\alpha_{k0} + \alpha_{k1}^{\dagger}\alpha_{k1}\right) + \sum_{\underset{\sim}{p}} \tilde{\omega}(\underset{\sim}{p})\beta_p^{\dagger}\beta_p \tag{2.6}$$

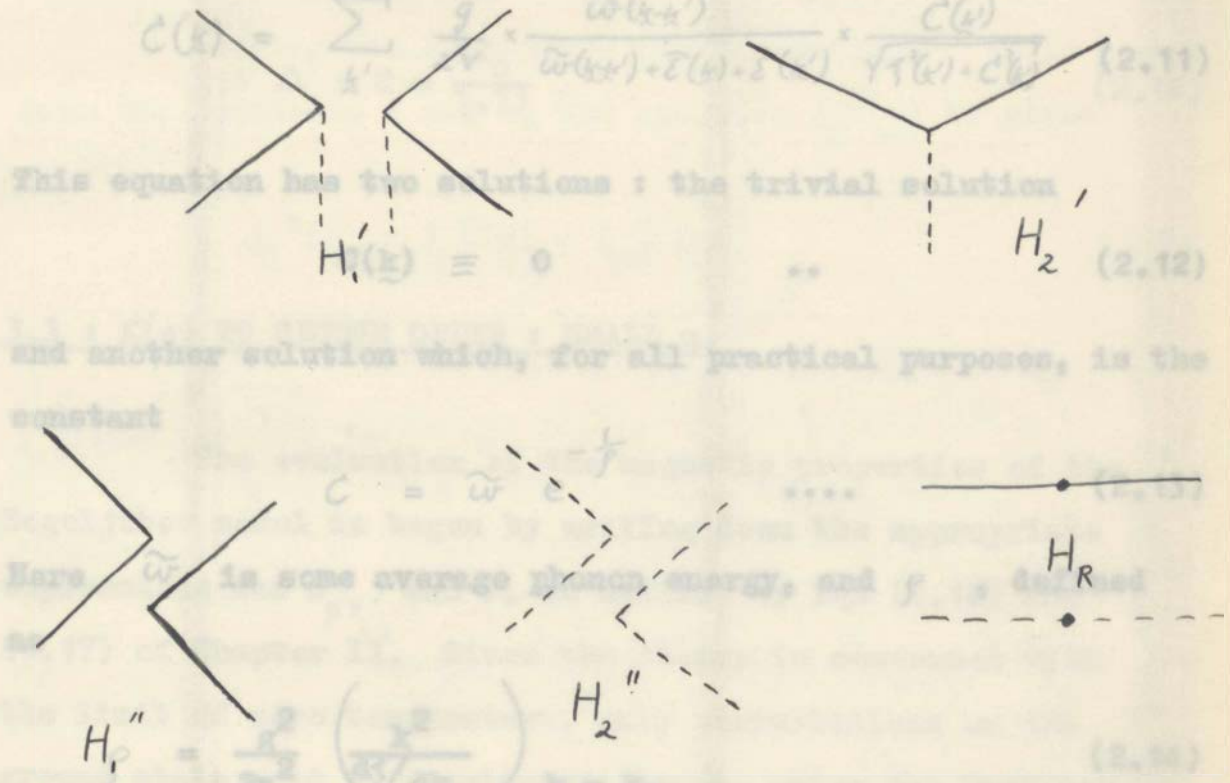
and the remaining terms are given by

$$\left.\begin{aligned}
H_1' &= \sum_{\substack{\underset{\sim}{k}\underset{\sim}{k}' \\ (\underset{\sim}{k}'-\underset{\sim}{k}=\underset{\sim}{p})}} g(\underset{\sim}{p})\left(\frac{\omega(\underset{\sim}{p})}{2V}\right)^{\frac{1}{2}}\left(u_k v_{k'} + v_k u_{k'}\right)\left(\mu_p + \lambda_p\right) \times \\
&\qquad \times \left(\alpha_{k0}^{\dagger}\alpha_{k'1}^{\dagger} + \alpha_{k1}\alpha_{k'0}\right)\left(\beta_p^{\dagger} + \beta_{-p}\right) \\
H_2' &= \sum_{\substack{\underset{\sim}{k}\underset{\sim}{k}' \\ (\underset{\sim}{k}'-\underset{\sim}{k}=\underset{\sim}{p})}} g(\underset{\sim}{p})\left(\frac{\omega(\underset{\sim}{p})}{2V}\right)^{\frac{1}{2}}\left(u_k u_{k'} - v_k v_{k'}\right)\left(\mu_p + \lambda_p\right) \times \\
&\qquad \times \left(\alpha_{k0}^{\dagger}\alpha_{k'0} + \alpha_{k'1}^{\dagger}\alpha_{k1}\right)\left(\beta_p^{\dagger} + \beta_{-p}\right) \\
H_1'' &= \sum_{\underset{\sim}{k}} \left(E(\underset{\sim}{k}) - \lambda\right) 2\, u_k v_k \left(\alpha_{k0}^{\dagger}\alpha_{k1}^{\dagger} + \alpha_{k1}\alpha_{k0}\right) \\
H_2'' &= \sum_{\underset{\sim}{p}} \omega(\underset{\sim}{p})\,\mu_p\lambda_p\left(\beta_p^{\dagger}\beta_{-p}^{\dagger} + \beta_{-p}\beta_p\right) \\
H_R &= \sum_{\underset{\sim}{k}} \left\{\left(E(\underset{\sim}{k}) - \lambda\right)\left(u_k^2 - v_k^2\right) - \tilde{\mathcal{E}}(\underset{\sim}{k})\right\}\left\{\alpha_{k0}^{\dagger}\alpha_{k0} + \alpha_{k1}^{\dagger}\alpha_{k1}\right\} + \\
&\qquad + \sum_{\underset{\sim}{p}} \left\{\omega(\underset{\sim}{p})\left(\mu_p^2 + \lambda_p^2\right) - \tilde{\omega}(\underset{\sim}{p})\right\}\beta_p^{\dagger}\beta_p
\end{aligned}\right\} \tag{2.7}$$

The remaining term is a constant,

$$U = \sum_{\underset{\sim}{k}} (E(\underset{\sim}{k}) - \lambda)\, 2v_k^2 + \sum_{\underset{\sim}{p}} \omega(\underset{\sim}{p})\, \mu_p^2 \quad .. \qquad (2.8)$$

The terms (2.7) are described in figure 5 by Feynman graphs: unbroken lines represent fermions, broken lines phonons. Time runs from left to right.



(Fig. 5)

The transformation parameters u, v and μ, λ are determined by the criterion that 'dangerous' processes (creation of a virtual pair of fermions or phonons from the vacuum) should compensate. One then writes u_k, v_k in terms of a function $C(\underset{\sim}{k})$ as

$$u_k^2 = \frac{1}{2}\left\{1 + \frac{\xi(k)}{\sqrt{\xi^2(k)+C^2(k)}}\right\} \; ; \; v_k^2 = \frac{1}{2}\left\{1 - \frac{\xi(k)}{\sqrt{\xi^2(k)+C^2(k)}}\right\} \qquad (2.9)$$

where $\xi(\underset{\sim}{k}) = E(\underset{\sim}{k}) - E_F$ (2.10)

and $C(\underset{\sim}{k})$ is to be determined (to second order) from

$$C(\underset{\sim}{k}) = \sum_{\underset{\sim}{k}'} \frac{g^2}{2V} \times \frac{\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k}')}{\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k}') + \tilde{\mathcal{E}}(\underset{\sim}{k}) + \tilde{\mathcal{E}}(\underset{\sim}{k}')} \times \frac{C(\underset{\sim}{k}')}{\sqrt{\xi^2(\underset{\sim}{k}') + C^2(\underset{\sim}{k}')}} \qquad (2.11)$$

This equation has two solutions : the trivial solution

$$C(\underset{\sim}{k}) \equiv 0 \qquad .. \qquad (2.12)$$

and another solution which, for all practical purposes, is the constant

$$C = \tilde{\omega}\, e^{-\frac{1}{\rho}} \qquad .... \qquad (2.13)$$

Here $\tilde{\omega}$ is some average phonon energy, and ρ, defined as

$$\rho = \frac{g^2}{2\pi^2}\left(\frac{k^2}{d\xi/dk}\right)_{k = k_F} \qquad (2.14)$$

is required to be small. The trivial solution (2.12) corresponds to the normal state, which has a higher ground state energy than the superconducting state, given by (2.13).

Finally, we mention that, to second order, the renormalized fermion energy $\left(\tilde{\mathcal{E}}^{(1)}(\underset{\sim}{k})\right)$ is given by

$$\tilde{\varepsilon}^{(1)}(\underset{\sim}{k})\left[1 + \sum_{\underset{\sim}{k'}} \frac{g^2}{2V} \times \frac{\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k'})\left(u_k^2 u_{k'}^2 + v_k^2 v_{k'}^2\right)}{\left[\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k'}) + \tilde{\varepsilon}(\underset{\sim}{k'})\right]^2 - \tilde{\varepsilon}^2(\underset{\sim}{k})}\right] = \sqrt{\xi^2(\underset{\sim}{k}) + C^2(\underset{\sim}{k})} \quad (2.15)$$

The noteworthy feature is that this fermion excitation spectrum has an energy gap Δ above the ground state; the magnitude of this gap is

$$\Delta = C = \frac{kT_c}{1.13} \quad (2.16)$$

3.3 : K(q) TO SECOND ORDER : SMALL q.

The evaluation of the magnetic properties of the Bogoljubov model is begun by writing down the appropriate expressions for $S_{\mu\nu}$ and L, as defined by Eqs (1.16) and (1.17) of Chapter II. Since the theory is concerned with the limit of zero temperature, only perturbations on the ground state need be considered: hence, using the Frohlich hamiltonian,

$$L = \frac{e^2 N}{mc^2} \quad (3.1)$$

$$S_{\mu\nu} = -\frac{1}{c^2} \sum_{\underset{\sim}{k}} \frac{\langle o | j_\mu^{\,o}(\underset{\sim}{q}) | k \rangle \langle k | j_\nu^{\,o}(-\underset{\sim}{q}) | o \rangle}{E_o - E_k} + \text{c.c.} \quad (3.2)$$

with the operator $j_\mu{}^o(\underset{\sim}{q})$ (Eq (1.8) of Chapter II) in second quantized form

$$j_\mu{}^o(\underset{\sim}{q}) = \frac{e}{2m} \sum_{\substack{\underset{\sim}{k},\underset{\sim}{k}',s \\ (\underset{\sim}{k}-\underset{\sim}{k}'=\underset{\sim}{q})}} (k+k')_\mu \; a^\dagger_{\underset{\sim}{k}s} \; a_{\underset{\sim}{k}'s} \tag{3.3}$$

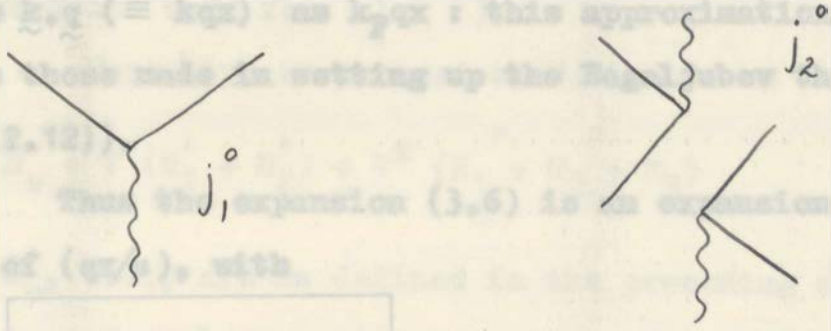
Making the Bogoljubov transformation(*) (2.2) into the operators $\alpha^\dagger$ and α, the operator $j_\mu{}^o(\underset{\sim}{q})$ is given (exactly) as

$$j_\mu{}^o(\underset{\sim}{q}) = j_{\mu 1}{}^o(\underset{\sim}{q}) + j_{\mu 2}{}^o(\underset{\sim}{q}) \tag{3.4}$$

$$\left.\begin{aligned} j_{\mu 1}{}^o(\underset{\sim}{q}) &= -\frac{e}{m} \sum_{\underset{\sim}{k}} k_\mu \left(u_{k+\frac{q}{2}} \, u_{k-\frac{q}{2}} + v_{k+\frac{q}{2}} \, v_{k-\frac{q}{2}} \right) \times \\ &\quad \times \left(\alpha^\dagger_{k-\frac{q}{2},0} \; \alpha_{k+\frac{q}{2},0} - \alpha^\dagger_{k+\frac{q}{2},1} \; \alpha_{k-\frac{q}{2},1} \right) \\ j_{\mu 2}{}^o(\underset{\sim}{q}) &= -\frac{e}{m} \sum_{\underset{\sim}{k}} k_\mu \left(u_{k-\frac{q}{2}} \, v_{k+\frac{q}{2}} - u_{k+\frac{q}{2}} \, v_{k-\frac{q}{2}} \right) \times \\ &\quad \times \left(\alpha^\dagger_{k-\frac{q}{2},0} \; \alpha^\dagger_{k+\frac{q}{2},1} - \alpha_{k-\frac{q}{2},1} \; \alpha_{k+\frac{q}{2},0} \right) \end{aligned}\right\} \tag{3.5}$$

*) It is to be noted that a Bogoljubov transformation (2.2), with fixed, field independent coefficients u and v does not destroy the gauge-covariance of the hamiltonian.

The vectors $\underset{\sim}{k}$, $\underset{\sim}{k}'$ of equation (3.3) have been rewritten as $\underset{\sim}{k} \to \underset{\sim}{k} - \underset{\sim}{q}/2$, $\underset{\sim}{k}' \to \underset{\sim}{k} + \underset{\sim}{q}/2$. Invoking graphical representation, $j_1^{\,o}$ and $j_2^{\,o}$ may be expressed as in figure 6. (Wavy lines represent the action of the external field, $\underset{\sim}{A}$.)



(Fig. 6)

The qualitative nature of the M-O effect is described by the behaviour of K(q) in the limit $q \to 0$ (cf. Eq(1) in the Preamble). We therefore expand the matrix elements in (3.5) in this limit,

$$\left.\begin{aligned}\left(u_{k+\frac{q}{2}}\, u_{k-\frac{q}{2}} + v_{k+\frac{q}{2}}\, v_{k-\frac{q}{2}}\right) &= 1 - \left(\frac{\underset{\sim}{k}\cdot\underset{\sim}{q}}{2m}\right)^2 \frac{c^2}{\left(c^2 + \xi_o^{\,2}\right)^2} + \mathcal{O}\left[\frac{(\underset{\sim}{k}\cdot\underset{\sim}{q})}{2mc}\right]^4 \\ \left(u_{k-\frac{q}{2}}\, v_{k+\frac{q}{2}} - u_{k+\frac{q}{2}}\, v_{k-\frac{q}{2}}\right) &= -\left(\frac{\underset{\sim}{k}\cdot\underset{\sim}{q}}{2m}\right) \times \frac{c}{c^2 + \xi_o^{\,2}} + \mathcal{O}\left[\frac{\underset{\sim}{k}\cdot\underset{\sim}{q}}{2mc}\right]^3\end{aligned}\right\} \quad (3.6)$$

where

$$\xi_o \equiv \frac{1}{2m}\left(k^2 + \frac{q^2}{4} - k_F^{\,2}\right) \quad (3.7)$$

(From now on we neglect the q dependence embodied in ξ_0, as it gives rise to correction factors of order $(q/k_F)^2$, which are negligible for all q of any interest.) Moreover, since all integrals over $\underset{\sim}{k}$ have their dominating contribution from the region $|\underset{\sim}{k}| \approx k_F$, in (3.6) we rewrite $\underset{\sim}{k}.\underset{\sim}{q}$ ($\equiv kqx$) as $k_F qx$: this approximation is as good as those made in setting up the Bogoljubov theory (e.g. (2.12)).

Thus the expansion (3.6) is an expansion in powers of (qx/μ), with

$$\boxed{\mu \equiv \frac{2mC}{k_F}} \qquad (3.8)$$

Hence by "small q" we mean $q < \mu$: we shall now derive $K(q)$ in this limit, as a power series in (q/μ). The case of $q > \mu$ ("large q"), which is relevant to penetration phenomena, is deferred to section 4.

It is important to note that in the limit $q < \mu$, the matrix element associated with $j_1^{\,0}$ (i.e. scattering of a fermion by the field) is of order unity; whereas that associated with $j_2^{\,0}$ (emission or absorption of a pair by the field) is of order $\frac{q}{\mu}$.

In evaluating $S_{\mu\nu}$, only those terms which contain either $j_1^{\,0}$ or $j_2^{\,0}$ twice are pertinent : any term containing each of $j_1^{\,0}$ and $j_2^{\,0}$ once is odd in $\underset{\sim}{k}$, and thus vanishes identically on summation.

The scheme so far is exact and gauge-covariant — the approximation now enters, when the Bogoljubov treatment is used to provide approximate eigenvalues and eigenvectors of the field-free hamiltonian, to calculate $\hat{S}_{\mu\nu}$. (The quantity L is, of course, exact, independent of the approximation used for $\hat{S}_{\mu\nu}$).

Formally, we proceed as follows:- we write

$$H = H_0 + \gamma (H_1' + H_2') + \gamma^2 (H_1'' + H_2'' + H_R) \qquad (3.9)$$

where H_0, etc., are as defined in the preceding section, and γ is a formal expansion parameter, which we put = 1 finally. Terms of order γ^{2n} correspond, in effect, to graphs with n closed phonon lines.

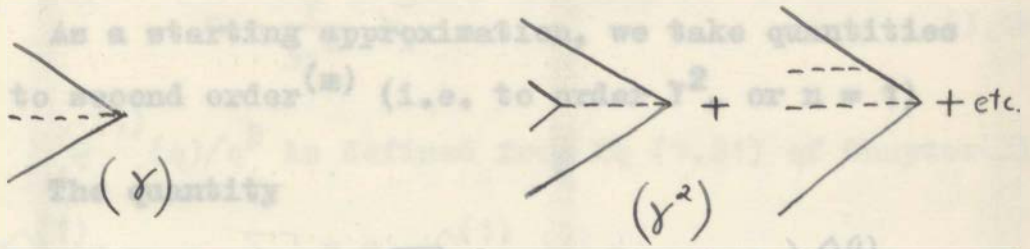
For order γ^{2n}, H_0 contains the energies of fermions and phonons renormalized to this order. Hence the eigenvalues for the energy denominators in $\hat{S}_{\mu\nu}$ are known.

By application of perturbation theory (with corrected energy denominators - cf. Morse and Feshbach 1953) eigenvectors are then calculated. [The eigenvector for the state with, say, fermions $k_1 0$, $k_2 1$, ... , $k_{N_1} 1$ and phonons p_1, p_2, ... , p_{N_2} is represented in zeroth order by $|k_1 0, k_2 1, \ldots\ldots k_{N_1} 1; p_1, p_2, \ldots\ldots, p_{N_2}\rangle$, and by $\left\{ |k_1 0, \ldots\ldots, k_{N_1} 1; p_1, \ldots, p_{N_2}\rangle \right\}_n$ when corrected to order γ^{2n}.] For example, to second order, the ground state is

$$|0\rangle + \gamma\,|k0,k'1;p(=k'-k)\rangle\langle k0,k'1;p|H_1'|0\rangle$$

$$\{|0\rangle\}_2 = +\gamma^2 \begin{cases} |k0,k'1,k''0,k'''1\rangle\langle k0,k'1,k''0,k'''1|H_1'|k0,k'1;p\rangle\times \\ \qquad \times\langle k0,k'1;p|H_1'|0\rangle \\ +|k''0,k'1;p,p'\rangle\langle k''0,k'1;p',p|H_2'|k0,k'1;p\rangle\times \\ \qquad \times\langle k0,k'1;p|H_1'|0\rangle \\ +\text{etc.} \end{cases} \tag{3.10}$$

where these perturbation terms have the graphical representations



(Fig.7)

Using eigenvalues and eigenvectors calculated to order γ^{2n}, a $\hat{S}^{(n)}_{\mu\nu}$ is found. It may be shown (e.g. Wentzel 1958) that in the Bogoljubov approximation gauge-covariance is no longer fulfilled identically to each order in γ : i.e. $\hat{S}^{(n)}_{\mu\nu}$ gives rise to a $\hat{G}^{(n)}$ which violates the identity (1.21) of Chapter II. This difficulty is overcome by using the technique developed in Chapter II to choose a best value for α in $\hat{K}^{(n)}(q,\alpha)$.

In principle, this is done by choosing $\alpha = \alpha_1$ such that $\hat{K}^{(n)}(q,\alpha_1)$ is a stationary approximation to $K(q)$: in detail, we calculate $\hat{K}^{(n+1)}(q,\alpha)$ by use of wave-

functions and energy values correct to the next highest order, and then choose $\alpha = \alpha_1$, such that the difference

$$\Delta \hat{K}^{(n)}(q,\alpha) = \hat{K}^{(n+1)}(q,\alpha) - \hat{K}^{(n)}(q,\alpha) \qquad (3.11)$$

is minimized. In this way, our non gauge-invariant $\hat{K}^{(n)}(q,\alpha)$ may be used to get a well defined approximation, of order γ^{2n}, to $K(q)$.

* * * * *

As a starting approximation, we take quantities correct to second order(*) (i.e. to order γ^2, or $n = 1$)

The quantity

$$\hat{K}_B^{(1)}(q) = \frac{1}{q^2} \sum_{\mu\nu} \left(\frac{1}{2} \delta_{\mu\nu} - \frac{3}{2} \frac{q_\mu q_\nu}{q^2} \right) \hat{S}_{\mu\nu}^{(1)} \qquad (3.12)$$

is regular as q tends to zero : this is because all terms of order $1/q^2$ involve an angular integration of the form

---

*) We avoid use of the zero order eigenfunctions, since the continuous energy spectrum so obtained is qualitatively at fault in describing a spectrum with a gap. If one uses such quantities, one encounters difficulties stemming from the expansion of a spectrum with a gap around a continuum.

$$\int_0^{\pi} \left(\frac{1}{2} - \frac{3}{2}\cos^2\theta\right) d(\cos\theta) = 0 \qquad (3.13)$$

The leading term in $\hat{K}_B^{(1)}(q)$ is then of order γ^0, obtained by the operator j_2^0 creating and then destroying a pair of fermions.

$$\hat{K}_B^{(1)}(q) = \frac{1}{q^2}\frac{2}{c^2}\left(\frac{e}{m}\right)^2 \sum_{\mu\nu,\underline{k}} \frac{\left(\frac{1}{2}\delta_{\mu\nu} - \frac{3}{2}\frac{q_\mu q_\nu}{q^2}\right) k_\mu k_\nu \left(u_{k+\frac{q}{2}} v_{k-\frac{q}{2}} - u_{k-\frac{q}{2}} v_{k+\frac{q}{2}}\right)^2}{\left(\tilde{\mathcal{E}}^{(1)}(k+\frac{q}{2}) + \tilde{\mathcal{E}}^{(1)}(k-\frac{q}{2})\right)} + \mathcal{O}(\gamma^2) \qquad (3.14)$$

For the case of $q<\mu$, this reduces to

$$\hat{K}_B^{(1)}(q) = -\frac{4}{15}\frac{L}{\mu^2}\left\{1 + \mathcal{O}\left(\frac{q}{\mu}\right)^2 + \mathcal{O}(\gamma^2)\right\} \qquad (3.15)$$

In simplifying (3.14), we have used the relation

$$N = \frac{V}{3\pi^2} k_F^3 \qquad (3.16)$$

$\hat{G}^{(1)}(q)/q^2$ is defined from Eq (1.21) of Chapter II by

$$\frac{\hat{G}^{(1)}(q)}{q^2} = \sum_{\mu\nu} \frac{q_\mu q_\nu}{q^4} \hat{S}_{\mu\nu}^{(1)} - \frac{L}{q^2} \qquad (3.17)$$

The $1/q^2$ term due to $\hat{S}_{\mu\nu}^{(1)}$ has its leading coefficient of order γ^2. This is because terms proportional to $1/q^2$ must arise from the operator j_1^0 (cf. (3.6)); but since j_1^0 is a scattering operator, fermions must first be created from, and finally destroyed to, the vacuum, by perturbations on the ground state, $|0\rangle$, which are at least of order γ. Hence,

$$\frac{\hat{G}^{(1)}(q)}{q^2} = -\frac{L}{q^2}\left\{1 + \mathcal{O}\left(\frac{q}{\mu}\right)^2 + \mathcal{O}(\gamma^2)\right\} \qquad (3.18)$$

and, as we expected, the approximate wave-functions and energies have violated the gauge condition $G(q) \equiv 0$.

So our approximate kernel is to be chosen from the infinite linear family

$$\hat{K}^{(1)}(q) = -\left(\frac{4}{15\mu^2} + \frac{\alpha}{q^2}\right) L \qquad (3.19)$$

We therefore proceed to construct the quantity $\Delta\hat{K}^{(1)}(q,\alpha)$, as defined by Eq (3.11). The lowest order terms in $\Delta\hat{K}^{(1)}(q,\alpha)$ are clearly of order γ^4 - that is to say

$$\Delta\hat{K}^{(1)}(q,\alpha) = \gamma^4 \mathcal{K}^{(1)}(q,\alpha)\left[1 + O(\gamma^2)\right] \qquad (3.20)$$

A well-defined approximation to the exact kernel $K(q)$ may now be obtained from Eq(3.19) by choosing $\alpha = \alpha_1$, such that

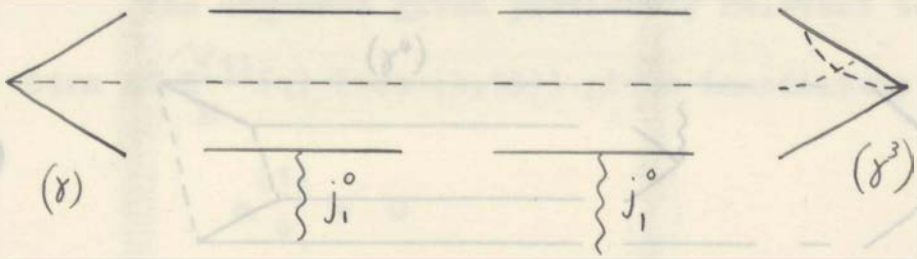
$$\mathcal{K}^{(1)}(q,\alpha_1) = 0 \qquad (3.21)$$

i.e.

$$\mathcal{K}_B^{(1)}(q) + \alpha_1 \frac{\not{q}^{(1)} \not{q}}{q^2} = 0 \qquad (3.22)$$

Bearing in mind that $S_{\mu\nu}$ contains either the pair of operators j_1^0, j_1^0 or the pair j_2^0, j_2^0, it is seen that the lowest order (γ^4) terms in the difference $\left\{\hat{K}^{(2)}(q,\alpha) - \hat{K}^{(1)}(q,\alpha)\right\}$ arise basically in three ways.

(i) The j_1° operator scatters a fermion of a pair which is created and destroyed by perturbations on the zero-order ground state, $|o\rangle$, of orders γ and γ^3. Schematically, such terms correspond to graphs such as shown in figure 8. (We have 'exploded' the graph, into its successive components).

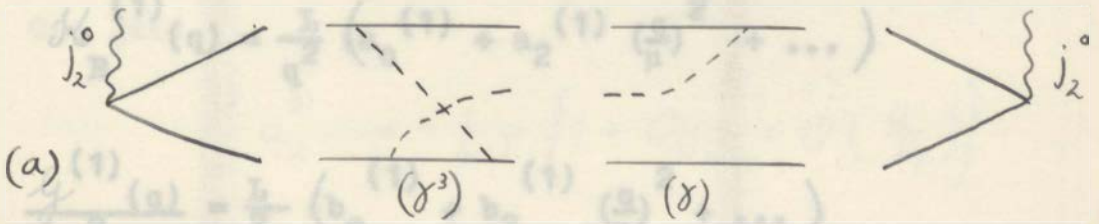


(Fig.8)

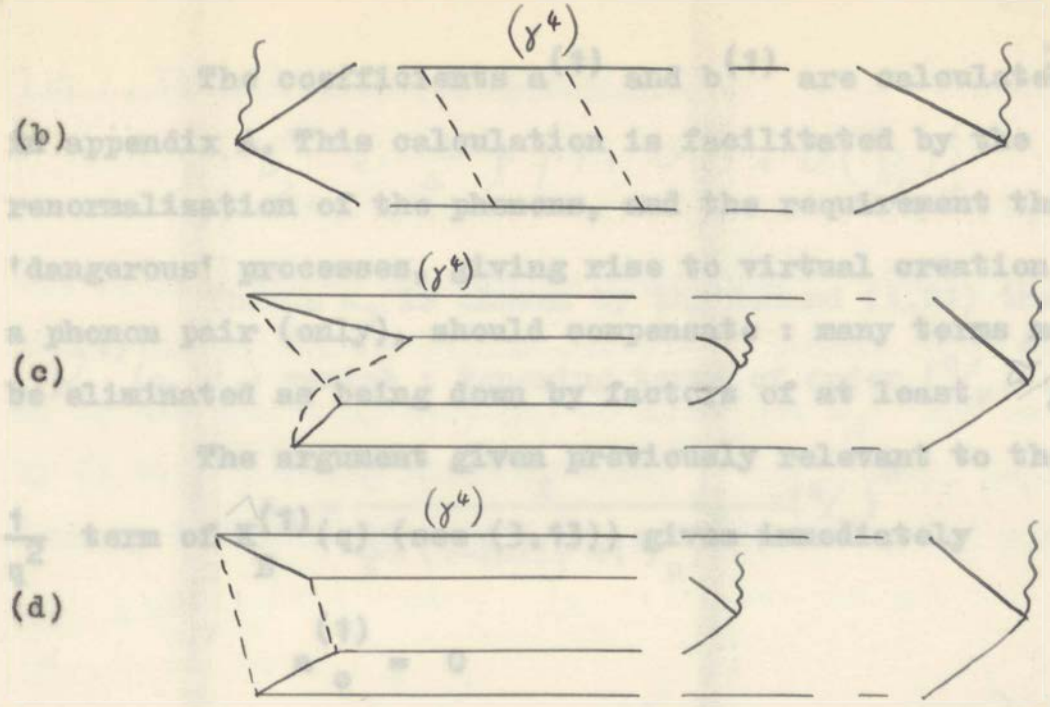
Such terms have a leading component of order $1/q^2$.

(ii) A j_2° operator creates a pair from the vacuum, and destroys it back into the vacuum; the wave functions in between having perturbations of order γ and γ^3, or else of order γ^4 coupled to an unperturbed function.

Also in this class we include terms arising when successive j_2° operators create (or annihilate) four fermions from the vacuum, and these fermions are annihilated (or created) by perturbations to the zero-order vacuum of order γ^4.



(Fig. 9)



Here the leading term will be of order $1/\mu^2$.

(iii) There is also a term of order γ^4 in the difference between $\hat{S}_{\mu\nu}^{(1)}$ and $\hat{S}_{\mu\nu}^{(2)}$ arising from the difference in the two denominators (i.e. from the fact that $\tilde{\mathcal{E}}^{(2)}(\underset{\sim}{k}) - \tilde{\mathcal{E}}^{(1)}(\underset{\sim}{k}) \sim \gamma^4$). This, in conjunction with unperturbed wave functions, gives a contribution to $\mathcal{K}^{(1)}(q,\alpha)$, which is of order $1/\mu^2$.

The quantities $\mathcal{K}_B{}^{(1)}(q)$ and $\frac{\mathcal{G}^{(1)}(q)}{q^2}$, defined in (3.22), may be expanded in powers of $(\frac{q}{\mu})^2$:

$$\mathcal{K}_B{}^{(1)}(q) = \frac{L}{q^2}\left(a_0{}^{(1)} + a_2{}^{(1)}\left(\frac{q}{\mu}\right)^2 + \ldots\right) \qquad (3.23)$$

$$\frac{\mathcal{G}^{(1)}(q)}{q^2} = \frac{L}{q^2}\left(b_0{}^{(1)} + b_2{}^{(1)}\left(\frac{q}{\mu}\right)^2 + \ldots\right) \qquad (3.24)$$

The coefficients $a^{(1)}$ and $b^{(1)}$ are calculated in appendix A. This calculation is facilitated by the renormalization of the phonons, and the requirement that 'dangerous' processes, giving rise to virtual creation of a phonon pair (only), should compensate : many terms may be eliminated as being down by factors of at least $\tilde{\omega}/E_F$.

The argument given previously relevant to the $\frac{1}{q^2}$ term of $\hat{K}^{(1)}_B(q)$ (see (3.13)) gives immediately

$$a_o^{(1)} = 0 \tag{3.15}$$

Evaluation of terms of type (i) yields (neglecting terms of relative order $\rho \exp(-1/\rho)$ and $\tilde{\omega}/E_F \ln \tilde{\omega}/E_F$)

$$b_o^{(1)} = \frac{4}{3}(1 - \ln 2)\,\rho^2 \tag{3.26}$$

To find $a_2^{(1)}$ and $b_2^{(1)}$, terms of all three types (i), (ii) and (iii) must be considered. It is found that the dominant contribution comes from the 'ladder graph' type of terms in (ii) illustrated by fig. 9 (b) and (d) : such terms are characterized by the fact that each alternate energy denominator, in perturbation theory, contains only fermions, and no phonons.

One gets

$$a_2^{(1)} = -\frac{1}{4}\rho\left\{1 + O(\rho) + O\left(\frac{\tilde{\omega}}{E_F}\right)\right\} \tag{3.27}$$

$$b_2^{(1)} = \frac{1}{4}\rho\left\{1 + \mathcal{O}(\rho) + \mathcal{O}\left(\frac{\omega}{E_F}\right)\right\} \qquad (3.28)$$

Thence α_1 is chosen by the demand (3.21) that $\mathcal{K}^{(1)}(q, \alpha_1)$ vanish : ignoring terms of order $(q/\mu)^4$,

$$\alpha_1 = \frac{1}{\frac{16}{3}(1-\ln 2)\rho + (q/\mu)^2} \times (q/\mu)^2 \qquad (3.29)$$

$$\doteq \frac{3}{16(1-\ln 2)\rho} \cdot \frac{q^2}{\mu^2}\left\{1 + \mathcal{O}(q/\mu)^2\right\} \qquad (3.30)$$

and finally substituting into (3.19), to second order in γ, we get the kernel in the limit $q<\mu$ as

$$K(q) \approx \hat{K}^{(1)}(q, \alpha_1)$$

$$= -\left(\frac{4}{15} + \frac{3}{16(1-\ln 2)\rho}\right)\frac{L}{\mu^2} \qquad (3.31)$$

Such a kernel describes a large diamagnetism, rather than a London M-O effect.

3.4 : K(q) TO SECOND ORDER: LARGE q.

In the region $q > \mu$ (although still $q \ll k_F \sim 10^{8-1}$ cm^{-1}) the calculation of K(q) is straightforward. Using wave-functions and energy values correct to second order in γ, as in the preceding section, we again get $\hat{K}_B^{(1)}(q)$ as given by (3.14), ignoring terms of order ρ and higher. Replacing sums by integrals in (3.14) and making a change of variables $\xi_0 = (\frac{q}{\mu}c)y$,

$$\hat{K}_B^{(1)}(q) = -\frac{3}{2}\frac{L}{q^2}\int_0^\infty dy \int_0^1 dx \frac{(3x^2-1)}{\sqrt{(y+x)^2+\delta^2}+\sqrt{(y-x)^2+\delta^2}} \times \left\{1 - \frac{(y^2-x^2+\delta^2)}{\sqrt{(y+x)^2+\delta^2}\sqrt{(y-x)^2+\delta^2}}\right\} \tag{4.1}$$

which is to be evaluated in the limit $\delta < 1$, with $\delta \equiv \frac{\mu}{q}$. This evaluation, carried out in appendix B, yields

$$\hat{K}_B^{(1)}(q) = -\frac{9\pi^2}{16} \times \frac{\mu}{q^3}\left\{1 + \frac{32}{3\pi^2}\frac{\mu}{q}\ln\left(\frac{\mu}{q}\right) + \mathcal{O}\left(\frac{\mu}{q}\right)\right\} L \tag{4.2}$$

Also we have

$$\frac{\hat{G}^{(1)}(q)}{q^2} = \frac{1}{q^2}\left\{\frac{2}{c^2}\left(\frac{e}{m}\right)^2 \sum_{\underset{\sim}{k}} \frac{(\underset{\sim}{k}\cdot\underset{\sim}{q})^2}{q^2} \times \frac{\left(u_{\underset{\sim}{k}+\frac{q}{2}}^{\nu} u_{\underset{\sim}{k}-\frac{q}{2}}^{-u} - u_{\underset{\sim}{k}-\frac{q}{2}}^{\nu} u_{\underset{\sim}{k}+\frac{q}{2}}^{}\right)^2}{\left(\mathcal{E}^{(1)}(\underset{\sim}{k}+\frac{q}{2}) + \mathcal{E}^{(1)}(\underset{\sim}{k}-\frac{q}{2})\right)} - L\right\} \tag{4.3}$$

Again we may expand in powers of $\frac{\mu}{q}$:

$$\frac{\hat{G}^{(1)}(q)}{q^2} = \frac{9\pi^2}{16} \times \frac{\mu}{q^3} \left\{ 0 - \frac{16}{3\pi^2} \frac{\mu}{q} \ln\left(\frac{\mu}{q}\right) + \mathcal{O}\left(\frac{\mu}{q}\right) \right\} L \qquad (4.4)$$

Comparing equations (4.2) and (4.4), it is apparent that, in the limit $\frac{\mu}{q} \ll 1$,

$$\hat{K}_B^{(1)}(q) \gg \frac{\hat{G}^{(1)}(q)}{q^2} \qquad (4.5)$$

This then implies that $\hat{K}^{(1)}(q,\alpha)$ is very insensitive to variations in α.

α_1 is evaluated, according to our criterion, in Appendix C. In carrying out the resulting calculations, we find it convenient to subdivide the region $q > \mu$ into two parts:

$$\text{(a)} \quad \mu < q < \mu \exp\left(\tfrac{1}{\rho}\right) \qquad (4.6)$$

$$\text{(b)} \quad k_F > q > \mu \exp\left(\tfrac{1}{\rho}\right)$$

Physically, region (a) is the more interesting one, since it is relevant to $q \lesssim 10^6 \text{cm}^{-1}$. In this region, both $\mathcal{K}_B^{(1)}(q)$ and $\mathcal{G}^{(1)}(q)/q^2$ have leading terms which differ from $L\rho^2/q^2$ only by numerical factors. α_1 is thus a purely numerical constant, containing any q dependence only in correction terms. Hence, in region (a),

$$K(q) = -\frac{9\pi^2}{16} \times \frac{\mu}{q^3} \left\{ 1 + \mathcal{O}\left(\frac{\mu}{q} \ln \frac{\mu}{q}\right) \right\} L \qquad (4.7)$$

In region (b), $\hat{G}^{(1)}(q)/q^2$ is smaller than $\hat{K}_B^{(1)}(q)$ by a factor of less than $\frac{1}{\rho}\exp\left(-\frac{1}{\rho}\right)$. We find (see (C.13))

$$\alpha_1 = \sigma \frac{q}{\mu} \exp\left(-\frac{1}{\rho}\right)\left\{1+\mathcal{O}\left(\frac{\mu}{q}e^{\frac{1}{\rho}}\ln\left(\frac{\mu}{q}e^{\frac{1}{\rho}}\right)\right)\right\} \quad (4.8)$$

with σ some numerical constant. The ensuing term $\alpha_1\hat{G}^{(1)}/q^2$ in $\hat{K}(q, \alpha_1)$ is, however, still smaller than $\hat{K}_B^{(1)}$ throughout the region (b), by a factor $(\exp\left(\frac{-1}{\rho}\right)\ln\frac{\mu}{q})$. That is, in region (b),

$$K(q) = -\frac{9\pi^2}{16}\frac{\mu}{q^3}\left\{1+\mathcal{O}\left(\exp\left(\frac{-1}{\rho}\right)\ln\frac{\mu}{q}\right)\right\} L \quad (4.9)$$

The results (4.7) and (4.9) may be collected together by writing the kernel, in the limit $q > \mu$, as

$$K(q) = -\frac{9\pi^2}{16}\frac{\mu}{q^3}\left\{1+\mathcal{O}\left(\left(\frac{\mu}{q}+\exp\left(\frac{-1}{\rho}\right)\right)\ln\frac{\mu}{q}\right)\right\} L \quad (4.10)$$

3.5 : K(q) TO HIGHER ORDER IN THE APPROXIMATION SCHEME.

The evaluation of the kernel is extended to nth order by calculating $\hat{K}_B^{(n)}$ and $\hat{G}^{(n)}/q^2$ with eigenfunctions correct up to terms proportional to γ^{2n}, and choosing $\alpha_1^{(n)}$ by the criterion (3.11)

$$\Delta\hat{K}^{(n)}(q,\alpha_1) \equiv \hat{K}^{(n+1)}(q,\alpha_1) - \hat{K}^{(n)}(q,\alpha_1) \tag{5.1}$$

$$= 0 \tag{5.2}$$

($\hat{K}^{(n+1)}(q,\alpha)$ is the kernel calculated with eigenfunctions correct to the next highest order.)

The quantities $\hat{K}_B^{(n)}$ and $\hat{G}^{(n)}/q^2$ now have the form

$$\hat{K}_B^{(n)} = \hat{K}_B^{(1)}\left(1+ \text{terms of higher order in } \gamma^2\right) \tag{5.3}$$

$$\frac{\hat{G}^{(n)}}{q^2} = \frac{\hat{G}^{(1)}}{q^2}\left(1+ \text{terms of higher order in } \gamma^2\right) \tag{5.4}$$

The leading terms are as calculated in the preceding sections.

Also, as the lowest order terms in $\Delta\hat{K}^{(n)}(q,\alpha)$ are obviously of order $\gamma^{2(n+1)}$, we can write

(5.5)

$$\Delta\hat{K}_B^{(n)} = \gamma^{2(n+1)}\mathcal{K}_B^{(n)}\left(1+ \text{terms of higher order in } \gamma^2\right)$$

$$\Delta\frac{\hat{G}^{(n)}}{q^2} = \gamma^{2(n+1)}\frac{\mathcal{G}^{(n)}}{q^2}\left(1+ \text{terms of higher order in } \gamma^2\right) \tag{5.6}$$

where $\mathcal{K}_B^{(n)}$, $\mathcal{G}^{(n)}/q^2$ are found from those terms corresponding to graphs with $(n+1)$ phonon lines. Then $\alpha_1^{(n)}$ is derived as

$$\alpha_1^{(n)} = -\, q^2 \frac{\mathcal{H}_B^{(n)}}{\mathcal{G}^{(0)}} \left\{ 1 + \text{terms of higher order in } \gamma^2 \right\} \quad (5.7)$$

The leading term of $\alpha_1^{(n)}$ is, of course, of zeroth order in γ for all n.

Thus we have the result

$$\hat{K}^{(n)}(q,\alpha_1) = \left\{ \hat{K}_B^{(1)} - \frac{\mathcal{H}_B^{(n)} \hat{G}^{(1)}}{\mathcal{G}^{(0)}} \right\} \left\{ 1 + \text{terms of higher order in } \gamma^2 \right\} \quad (5.8)$$

Strictly, a calculation of $\hat{K}^{(n)}(q,\alpha_1)$ would involve summation over all terms up to order γ^{2n} in equations (5.3), (5.4), (5.5) and (5.6). Although this summation is mathematically intractable, we may still improve the second order calculation by taking $\hat{K}^{(n)}(q,\alpha_1)$ to be given by the first bracket in Eq(5.8), ignoring the terms of relative order γ^2 and higher. Such a procedure avoids questions as to whether the Bogoljubov expansion is uniformly convergent, or, rather, is some form of asymptotic expansion.

This method for improving the second order approximation to K(q) is justified if and only if the resulting $\hat{K}^{(n)}(q)$ tends uniformly to a limit as n tends to infinity.

For the calculation of $\mathcal{H}_B^{(n)}$ and $\mathcal{G}^{(n)}/q^2$, and thence $\hat{K}^{(n)}(q,\alpha_1)$, we again consider separately the regions $q < \mu$ and $q > \mu$.

(a) The region $q < \mu$:-

In analogy to Eqs. (3.23) and (3.24), we expand in powers of $(q/\mu)^2$ as follows:

$$\mathcal{K}_B^{(n)}(q) = \frac{L}{q^2}\left(a_o^{(n)} + a_2^{(n)}\left(\frac{q}{\mu}\right)^2 + \ldots\right) \tag{5.9}$$

$$\frac{\mathcal{G}^{(n)}(q)}{q^2} = \frac{L}{q^2}\left(b_o^{(n)} + b_2^{(n)}\left(\frac{q}{\mu}\right)^2 + \ldots\right) \tag{5.10}$$

The methods used in appendix A to find the coefficients $a^{(1)}$ and $b^{(1)}$ may be extended to higher orders to get (appendix D)

$$\begin{cases} a_o^{(n)} = 0 & (5.10) \\ a_2^{(n)} = -\tau_1 \rho\left(1 + \mathcal{O}(\rho)\right) & (5.11) \\ b_o^{(n)} = \tau_2 \rho^{n+1} & (5.12) \\ b_2^{(n)} = -a_2^{(n)}\left(1 + \mathcal{O}(\rho^n)\right) & (5.13) \end{cases}$$

where τ_1, τ_2 are numerical constants. (Terms of relative orders $\tilde{\omega}/E_F \ln(\tilde{\omega}/E_F)$ and $\frac{1}{\rho}\exp\left(-\frac{1}{\rho}\right)$ have been neglected.) From these equations it follows that

$$-\frac{q^2 \mathcal{K}_B^{(n)}}{\mathcal{G}^{(n)}} = \frac{q^2}{f\rho^n\mu^2 + q^2}\left\{1 + \mathcal{O}(\rho) + \mathcal{O}\left(\frac{q}{\mu}\right)^2\right\} \tag{5.14}$$

with f a numerical factor of order unity.

The improved approximate kernel, $\hat{K}^{(n)}(q,\alpha_1)$, is now given by Eqs (3.15), (3.18), (5.8) and (5.14) :

$$\hat{K}^{(n)}(q) \approx -\frac{1}{q^2 + f\rho^n \mu^2} \cdot L \qquad (5.15)$$

The behaviour of this kernel is depicted qualitatively in figure 10 (with $\rho \approx 1/4$).

The kernel has a $1/q^2$ singularity, which is cut off below some $q_o^{(n)}$,

$$q_o^{(n)} = \rho^{n/2} \mu \qquad (5.16)$$

As we take higher and higher orders of perturbation theory (i.e. n very large, and $\rho^{n/2}$ very small), the cut-off occurs at smaller and smaller values of q, becoming indistinguishable from the London kernel :

$$\lim_{n \to \infty} \hat{K}^{(n)}(q) = -\frac{L}{q^2} \qquad (5.17)$$

This result agrees with that of Blatt and Matsubara, and that of Bogoljubov (1958 (c); 1959). This is to be expected, since our calculation (in which the ladder graphs play a central role) is one way of treating the leading contributions from high order terms, while the collective excitation formalism (which involves a summation over terms analogous to our ladder graphs) and the "method of the self-consistent field" are alternative approaches

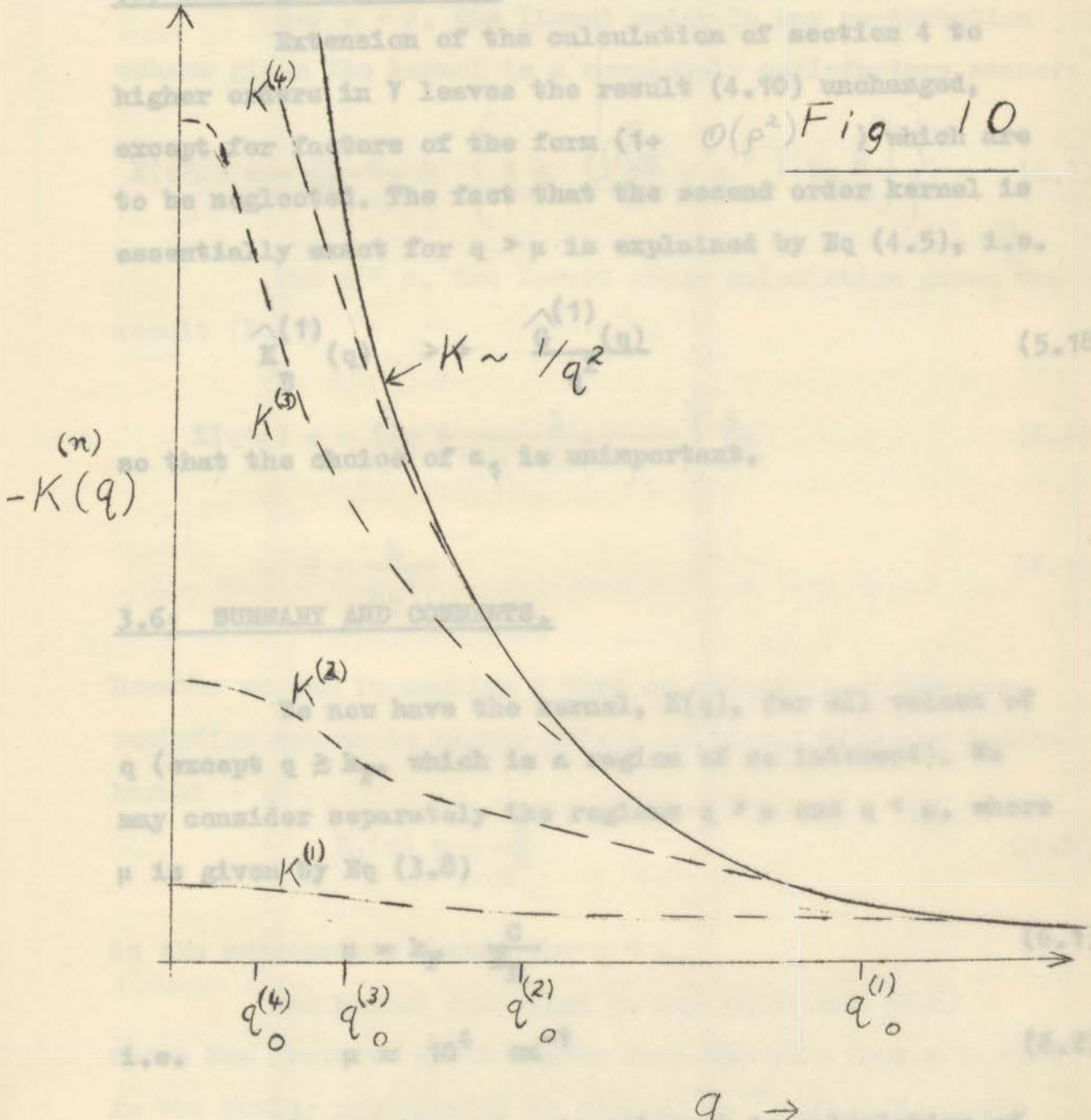


Fig 10

to these higher order terms.

(b) The region $q > \mu$: -

Extension of the calculation of section 4 to higher orders in γ leaves the result (4.10) unchanged, except for factors of the form $(1+ \mathcal{O}(\rho^2))$ which are to be neglected. The fact that the second order kernel is essentially exact for $q > \mu$ is explained by Eq (4.5), i.e.

$$\hat{K}_B^{(1)}(q) \; >> \; \frac{\hat{G}^{(1)}(q)}{q^2} \tag{5.18}$$

so that the choice of α_1 is unimportant.

3.6: SUMMARY AND COMMENTS.

We now have the kernel, $K(q)$, for all values of q (except $q \gtrsim k_F$, which is a region of no interest). We may consider separately the regions $q > \mu$ and $q < \mu$, where μ is given by Eq (3.8)

$$\mu = k_F \frac{C}{E_F} \tag{6.1}$$

i.e. $$\mu \approx 10^4 \text{ cm}^{-1} \tag{6.2}$$

The region $q > \mu$ is relevant to calculation of the penetration depth, as measured in static and microwave experiments, and allied quantities. The behaviour of $K(q)$

in the limit $q \to 0$ describes the law of field penetration at large distances within the superconductor - that is, it describes the qualitative nature of the M-O effect.

For $q > \mu$, the lowest order in our perturbation scheme gives the kernel in a completely satisfactory manner:

$$K(q>\mu) = -\frac{9\pi^2}{16}\frac{\mu}{q^3} L \left\{ 1 + \mathcal{O}\left[\left(\frac{\mu}{q} + e^{-\frac{1}{\rho}}\right) \ln \frac{\mu}{q}\right]\right\} \qquad (6.3)$$

For $q < \mu$, the lowest order calculation gives the result (3.31)

$$K(q<\mu) = -\left(\frac{4}{15} + \frac{3}{16(1-\ln^2)\rho}\right)\frac{L}{\mu^2} \qquad (6.4)$$

$$\equiv -\frac{L}{\mu_1^2} \qquad (6.5)$$

However we saw in section 5 that an extension of the perturbation scheme to higher orders indicates that the London kernel

$$K_L(q) = -\frac{L}{q^2} \qquad (6.6)$$

is the appropriate result for $q < \mu$.

The kernel described by Eqs (6.3) and (6.6) above has features which differ from the pure London kernel in the manner anticipated by Pippard (μ^{-1} being Pippard's "coherence length"). When treating penetration phenomena, the so-called "London penetration depth",

$$\lambda_L = \left(\frac{4\pi e^2 n}{mc^2}\right)^{-1/2} \qquad (6.7)$$

must be replaced by a penetration depth d,

$$d = \frac{4}{3\sqrt{3}} \times \frac{\lambda_L}{(\mu' \lambda_L)^{1/3}} \left\{ 1 + \frac{3\sqrt{3}}{4\pi} (\mu' \lambda_L)^{4/3} + \ldots \right\} \qquad (6.8)$$

with

$$\mu' \equiv \frac{9\pi^2}{16} \mu \qquad (6.9)$$

$$= \frac{9\pi^2}{16} \times \frac{kT_c}{1.13E_F} \times k_F \qquad (6.10)$$

The calculation of d, for specimens of size $R >> d$, follows the course outlined in section 1.3.

This expression agrees well with experimental results. For example, the experimentally measured penetration depth at absolute zero, d_o, for tin is

$$d_o(\text{Sn, expt.}) = 1.8 \ \lambda_L \qquad (6.11)$$

(London interpreted this fact as implying that 30°/o of the electrons were superconducting at zero temperature). Substituting the relevant parameters for tin in Eq (6.8) gives

$$d_o(\text{Sn, theoret.}) = 1.8 \ \lambda_L \qquad (6.12)$$

A point worth noting at this stage is the following:- the kernel calculated in lowest order remains finite in the limit $q \to o$ (Eq (6.4)). Comparison with the discussion of section 1.3 shows that there will be a small residual field at great distances inside a specimen:

$$B_\infty = B_o \left(\mu_1 \lambda_L\right)^2 \tag{6.13}$$

This is in contrast to the complete field expulsion of the kernel (6.6). However, experimental difficulties due to small locked-in magnetic fluxes are such as to make a detection of the effect (6.13) extremely difficult if $(\mu_1)^{-1}$ is greater than 10^{-4}cm (Casimir 1958). That is, the kernel calculated in lowest order (Eqs (6.3) and (6.4)), and that found in the limit of infinite order (Eqs (6.3) and (6.6), are from an experimental point of view indistinguishable. There remain significant differences in principle.

An experimental test as to the nature of the kernel at large q is provided by measurements of the magnetic susceptibility, χ , of a very fine-grained colloidal suspension of superconducting material. The kernel (6.3) and (6.6) anticipates that χ is given by (May and Schafroth, 1959)

$$\frac{\chi}{\chi_o} = 0.0108 \, \frac{\langle R^6 \rangle}{d^3 \langle R^3 \rangle} \left(1 + \mathcal{O}\left(\frac{\langle R^3 \rangle}{d^3}\right)\right) \tag{6.14}$$

Here χ_o is the susceptibility corresponding to no field penetration at all, and $\langle R^n \rangle$ is defined by

$$\langle R^n \rangle = \frac{\int R^n \rho(R)\, dR}{\int \rho(R)\, dR} \tag{6.15}$$

with ρ (R) dR being the number of (spherical) particles with radius between R and R + dR. The expression (6.14) is in contrast to that obtained from a pure London kernel, which predicts

$$\frac{\chi}{\chi_o} = \frac{1}{15} \frac{\langle R^5 \rangle}{d^2 \langle R^3 \rangle} \left(1 + \mathcal{O}\left(\frac{\langle R^2 \rangle}{d^2}\right)\right) \qquad (6.16)$$

Experimental results for χ/χ_o (Whitehead 1957) are consistent with the $(R/d)^3$ dependence of (6.14) and <u>not</u> with the $(R/d)^2$ London result. This fact gives rise to an experimental paradox : experiments on macroscopic specimens ($R >> d$) imply that d (T) varies like $\left[1 - (T/T_c)^4\right]^{-1/2}$, whereas experiments on microscopic specimens imply a $\left[1-(T/T_c)^4\right]^{-1/3}$ variation. This conflict of results (which does not arise if experiments on colloids are interpreted with the London kernel) is as yet unresolved.

APPENDIX A : CALCULATIONS FOR α_1 IN 3.3

The coefficients $a_o^{(1)}$, $a_2^{(1)}$, $b_o^{(1)}$ and $b_2^{(1)}$, defined by equations (3.23) and (3.24), are calculated in this appendix. In evaluating integrals arising in the Bogoljubov theory, we may utilize the fact that the dominant contribution comes from the Fermi surface: i.e. we replace $g^2/2\pi^2 \int k^2 dk$ by $\rho \int d\xi$. Also, in general, we replace the phonon energy $\omega(\underset{\sim}{k}-\underset{\sim}{k}')$ by an average energy, $\tilde{\omega}$, with $\tilde{\omega} \ll E_F$.

The coefficients are calculated under the assumption that ρ is small, compared to unity : in getting final results, quantities of order

$$\frac{\tilde{\omega}}{E_F} \ln \frac{\tilde{\omega}}{E_F} \ll 1 \; ; \quad \frac{1}{\rho} \exp\left(-\frac{1}{\rho}\right) \ll 1 \qquad (A.1)$$

are ignored, compared to unity.

(1) $a_o^{(1)}$, $b_o^{(1)}$:

First, for the $\frac{1}{q^2}$ coefficients, only terms of type (i) (see Section 3) need be considered. By an earlier argument, exemplified by (3.13), we get immediately

$$a_o^{(1)} = 0 \qquad (A.2)$$

A variety of terms contribute to $b_o^{(1)}$: these we have evaluated. It is found that, for various reasons,

many may be neglected as being smaller than the leading contribution by factors of at least $\frac{\tilde{\omega}}{E_F} \ln \frac{\tilde{\omega}}{E_F}$ or $\frac{1}{\rho} \exp(-\frac{1}{\rho})$ (cf. A.1).

The Bogoljubov formalism employed here leads to the following simplications:

(a) The choice of the parameters u, v and μ, λ such that "dangerous" graphs compensate means that all graphs with either two fermions or two phonons (only) in an intermediate must compensate, to give zero contribution

(b) Due to renormalization of phonon energies, graphs which contain internal phonon self-energy lines (e.g. fig. 11(a)) give contributions smaller than the leading one by factors of at least $\tilde{\omega}/E_F$. (cf. Bogoljubov 1958(b)).

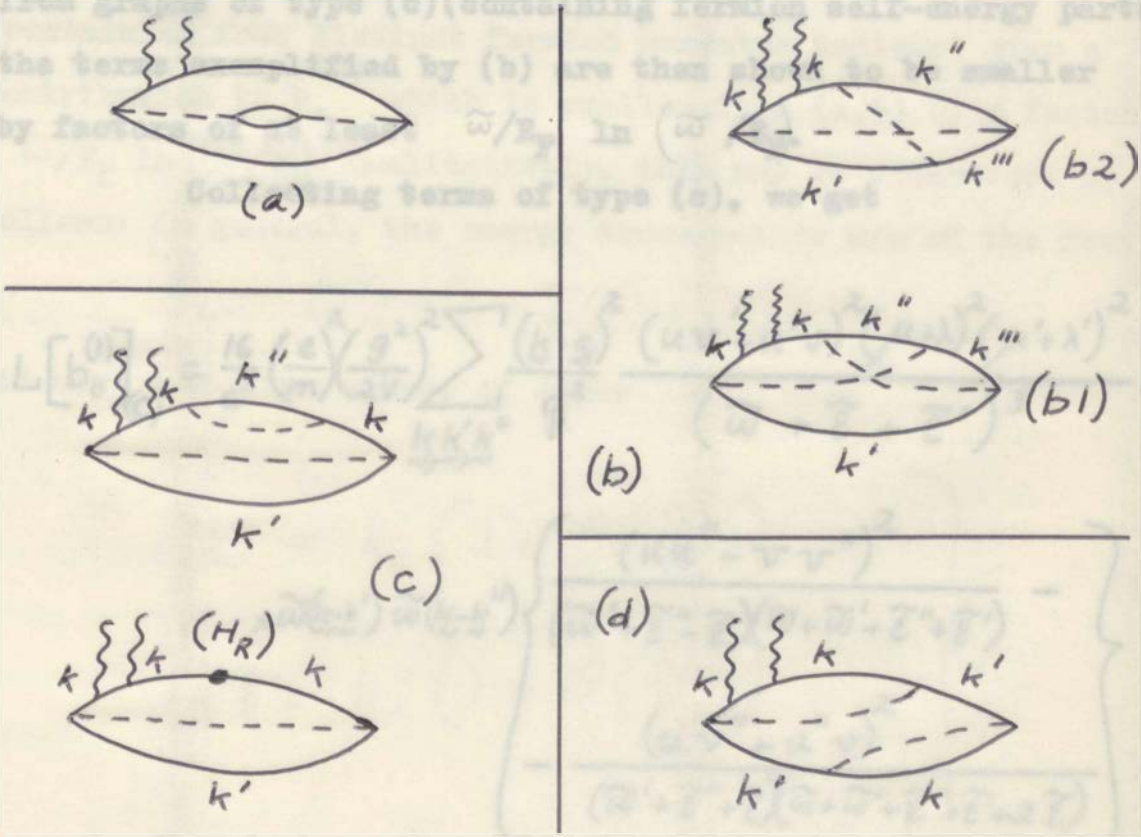


Fig. 11

Most of the remaining graphs (e.g. fig. 11(b)) contain four distinct fermion momenta ($\underset{\sim}{k}$, $\underset{\sim}{k}'$, $\underset{\sim}{k}''$, $\underset{\sim}{k}'''$) related by the requirement that

$$\underset{\sim}{k} + \underset{\sim}{k}''' = \underset{\sim}{k}' + \underset{\sim}{k}'' \qquad (A.3)$$

The other graphs contain not more than three distinct momentum indices, being of the type illustrated by figs. 11(c) and (d).

It is found that contributions from graphs of type (d) differ from those of type (c) by factors $\frac{1}{p}\exp(-\frac{1}{p})$: they are therefore ignored.

We now calculate the total contribution to $b_o^{(1)}$ from graphs of type (c)(containing fermion self-energy parts): the terms exemplified by (b) are then shown to be smaller by factors of at least $\tilde{\omega}/E_F \ln(\tilde{\omega}/E_F)$.

Collecting terms of type (c), we get

$$L\left[b_o^{(1)}\right]_{(c)} = \frac{16}{c^2}\left(\frac{e}{m}\right)^2\left(\frac{g^2}{2V}\right)^2 \sum_{\underset{\sim}{k}\underset{\sim}{k}'\underset{\sim}{k}''} \frac{(\underset{\sim}{k}\cdot\underset{\sim}{q})^2}{q^2} \frac{(uv'+u'v)^2(\mu+\lambda)^2(\mu'+\lambda')^2}{(\tilde{\omega}+\tilde{\varepsilon}+\tilde{\varepsilon}')^3} \times$$

$$\times \tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k}')\,\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k}'') \left\{ \frac{(uu''-vv'')^2}{(\tilde{\omega}'+\tilde{\varepsilon}''-\tilde{\varepsilon})(\tilde{\omega}+\tilde{\omega}'+\tilde{\varepsilon}''+\tilde{\varepsilon}')} - \right.$$

$$\left. - \frac{(uv''+u''v)^2}{(\tilde{\omega}'+\tilde{\varepsilon}''+\tilde{\varepsilon})(\tilde{\omega}+\tilde{\omega}'+\tilde{\varepsilon}''+\tilde{\varepsilon}'+2\tilde{\varepsilon})} \right\} \qquad (A.4)$$

(where $\tilde{\varepsilon}'$ means $\tilde{\varepsilon}^{(i)}(\underset{\sim}{k}')$, and so on). Utilizing the remarks made at the beginning of this appendix, we have $\left[b_o^{(1)}\right]_{(c)}$, to the approximation (A.1), as

$$\left[b_o^{(1)}\right]_{(c)} = 4\rho^2 \int_0^\infty\int_0^\infty\int_0^\infty \frac{d\xi\, d\xi'\, d\xi''}{(\tilde{\omega}+\xi+\xi')^3} \left\{ \frac{\tilde{\omega}\,\tilde{\omega}'}{(\tilde{\omega}'+\xi''-\xi)(\tilde{\omega}+\tilde{\omega}'+\xi''+\xi')} - \frac{\tilde{\omega}\,\tilde{\omega}'}{(\tilde{\omega}'+\xi''+\xi)(\tilde{\omega}'+\tilde{\omega}+\xi''+\xi'+2\xi)} \right\} \tag{A.5}$$

This expression reduces to

$$\left[b_o^{(1)}\right]_{(c)} = \frac{4}{3}(1-\ln 2)\,\rho^2 \tag{A.6}$$

We have yet to show that terms of type (b) (containing four distinct fermion momentum indices) give a contribution to $b_o^{(1)}$ which is smaller than (A.6) by a factor $\tilde{\omega}/E_F \ln(\tilde{\omega}/E_F)$. Qualitatively, this may be understood as follows: in general, the energy denominators are of the form

$$\tilde{\omega}(\underset{\sim}{k}-\underset{\sim}{k}') + \tilde{\varepsilon}(\underset{\sim}{k}) + \tilde{\varepsilon}(\underset{\sim}{k}')$$

and have a minimum value, of order $\tilde{\omega}$, when

$$\left.\begin{aligned} |\underset{\sim}{k}| &= k_F\left(1+\mathcal{O}\left(\frac{\tilde{\omega}}{E_F}\right)\right) \\ |\underset{\sim}{k}'| &= k_F\left(1+\mathcal{O}\left(\frac{\tilde{\omega}}{E_F}\right)\right) \end{aligned}\right\} \tag{A.7}$$

Consequently, when we come to integrate over fermion momenta, the dominant contributions occur when all the momenta have moduli of order k_F. At this stage, the condition (A.3) imposes a limitation on graphs of type (b) - if $|\underset{\sim}{k}'|$, $|\underset{\sim}{k}''|$ and $|\underset{\sim}{k}'''|$ be chosen to satisfy (A.7), only a fraction of those $\underset{\sim}{k}$ allowed by (A.3) will satisfy (A.7). Moreover, since this fraction is roughly $\tilde{\omega}/E_F$, it is not surprising that a quantitative evaluation of these integrals leads to a contribution to $b_o^{(1)}$ which is smaller, by such a fraction, than the contribution from integrals without a constraint like (A.3). As a quantitative example, we consider the graph described by fig. 11 (b1) :

$$L\left[b_o^{(1)}\right]_{(b1)} = \frac{2}{c^2}\left(\frac{e}{m}\right)^2\left(\frac{g^2}{2V}\right)^2 \sum_{\substack{\underset{\sim}{k},\underset{\sim}{k}',\underset{\sim}{k}'',\underset{\sim}{k}''' \\ (\underset{\sim}{k}'''=\underset{\sim}{k}'+\underset{\sim}{k}''-\underset{\sim}{k})}} \tilde{\omega}\tilde{\omega}\frac{(\underset{\sim}{k}\cdot\underset{\sim}{q})^2}{q^2}(\mu+\lambda)^2(\mu'+\lambda')^2 \times \tag{A.8}$$

$$\times \frac{(uv'+u'v)(u'v'''+u'''v')(uu''-vv'')(u''u'''-v''v''')}{(\tilde{\omega}+\tilde{\varepsilon}+\tilde{\varepsilon}')^3(\tilde{\omega}+\tilde{\omega}'+\tilde{\varepsilon}'+\tilde{\varepsilon}'')(\tilde{\omega}'+\tilde{\varepsilon}'+\tilde{\varepsilon}''')}$$

That is, replacing sums by integrals in the customary fashion,

$$\left[b_o^{(1)}\right]_{(b1)} = \frac{1}{2}\rho^2 \int_0^\infty\int_0^\infty\int_0^\infty \frac{d\xi\, d\xi'\, d\xi''}{(\tilde{\omega}+\xi+\xi')^3(\tilde{\omega}+\tilde{\omega}'+\xi'+\xi'')} \times \tag{A.9}$$

$$\times \frac{1}{8\pi}\int_{-1}^{+1}dx\int_{-1}^{+1}dx'\int_0^{2\pi}d\phi\, \frac{\tilde{\omega}\,\tilde{\omega}'}{(\tilde{\omega}'+\xi'+\xi''')}$$

where

$$\xi''' = \xi+\xi'+\xi''+2E_F\left(1-x-x'+\left[xx'+\sqrt{(1-x^2)(1-x'^2)}\cos\phi\right]\right).$$

Finally, Eq (A.9) reduces to

$$\left[b_o^{(1)}\right]_{(b7)} = \frac{1}{2}\rho^2\tilde{\omega}^2 \int_0^\infty\int_0^\infty \frac{d\xi\, d\xi'}{(\tilde{\omega}+\xi+\xi')^3} \times \frac{\ln 2}{E_F}\left\{\ln\frac{E_F}{\tilde{\omega}} + \mathcal{O}(1)\right\} \qquad (A.10)$$

$$= -\frac{\ln 2}{4}\,\rho^2\left(\frac{\tilde{\omega}}{E_F}\ln\frac{\tilde{\omega}}{E_F}\right) \quad \ldots \qquad (A.11)$$

which justifies the remarks above.

Hence, collecting all terms but neglecting relative orders $\tilde{\omega}/E_F \ln(\tilde{\omega}/E_F)$ and $1/\rho\ \exp(-1/\rho)$, $b_o^{(1)}$ is found from Eq (A.6) :

$$b_o^{(1)} = \frac{4}{3}(1-\ln 2)\,\rho^2 \qquad (A.12)$$

(2) $a_2^{(1)}$, $b_2^{(1)}$:

Now we must consider terms of the general type (ii) and (iii)(whose leading terms are proportional to $\frac{1}{\mu^2}$), as well as the second order terms in the expansion of type (i) in powers of $(\frac{q}{\mu})$. We can pick out certain terms, of type (ii), which give a contribution larger than others by a factor of (at least) $1/\rho$. These are the so-called ladder graph terms, as illustrated by fig. 9 (b) and (d) - but not by (a) and (c). They are characterized by the fact that each alternate energy denominator contains no phonon terms (see e.g. equation (A.17) below). They do not contain either fermion or phonon self-energy parts (such graphs are found to give contributions

smaller than those due to ladder graphs by factors of at least ρ (fermion self-energy) or $\tilde{\omega}/E_F$ (phonon self-energy)); nor do they contain the process whereby a fermion pair is annihilated and re-created by a phonon (these have been found to differ from ladder graphs by factors of at least $\frac{q}{\mu} \cdot \frac{\tilde{\omega}}{E_F}$).

An important property of graphs of type (ii) is that their contributions to $\mathcal{K}_B^{(1)}(q)$ and to $\mathcal{G}^{(1)}(q)/q^2$, $\left\{ \left[\mathcal{K}_B^{(1)}(q)\right]_{ii} \text{ and } \left[\mathcal{G}^{(1)}(q)/q^2\right]_{ii} \text{ say} \right\}$, are equal in magnitude, but opposite in sign. This may be proved as follows:

In these graphs, the matrix elements for the two j_2^o operators contain different momentum indices : such is not the case in types (i) and (iii). The consequent $\left[\mathcal{K}_B^{(1)}(q)\right]_{ii}$ assumes the form

$$\left[\mathcal{K}_B^{(1)}(q)\right]_{ii} = \sum_{\underset{\sim}{k},\underset{\sim}{k}'} \left(\frac{1}{2}\,\underset{\sim}{k}.\underset{\sim}{k}' - \frac{3}{2}\,\frac{(\underset{\sim}{k}.\underset{\sim}{q})(\underset{\sim}{k}'.\underset{\sim}{q})}{q^2}\right) f\left(|\underset{\sim}{k}|, \underset{\sim}{k}.\underset{\sim}{q}, |\underset{\sim}{k}'|, \underset{\sim}{k}'.\underset{\sim}{q}\right) \qquad (A.13)$$

Writing

$$(\underset{\sim}{k}.\underset{\sim}{k}') = \frac{1}{q^2}\left\{(\underset{\sim}{k}.\underset{\sim}{q})(\underset{\sim}{k}'.\underset{\sim}{q}) + (\underset{\sim}{k}\times\underset{\sim}{q}).(\underset{\sim}{k}'\times\underset{\sim}{q})\right\} \qquad (A.14)$$

(A.13) reduces to

$$\left[\mathcal{K}_B^{(1)}(q)\right]_{ii} = -\sum_{\underset{\sim}{k}\,\underset{\sim}{k}'} \frac{(\underset{\sim}{k}.\underset{\sim}{q})(\underset{\sim}{k}'.\underset{\sim}{q})}{q^2} f\left(|\underset{\sim}{k}|, \underset{\sim}{k}.\underset{\sim}{q}, |\underset{\sim}{k}'|, \underset{\sim}{k}'.\underset{\sim}{q}\right) \qquad (A.15)$$

i.e.

$$\left[\mathcal{K}_B^{(1)}(q)\right]_{ii} = -\left[\mathcal{G}^{(1)}(q)/q^2\right]_{ii} \qquad (A.16)$$

Thus for terms of type (ii), there is no need to find $a_2^{(1)}$ and $b_2^{(1)}$ separately.

Now we calculate a typical member of the ladder graph terms, namely that corresponding to fig. 9(d). The contribution to $b_2^{(1)}$ from this graph ($[b_2^{(1)}]_1$, say) is

$$L[b_2^{(1)}]_1 = \frac{2}{c^2}\left(\frac{e}{m}\right)^2 \sum_{\underset{\sim}{k}\,\underset{\sim}{k}'\,\underset{\sim}{k}''} \frac{(\underset{\sim}{k}.\underset{\sim}{q})^2(\underset{\sim}{k}'.\underset{\sim}{q})^2}{kk'\,q^4}\left(\frac{g^2}{2V}\right)^2\left(\frac{c^2}{c^2+\xi^2}\right)\left(\frac{c^2}{c^2+\xi'^2}\right)\times$$

$$\times\,\tilde{\omega}\,\tilde{\omega}' \times \frac{(\mu+\lambda)^2(\mu'+\lambda')^2(uv''+u''v)^2(u'u''-v'v'')^2}{2\tilde{\varepsilon}(\tilde{\omega}+\tilde{\varepsilon}+\tilde{\varepsilon}'')(2\tilde{\varepsilon}''+2\tilde{\varepsilon})(\tilde{\omega}'+\tilde{\varepsilon}''+\tilde{\varepsilon}'+2\tilde{\varepsilon})(2\tilde{\varepsilon}'+2\tilde{\varepsilon})} \qquad (A.17)$$

We now replace sums by integrals in the usual manner, and perform the integration over ξ'' (noting that $\ln \tilde{\omega}/c = 1/\rho$).

$$[b_2^{(1)}]_1 = \frac{1}{48}\rho^2 \int_0^\infty \frac{dy}{(1+y^2)^{3/2}} \int_0^\infty \frac{dy'}{(1+y'^2)} \left\{\frac{1}{\sqrt{1+y^2}+\sqrt{1+y'^2}}\right\} \times$$

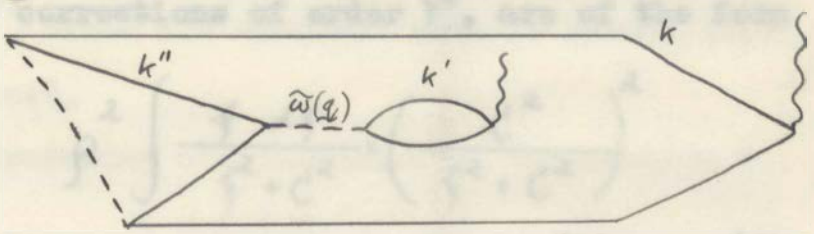
$$\times \left\{\frac{1}{\rho} + \left(\ln 2 - 1 + \frac{\sqrt{1+y^2}}{y}\ln\left(\sqrt{1+y^2}-y\right)\right) + O(e^{-1/\rho})\right\} \qquad (A.18)$$

$$= \frac{1}{96}\rho\left[1+O(\rho)\right] \qquad (A.19)$$

Summing over all ladder graphs leads to the result

$$\left[b_2^{(1)}\right]_{L.G.} = -\left[a_2^{(1)}\right]_{L.G.} = \tfrac{1}{4}\rho\left[1+\mathcal{O}(\rho)\right] \qquad (A.20)$$

The fact that this result is of order ρ, rather than ρ^2, is a consequence of alternate energy denominators containing no phonon contributions: the ensuing intermediate state denominator $\tilde{\mathcal{E}}(\underset{\sim}{k}'') + \tilde{\mathcal{E}}(\underset{\sim}{k})$ in (A.17), for example, then produces a factor $1/\rho$. It is thus easy to understand why the remaining terms of type (ii) (such as fig. 9(a) and (c)), which <u>do</u> contain phonons in the intermediate state, are found to be of order ρ^2. [At this stage, it is also easy to verify the remarks made on page 97-98 relevant to graphs which differ from ladder graphs by containing fermion or phonon self-energies, or the annihilation and re-creation of a fermion pair by a phonon. For example, to find the contribution to $b_2^{(1)}$ of the graph illustrated by fig. 12,



<u>Fig.12</u>

we make the following alterations to Eq (A.17):-

$$\text{(i)}\quad (u'u'' - v'v'')^2 \longrightarrow (u''_+v''_- + u''_-v''_+)(u'_+v'_- + u'_-v'_+)$$

where u'_+ means $u_{\underset{\sim}{k}'+\underset{\sim}{q}/2}$, etc.,

(ii) $\tilde{\omega}(\underset{\sim}{k}' - \underset{\sim}{k}'') \longrightarrow \tilde{\omega}(\underset{\sim}{q})$

(iii) $(\tilde{\omega}' + \tilde{\varepsilon}'' + \hat{\varepsilon}' + 2\tilde{\varepsilon}) \longrightarrow (\tilde{\omega}(\underset{\sim}{q}) + 2\hat{\varepsilon})$

The alteration (ii) produces a factor of order q/k_F, and (i) together with (iii) a factor $\tilde{\omega}/c$, resulting in a nett contribution to $b_2^{(1)}$ which is smaller than that for the true ladder graph by a factor $\frac{q}{k_F} \cdot \frac{\tilde{\omega}}{c} = \frac{q}{\mu} \cdot \frac{\tilde{\omega}}{E_F}$.]

Contributions to $b_2^{(1)}$ and $a_2^{(1)}$ also come from type (i) graphs, by expanding the matrix elements for j_1^o according to (3.6). The resultant integrals are similar to those for $b_o^{(1)}$, except for a factor of the form $c^4/(c^2+\xi^2)^2$. Inspecting the results for $b_o^{(1)}$, we find that introduction of such a modification produces a factor $\exp(\frac{-1}{\rho})$; thus, within the approximation defined above, (A.1), the contribution from type (i) terms is negligible.

Finally, type (iii) terms, which are proportional to the energy corrections of order γ^4, are of the form

$$\rho^2 \int \frac{\xi \, d\xi}{\xi^2 + c^2} \times \left(\frac{c^2}{\xi^2 + c^2} \right)^2 \qquad \text{(A.21)}$$

That is, the consequent contributions to $b_2^{(1)}$ and $a_2^{(1)}$ are proportional to ρ^2.

Using all these facts, and in particular the equation (A.20) for the ladder graphs, we get the results (3.27) and (3.28).

APPENDIX B : EVALUATION OF AN INTEGRAL.

In this appendix we evaluate the integral (4.1), pertinent to the magnetic response at large q. That is to say, we calculate

$$I(\delta) \equiv \int_0^\infty dy \int_0^1 dx \, \frac{(3x^2-1)}{\sqrt{(y+x)^2+\delta^2}+\sqrt{(y-x)^2+\delta^2}} \left\{ 1 - \frac{(y^2-x^2+\delta^2)}{\sqrt{((y+x)^2+\delta^2)((y-x)^2+\delta^2)}} \right\} \quad (B.1)$$

in the limiting case of $\delta < 1$

First, we note that, putting $\delta = 0$,

$$I\ (0) = \int_0^1 dy \int_y^1 dx \, \frac{(3x^2-1)}{x} \quad (B.2)$$

i.e. $$I\ (0) = 0 \quad (B.3)$$

A direct expansion of (B.1), as such, is difficult: we find it easier to expand the derivative of $I(\delta)$ with regard to δ. Since the constant term is known, (B.3), $I(\delta)$ is thus obtained.

Introducing new variables of integration :

$$\left.\begin{aligned} s &= y + x \\ t &= y - x \end{aligned}\right\} \quad (B.4)$$

(B.1) becomes

$$I(\delta) = \frac{1}{2}\left[\int_1^\infty ds \int_{s-2}^{s} dt + \int_0^1 ds \int_{-s}^{s} dt\right] \frac{\left(\frac{3}{4}(s-t)^2-1\right)}{\sqrt{s^2+\delta^2}+\sqrt{t^2+\delta^2}} \left\{ 1 - \frac{st+\delta^2}{\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} \right\} \quad (B.5)$$

Then, differentiating with respect to δ ,

$$\frac{dI(\delta)}{d\delta} = -\frac{\delta}{2} J \tag{B.6}$$

where, for convenience, J is separated in three parts:

$$J = J_1 + J_2 + J_3 \tag{B.7}$$

$$J_1 = \left[\int_1^\infty ds \int_{s-2}^{s} dt + \int_0^1 ds \int_{-s}^{s} dt\right] \frac{\frac{3}{4}(s-t)^2}{\left(\sqrt{s^2+\delta^2}+\sqrt{t^2+\delta^2}\right)\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} \times$$

$$\times \left\{3 - (st+\delta^2)\left(\frac{1}{s^2+\delta^2} + \frac{1}{\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} + \frac{1}{t^2+\delta^2}\right)\right\}$$

$$J_2 = \left[\int_1^\infty ds \int_{s-2}^{s} dt + \int_0^1 ds \int_{-s}^{s} dt\right] \frac{(st+\delta^2)}{\left(\sqrt{s^2+\delta^2}+\sqrt{t^2+\delta^2}\right)\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} \left\{\frac{1}{(s^2+\delta^2)} + \frac{1}{\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} + \frac{1}{(t^2+\delta^2)}\right\}$$

$$+ \left[\int_1^\infty ds \int_{s-2}^{s} dt\right] \frac{(-3)}{\left(\sqrt{s^2+\delta^2}+\sqrt{t^2+\delta^2}\right)\sqrt{(s^2+\delta^2)(t^2+\delta^2)}} \tag{B.8}$$

$$J_3 = -3 \int_0^1 ds \int_{-s}^{s} dt \frac{1}{\left(\sqrt{s^2+\delta^2}+\sqrt{t^2+\delta^2}\right)\sqrt{(s^2+\delta^2)(t^2+\delta^2)}}$$

From (B.6) it follows that those terms of J which are regular in δ give contributions to $I(\delta)$ which are, at most, of order δ^2 - this order we neglect. Thus we confine attention to those terms in J_1, J_2 and J_3 which are singular in the limit $\delta \to 0$.

In J_1 and J_2, putting $\delta = 0$ gives rise to, at worst, logarithmic singularities: these are then separated out, to give

$$J_1 = -12 \ln \delta + (\text{terms regular in } \delta) \qquad (B.9)$$

$$J_2 = 2\ln \delta + (\text{terms regular in } \delta) \qquad (B.10)$$

A more detailed treatment is required for J_3, which has a stronger (δ^{-1}) singularity. Performing the integration over t,

$$J_3 = -6 \int_0^1 \frac{dS}{S(S^2+\delta^2)^{1/2}} \ln \left\{ \frac{(S^2+\delta^2)^{1/2}}{\delta} \right\} \qquad (B.11)$$

This may be expressed as

$$J_3 = -\frac{6}{\delta} \left[\int_0^1 \frac{dr}{1-r^2} \ln(1/r) - \int_{1/\delta}^{\infty} \frac{dr}{r(1+r^2)^{1/2}} \ln\left\{(1+r^2)^{1/2}\right\} \right] \qquad (B.12)$$

$$= -\frac{3\pi^2}{4\delta} - 6\ln\delta + (\text{terms regular in } \delta) \qquad (B.13)$$

Thus, collecting together the expressions for J_1, J_2 and J_3, we have

$$\frac{dI(\delta)}{d\delta} = \frac{3\pi^2}{8} + 8\delta \ln \delta + \mathcal{O}(\delta) \qquad (B.14)$$

Using (B.3), the final expression, used in (4.2), is now obtained :

$$I(\delta) = \frac{3\pi^2}{8}\,\delta\left\{1+\frac{32}{3\pi^2}\,\delta\,\ln\delta + \mathcal{O}(\delta^2)\right\} \qquad (B.15)$$

The simplification of equation (4.3) for $\hat{G}^{(1)}(q)$ is carried through in a precisely analogous manner.

APPENDIX C : CALCULATIONS FOR α_1 IN 3.4.

The quantities $\mathcal{K}_B^{(1)}(q)$ and $\mathcal{G}^{(1)}(q)/q^2$, defined by (3.20), are found here in the case of $q > \mu$.

To illustrate the argument, we begin by evaluating the contributions $\left[\mathcal{K}_B^{(1)}(q)\right]_1$ and $\left[\mathcal{G}^{(1)}(q)/q^2\right]_1$, from the ladder graph shown in fig. 9 (d).

$$\left[\mathcal{G}^{(1)}(q)/q^2\right]_1 = -\left[\mathcal{K}_B^{(1)}(q)\right]_1$$

$$= \frac{1}{q^2}\times\frac{2}{c^2}\left(\frac{e}{m}\right)^2 \sum_{\underset{\sim}{k}\,\underset{\sim}{k}'\underset{\sim}{k}''} \frac{(\underset{\sim}{k}\cdot\underset{\sim}{\epsilon})(\underset{\sim}{k}'\cdot\underset{\sim}{\epsilon})}{q^2}\left(\frac{g^2\tilde{w}}{2V}\right)^2 (u+\lambda)^2(u'+\lambda')^2 \times \qquad (C.1)$$

$$\times \frac{(u_+v_+'' + u_+''v_+)(u_-v_-'' + u_-''v_-)(u_+'u_+'' - v_+'v_+'')(u_-'u_-'' - v_-'v_-'')(u_+v_- - u_-v_+)(u_+'v_-' - u_-'v_+')}{(\tilde{\varepsilon}_+ + \tilde{\varepsilon}_-)(\tilde{w} + \tilde{\varepsilon}_+'' + \tilde{\varepsilon}_-)(\tilde{\varepsilon}_+'' + \tilde{\varepsilon}_+ + \tilde{\varepsilon}_-'' + \tilde{\varepsilon}_-)(\tilde{w} + \tilde{\varepsilon}_+' + \tilde{\varepsilon}_-'' + \tilde{\varepsilon}_+ + \tilde{\varepsilon}_-)(\tilde{\varepsilon}_+' + \tilde{\varepsilon}_+ + \tilde{\varepsilon}_-' + \tilde{\varepsilon}_-)}$$

u_+' means $u_{\underset{\sim}{k}+\frac{\underset{\sim}{q}}{2}}'$, and so on.

We now replace sums by integrals, and make the change in variables $\xi = \frac{q}{\mu} Cy$, and $\underset{\sim}{k}\cdot\underset{\sim}{q} = k\,q\cos\theta = k\,q\,x$, etc. Terms of relative order $\left(\frac{\mu}{q}\right)^2$ are ignored: this corresponds to taking the normal state values of u and v. In such case, the presence of matrix elements $(u_+v_- - u_-v_+)$ amounts to the requirement $|x| > |y|$, while the occurrence of $(u_+u_- + v_+v_-)$ implies $|y| > |x|$. (C.1) now becomes

$$\left[\mathcal{G}^{(1)}(q)/q^2\right]_1 = -\left[\mathcal{K}_B^{(1)}(q)\right]_1 = \frac{3}{128}\rho^2\frac{L}{q^2}\int_0^1 dx\int_0^1 dx'\int_0^1 dx'' \, x \int_{-x}^{x} dy \int_{-x'}^{x'} dy' \int_{-x''}^{x''} dy'' \, \frac{xx'}{x(x+x')(x+x'')(\Lambda+x''+y''+x+y)(\Lambda+x'+y'+x''-y''+2x)} \qquad (C.2)$$

where

$$\Lambda \equiv \frac{\mu}{q} \times \frac{\omega}{c} \qquad (C.3)$$

Evaluation of (C.2), and all other integrals associated with $\mathcal{K}_B^{(1)}(q)$ and $\mathcal{G}^{(1)}(q)/q^2$, is simplified by considering two regions of q values separately:

$$\text{(a)} \quad \mu\frac{\omega}{c} > q \; (> \mu) \quad \Lambda > 1 \qquad (C.4)$$

$$\text{(b)} \quad \mu\frac{\omega}{c} < q \; (< k_F) \quad \Lambda < 1 \qquad (C.5)$$

Region (a):

Equation (C.2) becomes

$$\left[\mathcal{G}^{(1)}(q)/q^2\right]_1 = -\left[\mathcal{K}_B^{(1)}(q)\right]_1 = \frac{3}{16}\frac{L}{q^2}\rho^2 I\left\{1+\mathcal{O}\left(\frac{1}{\Lambda}\right)\right\} \qquad (C.6)$$

where I is a numerical constant $\left(I = \frac{1}{15}\left\{1+11\ln 2-6(\ln 2)^2-\frac{\pi^2}{2}\right\}\right)$.

A similar result holds for terms of type (ii) in general, so that for these terms, both $\mathcal{K}_B^{(1)}(q)$ and $\mathcal{G}^{(1)}(q)/q^2$ are

proportional to $\frac{L}{q^2}\rho^2$.

It is readily verified that when terms of types (i) and (iii) are calculated, by a procedure analogous to that for the example just given, they give contributions to $\mathcal{K}_B^{(1)}(q)$ and $\mathcal{G}^{(1)}(q)/q^2$ which are, in essence, of the form

$$\begin{bmatrix} \mathcal{G}^{(i)}(q)/q^2 \\ - - - - \\ \mathcal{K}_B^{(i)}(q) \end{bmatrix} \propto \frac{L}{q^2}\rho^2 \int_0^1 \frac{\Lambda^2 dx}{(\Lambda+x)^2} \begin{bmatrix} x^2 \\ - - - - - \\ 1-3x^2 \end{bmatrix} \qquad (C.7)$$

Thus for $\Lambda > 1$, the contribution of these terms to $\mathcal{G}^{(1)}(q)/q^2$ has a leading component $\frac{L}{q^2}\rho^2$, while their contribution to $\mathcal{K}_B^{(1)}(q)$ is smaller by a factor $1/\Lambda$.

To summarize, in region (a) we find by adding up all terms,

$$\mathcal{K}_B^{(1)}(q) = \sigma_1 \frac{L}{q^2}\rho^2 \left(1+\mathcal{O}(1/\Lambda)\right) \qquad (C.8)$$

$$\mathcal{G}^{(1)}(q)/q^2 = \sigma_2 \frac{L}{q^2}\rho^2 \left(1+\mathcal{O}(1/\Lambda)\right) \qquad (C.9)$$

where σ_1, σ_2 are numerical factors

Region (b) :

Returning to equation (C.2), we find that for $\Lambda < 1$ it becomes

$$\left[\mathcal{G}^{(1)}(q)/q^2\right]_1 = -\left[\mathcal{K}_B^{(1)}(q)\right]_1$$

$$= (\text{numerical constant}) \times \frac{L}{q^2} \rho^2 \Lambda^2 \left(1 + \mathcal{O}(\Lambda \ln \Lambda)\right) \qquad (C.10)$$

Results of this form hold generally for type (ii) terms, in the region (b) : they differ from those for region (a) by factors Λ^2.

For type (i) and (iii) terms, the form (C.7) may be simplified, to get a contribution to $\mathcal{G}^{(1)}(q)/q^2$ which is again like (C.10). However, the contribution to $\mathcal{K}_B^{(1)}(q)$ of such terms is seen to be proportional to $\frac{L}{q^2} \rho^2 \Lambda$:

that is, it is larger by a factor $1/\Lambda$ than contributions of type (ii).

Collecting the above results, in region (b) we have

$$\mathcal{K}_B^{(1)}(q) = \sigma_3 \frac{L}{q^2} \rho^2 \Lambda \left(1 + \mathcal{O}(\Lambda \ln \Lambda)\right) \qquad (C.11)$$

$$\mathcal{G}^{(1)}(q)/q^2 = \sigma_4 \frac{L}{q^2} \rho^2 \Lambda^2 \left(1 + \mathcal{O}(\Lambda \ln \Lambda)\right) \qquad (C.12)$$

where σ_3, σ_4 are again numerical factors.

Hence the result (4.8) follows

$$\alpha_1 = \sigma/\Lambda \ (1+ \mathcal{O}(\Lambda \ln \Lambda \ )) \qquad (C.13)$$

APPENDIX D : CALCULATIONS FOR α_1 IN 3.5.

We now extend the procedure of Appendix A to evaluate the coefficients $a_o^{(n)}$, $a_2^{(n)}$, $b_o^{(n)}$ and $b_2^{(n)}$ in nth order of our perturbation scheme. This task is greatly faciliated by the calculation for the case of n = 1 : most of the remarks made there may be generalized to arbitrary n.

(1) $a_o^{(n)}$:

It has been seen earlier ((3.13) and (A.2)) that the $\frac{1}{q^2}$ term in both $K_B^{(1)}(q)$ and $\mathcal{K}_B^{(1)}(q)$ has a coefficient zero. This property holds quite generally, for $\mathcal{K}_B^{(n)}(q)$. Thus

$$a_o^{(n)} = \sum_{\underset{\sim}{k}} \left\{ \frac{1}{2} \underset{\sim}{k}.\underset{\sim}{k} - \frac{3}{2} \frac{(\underset{\sim}{k}.\underset{\sim}{q})^2}{q^2} \right\} f(|\underset{\sim}{k}|) \qquad (D.1)$$

$$= 0 \qquad (D.2)$$

(2) $b_o^{(n)}$:

Only graphs of the general type (i) need be considered to find $b_o^{(n)}$. From the definition of $\mathcal{K}^{(n)}(q)$, such graphs will be of order $\gamma^{2(n+1)}$ - that is, they contain (n+1) internal phonon lines, each accompanied by a factor g^2. Thence, on replacing sums by integrals, a factor ρ^{n+1} arises.

Most of the possible graphs may be neglected, for the reasons detailed in dealing with the case of n = 1 : they give contributions smaller than the leading one by factors of $\frac{\tilde{\omega}}{E_F} \ln\left(\frac{E_F}{\tilde{\omega}}\right)$ or $\rho \exp(-1/\rho)$. As before, there remain graphs (containing fermion self-energy parts) which lead to a result for $b_o^{(n)}$ differing from ρ^{n+1} by a purely numerical factor (e.g. $\frac{4}{3}(1-\ln 2)$ for n = 1). Hence we get the equation (5.13).

(3) $a_2^{(n)}$, $b_2^{(n)}$:

We first consider type (ii) terms, which give contributions to $a_2^{(n)}$ and $b_2^{(n)}$ equal in magnitude, but opposite in sign.

The contribution from a typical ladder graph in nth order (as illustrated in fig. 13)

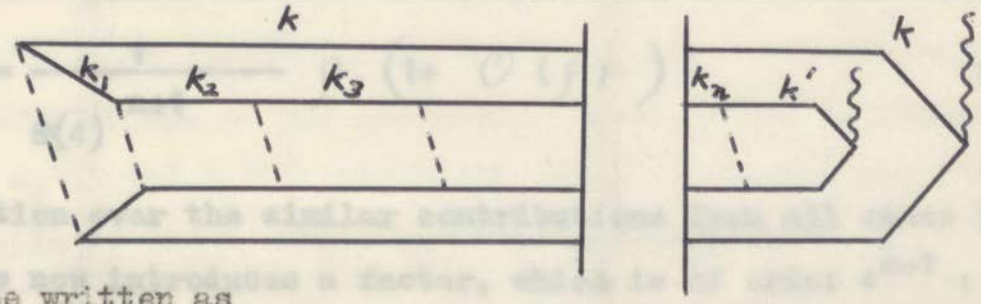


Fig.13.

may be written as

$$L\left[b_2^{(n)}\right]_1 = \frac{2}{c^2}\left(\frac{e}{m}\right)^2 \sum_{\underset{\sim}{k}\underset{\sim}{k}'\underset{\sim}{k}_1 \cdots \underset{\sim}{k}_n} \frac{(\underset{\sim}{k}\cdot\underset{\sim}{\xi})^2(\underset{\sim}{k}'\cdot\underset{\sim}{\xi})^2}{kk'q^4}\left(\frac{g^2\tilde{\omega}}{2V}\right)^{n+1}\left(\frac{c^2}{\xi^2+c^2}\right)\left(\frac{c^2}{\xi'^2+c^2}\right)\times$$

$$\times \frac{(uv_1+u_1v)^2(\lambda+\mu)^2(u_1u_2-v_1v_2)^2(\lambda_1+\mu_1)^2 \cdots\cdots (u_n u'-v_n v')^2}{2\tilde{\varepsilon}(\tilde{\omega}+\tilde{\varepsilon}+\tilde{\varepsilon}_1)(2\tilde{\varepsilon}_1+2\tilde{\varepsilon})(\tilde{\omega}+\tilde{\varepsilon}_1+\tilde{\varepsilon}_2+2\tilde{\varepsilon})\cdots(\tilde{\omega}+\tilde{\varepsilon}_n+\tilde{\varepsilon}'+2\tilde{\varepsilon})(2\tilde{\varepsilon}'+2\tilde{\varepsilon})} \qquad (D.3)$$

Making the usual approximations, this reduces to

$$\left[b_2^{(n)}\right]_1 = \frac{1}{3}\times\frac{\rho^{n+1}}{(2^{n+1})^2}\int_0^\infty \frac{C^2\,d\xi}{(C^2+\xi^2)^{3/2}}\int_0^\infty \frac{C^2\,d\xi'}{C^2+\xi'^2}\left\{\frac{1}{\sqrt{C^2+\xi^2}+\sqrt{C^2+\xi'^2}}\right\}\times \tag{D.4}$$

$$\times\int_0^\infty d\xi_1\int_0^\infty d\xi_2 \cdots \int_0^\infty d\xi_n \frac{(\widehat{\omega})^{n+1}}{(\widehat{\omega}+\widehat{\varepsilon}_1+\widehat{\varepsilon})(\widehat{\varepsilon}_1+\widehat{\varepsilon})\cdots\cdots(\widehat{\varepsilon}_n+\widehat{\varepsilon})(\widehat{\omega}+\widehat{\varepsilon}_n+\widehat{\varepsilon}'+2\widehat{\varepsilon})}$$

Performing the integrations over ξ_1, —, ξ_n, one by one, and keeping only the most important terms, we get the direct analogue of equation (A.18),

$$\left[b_2^{(n)}\right]_1 = \frac{1}{3}\left(\frac{\rho}{4}\right)^{n+1}\int_0^\infty \frac{dy}{(1+y^2)^{3/2}}\int_0^\infty \frac{dy'}{(1+y'^2)}\times$$

$$\times\left\{\frac{1}{\sqrt{1+y^2}+\sqrt{1+y'^2}}\right\}\ \frac{1}{\rho^n}\left\{1+\mathcal{O}(\rho)\right\} \tag{D.5}$$

$$= \frac{1}{6\times(4)^{n+1}}\,\rho\,\left(1+\mathcal{O}(\rho)\right) \tag{D.6}$$

Summation over the similar contributions from all other ladder graphs now introduces a factor, which is of order 4^{n+1} : thus we have that the contribution of the ladder graphs to $b_2^{(n)}$ is $\rho\,(1+\mathcal{O}(\rho))$, up to some purely numerical factor. As in the case of n = 1, all other possible graphs of type (ii) give contributions which are smaller than those due to ladder graphs by factors of at least ρ.

It is easily seen that type (i) contributions are at least of order ρ^{n+1} - energy denominators of the type which give rise to factors $1/\rho$ in the ladder graphs do not occur in type (i) graphs. Also, the argument used to show that for n = 1, type (iii) terms are proportional to ρ^2, is readily extended to show that, in general, these terms are of order ρ^{n+1}.

Thus the lowest order contribution to $a_2^{(n)}$ and $b_2^{(n)}$ from type (ii) terms is proportional to ρ, while that from types (i) and (iii) is proportional to ρ^{n+1}. The relation between the coefficients valid for type (ii) terms may then be utilized, to get

$$b_2^{(n)} = - a_2^{(n)} \left(1 + \mathcal{O}(\rho^n)\right) \qquad (D.7)$$

These results now give (5.12) and (5.14). The fact that they are indefinite up to purely numerical factors does not concern us, as the essential feature which is needed is that $a_2^{(n)}$ and $b_2^{(n)}$ remain of order ρ (being equal but opposite in sign), while $b_o^{(n)}$ is of order ρ^{n+1}.

CHAPTER IV

PAIR CORRELATIONS IN THE QUASICHEMICAL EQUILIBRIUM THEORY

4.1 : INTRODUCTION

4.1 : INTRODUCTION

The quasichemical equilibrium scheme is an approximation method for evaluating the partition function of a system of interacting fermions. It consists of treating statistical correlations exactly, but neglecting dynamical correlations between more than two particles; it is thus an extension of the Bloch free-electron theory when applied to metals.

The thermodynamic properties are obtained in the form of an equilibrium between the fermions ("atoms") and diatomic "pseudo-molecules", the latter obeying something like Bose statistics. Under certain conditions there is a singularity in the partition function - that is to say the thermodynamic properties of the system undergo a transition. Below this transition point, some of the pseudo-molecules will undergo a form of Bose-Einstein condensation, producing a superconducting state (cf. Schafroth 1955).

Any attempt at a detailed study of this system requires a knowledge of the eigenvalue spectrum of the "quenched 2-particle U-matrix" which is defined as follows:- The 2-particle U-matrix between the pair of fermion states k_1, k_2 and the states k_1', k_2' is

$$\langle k_1 k_2 | U_2 | k_1' k_2' \rangle = \langle k_1 k_2 | e^{-\alpha H} - e^{-\alpha H_o} | k_1' k_2' \rangle \qquad (1.1)$$

where H is the 2-fermion hamiltonian, complete with interactions, and H_o is that for two free fermions. The Fermi statistics of the system introduces "quenching" factors,

$$q(k) = \frac{1}{e^{\alpha(\mu - \varepsilon_k)} + 1} \qquad (1.2)$$

(with μ the chemical potential) to give the "quenched 2-particle U-matrix", $\tilde{U}_2$,

$$\langle k_1 k_2 | \tilde{U}_2 | k_1' k_2' \rangle = \left[q(k_1) q(k_2) \right]^{1/2} \langle k_1 k_2 | U_2 | k_1' k_2' \rangle \left[q(k_1') q(k_2') \right]^{1/2} \qquad (1.3)$$

These quenching factors, which appear as a consequence of the basic assumptions of the theory, are what one would expect on physical grounds - the Pauli principle forbids

any fully occupied state to take part in a correlation.

The eigenvalue spectrum, u_σ, is now obtained by bringing the $\widetilde{U}_2$ matrix into diagonal form:

$$\widetilde{U}_2 \mid \sigma > = u_\sigma \mid \sigma > \qquad (1.4)$$

Moreover it may be seen that if symmetrized and anti-symmetrized eigenfunctions are introduced by writing

$$<k_1k_2 \mid \sigma > = \frac{1}{\sqrt{2}} < [k_1k_2] \mid \sigma > + \frac{1}{\sqrt{2}} < \{k_1k_2\} \mid \sigma > \qquad (1.5)$$

$$<[k_1k_2] \mid \sigma > = - <[k_2k_1] \mid \sigma >; \; <\{k_1k_2\} \mid \sigma > = <\{k_2k_1\} \mid \sigma > \qquad (1.6)$$

then only the anti-symmetrized wave functions contribute to the partition function.

The grand canonical potential, Ω, — from which all other thermodynamic functions may be derived — may now be written (Schafroth, Butler and Blatt 1956)

$$\Omega = - kT \sum_{\underset{\sim}{k}} \ln\left(1+e^{\alpha(\mu - \varepsilon_k)}\right) + \qquad (1.7)$$

$$+kT \sum_{\sigma} \ln\left(1-e^{2\alpha\mu} u_\sigma\right)$$

(ε_k is the energy, and $e^{\alpha\mu}$ the activity, of the free fermions).

This grand canonical potential contains a singularity, and the system undergoes a phenomenon similar to Bose-Einstein condensation*), if and when the largest eigenvalue satisfies the relation

$$e^{2\alpha\mu} \max(u_\sigma) = 1 \qquad (1.8)$$

Two cases may be distinguished:- If the correlation matrix is negative definite ("purely repulsive"), then all $u_\sigma < 0$, and there is no transition: on the other hand, if at least one eigenvalue $u_\sigma > 0$, then for sufficiently large values of $\exp(2\alpha\mu)$ a thermodynamic transition does occur.

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*) The proof given by Schafroth, Butler and Blatt that the transition is identical to the Bose-Einstein transition has been shown to be inadequate (Blatt and Matsubara 1958(a)). While the existence of the transition remains unaltered, the nature of such a transition cannot be inferred from Eq(1.7), which ceases to be valid below the transition temperature, T_c. Although the actual evaluation of the partition function below T_c has yet to be performed, plausibility arguments indicate that the condensation is in all respects similar to a Bose-Einstein one.

It is thus clear that a computation of the quantity γ_M,

$$\gamma_M \equiv e^{2\alpha\mu} \max(u_\sigma) \qquad (1.9)$$

is of particular interest. Such a calculation, in conjunction with Eq (1.8), gives both a criterion for superconductivity, and an estimate of the superconducting transition temperature in terms of the inter-electron interaction parameters.

The actual interaction between electrons in metals consists of a screened Coulomb repulsion, together with the partly attractive Fröhlich interaction due to phonon exchange. Since calculation of $\tilde{U}_2$ in terms of this interaction is intractable, we employ model interactions, which contain the essential features, to investigate $\max(u_\sigma)$.

As has been seen, the prescription for obtaining $\tilde{U}_2$ consists of

(i) first calculating the pair-correlation matrix, U_2, by use of the total and free-particle hamiltonians (H and H_o) for unquenched electrons,

(ii) then finally multiplying by the statistical quenching factors to arrive at $\tilde{U}_2$.

The ensuing results, for a variety of model interactions, all indicate that this straight-forward calculation of the quenched pair-correlation matrix is not adequate, and leads to unphysical results. The trouble stems from the fact that we have first considered the electrons without any

quenching effects (step (i)), introducing such effects only as a final stage (step (ii)).

What is required is some form of self-consistent evaluation, which at no stage refers to unquenched electrons in the metal.

It should be noted that the failure to provide an adequate formula to calculate u_σ does not affect the validity of the thermodynamics of the quasichemical equilibrium theory (e.g. Eq(1.7)) : the thermodynamics involves only the spectrum u_σ , independent of its mode of evaluation.

Section 2 contains an account of the simplifying assumptions and formalism which are introduced in order to study γ_M. This maximum eigenvalue is then obtained for some particular model interactions in section 3. Finally the need for self-consistency is discussed in section 4 : it is stressed that before a quantitative theory of superconductivity can be derived from the quasichemical equilibrium approach, we must

(i) derive the correct expression for the partition function below the transition temperature, and

(ii) provide a self-consistent method of finding the quenched 2-particle correlation matrix.

Both these problems are as yet unsolved.

4.2 : EVALUATION OF THE MAXIMUM EIGENVALUE.

In order to study the eigenvalue spectrum, and in particular the maximum eigenvalue, of the quenched pair-correlation matrix, the following simplifying procedure is useful.

Particularizing to free electrons in a cubical box with periodic boundary conditions, the states k of the free electrons are described by a wave vector $\underset{\sim}{\varkappa}$ and a spin variable s. Furthermore, we only consider translationally - invariant interactions, so that $\tilde{U}_2$ conserves total momentum. Hence, introducing the centre-of-gravity momentum $\underset{\sim}{K}_{12} = \underset{\sim}{\varkappa}_1 + \underset{\sim}{\varkappa}_2$ and the relative momentum $\underset{\sim}{k}_{12} = \frac{1}{2}(\underset{\sim}{\varkappa}_1 - \underset{\sim}{\varkappa}_2)$, we have

$$\langle k_1 k_2 | \tilde{U}_2 | k_1' k_2' \rangle = \langle \underset{\sim}{k}_{12} s_1 s_2 | \tilde{U}_2(\underset{\sim}{K}_{12}) | \underset{\sim}{k}_{12}' s_1' s_2' \rangle \, \delta(\underset{\sim}{K}_{12} - \underset{\sim}{K}_{12}') \qquad (2.1)$$

The eigenvalues of $\tilde{U}_2$ may now be written $u_S(\underset{\sim}{K})$, and derived from the equation

$$\sum_{\underset{\sim}{k}_{12}', s_1' s_2'} \langle \underset{\sim}{K} S | \underset{\sim}{k}_{12}' s_1' s_2' \rangle \langle \underset{\sim}{k}_{12}' s_1' s_2' | \tilde{U}_2(\underset{\sim}{K}) | \underset{\sim}{k}_{12} s_1 s_2 \rangle = u_S(\underset{\sim}{K}) \langle \underset{\sim}{K} S | \underset{\sim}{k}_{12} s_1 s_2 \rangle \qquad (2.2)$$

where S represents some form of "internal quantum number" for the molecule. The eigenvectors of $\tilde{U}_2$, appropriately anti-symmetrized, have been written as

$$\langle \underset{\sim}{K}S \,|[\underset{\sim}{k}_1\underset{\sim}{k}_2]\rangle = \delta(\underset{\sim}{\varkappa}_1+\underset{\sim}{\varkappa}_2-\underset{\sim}{K})\langle \underset{\sim}{K}S|\underset{\sim}{k}_{12}s_1s_2\rangle \qquad (2.3)$$

with

$$\langle \underset{\sim}{K}S|\underset{\sim}{k}_{12}s_1s_2\rangle = -\langle \underset{\sim}{K}S|\underset{\sim}{k}_{21}s_2s_1\rangle \qquad (2.4)$$

Going to the limit of infinite volume, the spectrum $u_S(\underset{\sim}{K})$ is derived from the integral equation

$$\sum_{s_1's_2'} \int \underset{\sim}{dk}' \, \phi_{KS}(\underset{\sim}{k}'s_1's_2')\langle \underset{\sim}{k}'s_1's_2'|\tilde{U}_2(\underset{\sim}{K})|\underset{\sim}{k}s_1s_2\rangle =$$

$$= u_S(\underset{\sim}{K}) \, \phi_{KS}(\underset{\sim}{k}s_1s_2) \qquad (2.5)$$

The eigenfunctions of this equation, ϕ_{KS}, have the usual properties of orthogonality and completeness. They may be interpreted as the wave functions (in momentum space) which describe the pseudo-molecule.

At this stage we particularize to consideration of the <u>maximum</u> eigenvalue, and furthermore we make the assumption that this maximum is achieved for the centre-of-gravity momentum, $\underset{\sim}{K}$, equal to zero : i.e. we assume

$$\max\left[u_S(\underset{\sim}{K})\right] = \max\left[u_S(0)\right] \qquad (2.6)$$

[This assumption is demonstrably valid if the 2-particle interaction can be separated into a centre-of-gravity and a relative momentum part : even if this is not the case, the assumption is still in general a reasonable one.]

Also we assume that the electron-electron interaction is spin independent : this is indeed the case for the screened Coulomb and Fröhlich hamiltonians. This assumption eliminates the sum over spins in the integral equation (2.5).

With these two assumptions, the quantity γ_M (Eq(1.9)) is obtained as the maximum eigenvalue of the integral equation

$$\int \underset{\sim}{dk}' K(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2)\ \phi(\underset{\sim}{k}') = \gamma\ \phi(\underset{\sim}{k}) \qquad (2.7)$$

with the kernel

$$K(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2) = n(k) e^{k^2 t^2} \left\{ G(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2) - G_o(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2) \right\} \times \qquad (2.8)$$
$$\times\ e^{k'^2 t^2} n(k')$$

The functions G and G_o are defined in terms of the total and free-electron hamiltonians describing the relative motion of unquenched pairs (H_r and H_{ro}) :

$$G(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2) = \langle \underset{\sim}{k}s_1 s_2 |\ e^{-\alpha H_r}\ | \underset{\sim}{k}' s_1 s_2 \rangle \qquad (2.9)$$

$$G_o(\underset{\sim}{k}s_1 s_2 | \underset{\sim}{k}' s_1 s_2) = \langle \underset{\sim}{k}s_1 s_2 |\ e^{-\alpha H_{ro}} | \underset{\sim}{k}' s_1 s_2 \rangle \qquad (2.10)$$

[In deriving Eq(2.8), use has been made of the identity

$$n(k) = \frac{1}{e^{\alpha(\varepsilon_k - \mu)} + 1} = 1 - q(k) \qquad (2.11)$$

t, which differs from the thermal wave-length of Chapter I by a factor $\sqrt{4\pi}$, is defined as

$$t^2 = \frac{\alpha \hbar^2}{2m} \qquad (2.12)$$

with m the electron mass.]

We now make a Legendre expansion of $G(\underset{\sim}{k}, \underset{\sim}{k}')$ (forgetting the spin indices for the moment) to get

$$G(\underset{\sim}{k},\underset{\sim}{k}') = \sum_{l=0}^{\infty} (2l+1)\, \frac{G_l(k,k')}{kk'}\, P_l(\cos\theta) \qquad (2.13)$$

with θ the angle between the vectors $\underset{\sim}{k}$ and $\underset{\sim}{k}'$. Using the addition theorem for spherical harmonics, we may rewrite (2.13) in terms of the polar coordinates of the individual vectors $\underset{\sim}{k}$ and $\underset{\sim}{k}'$:

$$G(\underset{\sim}{k},\underset{\sim}{k}') = 4\pi \sum_{l=0}^{\infty} \sum_{m=-l}^{+l} \frac{G_l(k,k')}{kk'}\, Y_{lm}(\theta, \phi)\, Y_{lm}(\theta', \phi') \qquad (2.13a)$$

A precisely analogous expansion may be written down for the Fourier transform, $G(\underset{\sim}{r}, \underset{\sim}{r}')$, of this function. In this way

the 3-dimensional integral equation (2.7) for Υ may be reduced a set of 1-dimensional integral equations, with eigenvalues Υ_l corresponding to each value of l :

$$4\pi \int_0^\infty dk' K_l(k,k') \phi_l(k') = \Upsilon_l \phi_l(k) \qquad (2.14)$$

The eigenvectors $\phi(\underset{\sim}{k})$ have been expanded into "partial waves" in the usual manner

$$\phi(\underset{\sim}{k}) = \sum_{l=0}^{\infty} (2l+1) \frac{\phi_l(k)}{k} P_l(\cos\theta) \qquad (2.15)$$

Finally we observe that the calculation of $G_l(r,r')$, and thence $G_l(k,k')$ and $K_l(k,k')$, may be facilitated by a result derived by Blatt (1956) :

$$G_l(r,r') = \frac{2}{\pi} \int_0^\infty e^{-2K^2t^2} dK \psi_l(K,r) \psi_l(K,r') \qquad (2.16)$$

The functions $\psi_l(K,r)$ are obtained from a Legendre expansion of the eigenfunctions of the hamiltonian for relative motion: that is

$$-\frac{\hbar^2}{m} \frac{d^2\psi_l}{dr^2} + \left[V(r) + \frac{l(l+1)\hbar^2}{mr^2} \right] \psi_l = E(K) \psi_l \qquad (2.17)$$

where H_r has been written

$$H_r = -\frac{\hbar^2}{m} \nabla^2 + V(\underset{\sim}{r}) \qquad (2.18)$$

These functions $\psi_l(K,r)$ are required to satisfy the boundary conditions

$$\left.\begin{aligned} &\psi_l(K,r) = 0 \quad , \text{for } r = 0 \\ &\longrightarrow \quad \sin(Kr - \tfrac{\pi}{2}l + \delta_l) \, , \text{for } Kr \gg 1 \end{aligned}\right\} \tag{2.19}$$

(with δ_l being the asymptotic phase-shift for the l-th partial wave). The above expression (2.16) is invalid if there exists a solution of H_r corresponding to a bound state - such is not the case in any model pertinent to superconductors.

A Fourier transformation of $G(\underset{\sim}{r},\underset{\sim}{r}')$ leads to the result

$$G_l(k,k') = \frac{2}{\pi} \int_0^\infty e^{-2K^2t^2} \, dK \; \psi_l(K,k) \, \psi_l(K,k') \tag{2.20}$$

with

$$\psi_l(K,k) = \left(\frac{2}{\pi}\right)^{1/2} \int_0^\infty (kr) j_l(kr) \; \psi_l(K,r) \, dr \tag{2.21}$$

$j_l(kr)$ being the spherical Bessel function of order l.

Thus we see that, under the assumption (2.6), the matrix elements of $\widetilde{U}_2(\underset{\sim}{K}=0)$ are obtained by first using the relative motion hamiltonian to get wave-functions for the electron pairs: thence the unquenched correlation matrix is constructed by use of Eq(2.20), and the quenching effects are introduced as a final stage in Eq(2.8)

* * *

As has been pointed out in the introduction, we are obliged to use model interaction hamiltonians to study γ_M, owing to the intractable nature of the actual hamiltonian for electrons in metals.

The assumption that the interaction is spin independent has been justified above : thus the effects of electron spin enter only via the requirement that the eigenvectors of the $\widetilde{U}_2$ matrix be anti-symmetric. For pairs with opposite spins (and therefore singlet spin wave functions, which are anti-symmetric) the wave functions $\Psi(K,\underset{\sim}{r})$ must be symmetric; i.e. for anti-parallel spin pairs, the sum over l is restricted to <u>even</u> integers. Similarly, for pairs with parallel spins (triplet spin state), the sum over l is restricted to <u>odd</u> integers.

Moreover, since increasing l corresponds to an increasing centrifugal repulsion term in the relative motion hamiltonian (cf. (2.17)), that is to an increasing repulsive contribution to the pair correlations, we would expect the maximum eigenvalue of $\widetilde{U}_2$ to be achieved for $l = 0$. Thus our attention will be focused on the $l = 0$ partial wave. [The above arguments lead to an identification of the superconducting state with electron pairs of opposite spin - this is in accord with the basic assumption of the BCS theory. Also we observe that a gas of charged spinless bosons exhibits superconductivity below its transition temperature, T_c, while bosons of spin 1 give rise to ferromagnetism with a Curie temperature T_c - the fact that this

latter phenomenon ~~which~~ is comparatively rare is in harmony with our assumptions.]

To approximate the screened Coulomb repulsion together with the Fröhlich interaction, we use a potential V(r) which has some form of repulsive core for small r, but which is attractive at larger distances.

By using a Born approximation to generate a trial solution for use in the Friedman (1949) variation principle (see Blatt 1956), a quite general criterion may be given for the occurrence of a positive eigenvalue corresponding to the partial wave l = 0. Characterizing the potential by ranges (r_+, r_-) and heights (V_+, V_-) for the attractive and repulsive parts, the criterion becomes

$$V_+ r_+^3 > V_- r_-^3 \tag{2.22}$$

This result is derived by observing that a sufficient condition for $\tilde{U}_2$ to have at least one positive eigenvalue is that

$$\text{Trace } \tilde{U}_2 > 0 \tag{2.23}$$

It is to be noted that the requirement for a positive eigenvalue is qualitatively weaker (for $r_+ > r_-$) than that for a bound state — the criterion for a bound state has the general form

$$V_+ r_+^2 > V_- r_-^2 + \hbar^2/m \tag{2.24}$$

Although the prescription given for finding the matrix elements of $\widetilde{U}_2$ is found to lead to unphysical results, the criterion (2.22) remains valid : there is no need for self-consistency if we restrict ourselves to <u>diagonal</u> elements in an "improved Born approximation".

The specific model which is considered in detail in section 3(a) does not possess any repulsive core : however, it is easy to see that the unphysical results obtained are not qualitatively altered by the introduction of such a repulsion.

4.3 : RESULTS FOR SPECIFIC MODELS.

(a) A "Separable Potential".

If we consider the general form of Schrödinger's equation,

$$(T+V)\,\Psi = E\,\Psi \tag{3.1}$$

then those V-functions which can be written as

$$V\Psi = g(\underset{\sim}{r}) \int g(\underset{\sim}{r}') \,\Psi\,(\underset{\sim}{r}')\, d\underset{\sim}{r}' \tag{3.2}$$

define the class of "separable potentials". Such V-functions are not really potentials in the strict sense : they represent some form of velocity dependent interaction.

As a model interaction, we take a particular member of the class of separable potentials, given by

$$g(\underset{\sim}{r}) = \frac{\sigma\, e^{-\lambda r}}{r}, \qquad \sigma^2 = -\frac{\beta\, \hbar^2 \lambda^3}{4\pi m} \tag{3.3}$$

Qualitatively, this potential represents an attractive interaction with range λ^{-1} and "strength parameter" β. (It may be shown that $\beta \geq 2$ corresponds to a bound state - we of course restrict ourselves to $\beta \ll 1$).

Since the potential is isotropic, the partial wave expansion of $\Psi(\underset{\sim}{r})$ contains only a $l = 0$ (S-wave) term:

$$\Psi\,(\underset{\sim}{r}) = \frac{\psi\,(r)}{r} \tag{3.4}$$

Then $\psi\,(Kr)$ is obtained from the inhomogeneous differ-

ential equation

$$\frac{d^2\psi(K,r)}{dr^2} + K^2\psi(K,r) = -\beta\lambda^2 A(K)\, e^{-\lambda r} \qquad (3.5)$$

with A(K) defined by

$$A(K) = \lambda \int_0^\infty e^{-\lambda r'} \psi(K,r')\, dr' \qquad (3.6)$$

The solution of such a differential equation may be written down as the general solution for the corresponding homogeneous equation, together with a particular solution for the inhomogeneous case : doing this, and imposing the boundary conditions (2.19) on the ensuing solution, we finally get

$$\psi(K,r) = -\frac{\beta A(K/\lambda)}{1+(K/\lambda)^2}\left[e^{-\lambda r} - \cos Kr\right] + B(K/\lambda)\sin Kr \qquad (3.7)$$

The functions A(y) and B(y) are given by the definitions

$$A(y)\ (\equiv \sin\eta) = \frac{y}{\left[\left(y^2+\left\{1+\sqrt{\frac{\beta}{2}}\right\}^2\right)\left(y^2+\left\{1-\sqrt{\frac{\beta}{2}}\right\}^2\right)\right]^{1/2}} \qquad (3.8)$$

$$B(y)\ (\equiv \cos\eta) = \frac{1}{y}\left[(1+y^2)+\frac{\beta(y^2-1)}{2(y^2+1)}\right] A(y) \qquad (3.9)$$

In order to calculate the matrix elements of $\tilde{U}_2$ in a momentum-space representation, we require the Fourier transform of $\psi(K,r)$. Use of Eq (2.21) yields

$$\left(\frac{2}{\pi}\right)^{1/2} \psi(K,k) = e^{i\eta}\left(\delta_+(k-K) - \delta_+(-k-K)\right) + e^{-i\eta}\left(\delta_+(K-k) - \delta_+(k+K)\right) - \frac{2}{\pi}\frac{k}{k^2+\lambda^2}\sin\eta \qquad (3.10)$$

where η is defined by Eq (3.8), and the δ_+-function has its conventional definition. The above expression may be simplified to get

$$\left(\frac{2}{\pi}\right)^{1/2} \psi(K,k) = B(y)\left[\delta(y-x) - \delta(y+x)\right] + \frac{2\beta}{\pi\lambda} A(y) \frac{x}{1+x^2} \frac{\mathcal{P}}{x^2-y^2} \qquad (3.11)$$

with

$$\left.\begin{aligned} x &\equiv k/\lambda \\ y &\equiv K/\lambda \end{aligned}\right\} \qquad (3.12)$$

and the symbol $\mathcal{P}$ denotes that principal values are to be taken when integrating with respect to x or y. $G_{l=0}(k,k')$ may now be obtained from Eq. (220).

Thence γ_M is finally derived as the maximum eigenvalue of the integral equation (cf. (2.14)).

$$4\pi \int_0^\infty dx' \, K(x,x') \, \phi(x') = \gamma \, \phi(x) \qquad (3.13)$$

with the kernel $K(x,x')$ described by

$$K(x,x') = (B^2(x)-1)n(x)n(x')\ \delta(x-x') \qquad \text{(i)}$$

$$+\frac{2\beta}{\pi}\left\{\frac{A(x)B(x)}{(x'^2-x^2)}\frac{x'}{(1+x'^2)}\,q(x)n(x')\,e^{-t^2\lambda^2x'^2+a\mu}\right.$$

$$\left.+\frac{A(x')B(x')}{(x^2-x'^2)}\frac{x}{(1+x^2)}\,q(x')n(x)\,e^{-t^2\lambda^2x^2+a\mu}\right\} \qquad \text{(ii)}$$

$$+\frac{2\beta^2}{\pi}e^{2a\mu}\,q(x)\frac{q(x')xx'}{(1+x^2)(1+x'^2)}\left\{\frac{A^2(x)}{x(x^2-x'^2)}E_+(\sqrt{2}t\lambda x)\right.$$

$$+\frac{A^2(x')}{x'(x'^2-x^2)}E_+(\sqrt{2}t\lambda x')$$

$$-\frac{(\sqrt{\frac{2}{\beta}}-1)\,E_-(\sqrt{2}t\lambda\{1-\sqrt{\frac{\beta}{2}}\})}{4(x^2+\{1-\sqrt{\frac{\beta}{2}}\}^2)(x'^2+\{1-\sqrt{\frac{\beta}{2}}\}^2)}$$

$$\left.-\frac{(\sqrt{\frac{2}{\beta}}+1)\,E_-(\sqrt{2}t\lambda\{1+\sqrt{\frac{\beta}{2}}\})}{4(x^2+\{1+\sqrt{\frac{\beta}{2}}\}^2)(x'^2+\{1+\sqrt{\frac{\beta}{2}}\}^2)}\right\} \qquad \text{(iii)}$$

(3.14)

The following notation has been introduced:-

$$E_+(y) = -e^{-y^2}\frac{2}{\sqrt{\pi}}\int_0^y e^{z^2}\,dz \qquad (3.15)$$

t.o.

$$E_{-}(y) = e^{y^2} \frac{2}{\sqrt{\pi}} \int_{y}^{\infty} e^{-z^2} dz \qquad (3.15)$$

We now note one highly important physical fact:- above the transition temperature, when the expression (1.7) for the grand canonical potential Ω is perfectly regular, the pseudo-molecular contribution to Ω is unimportant. That is to say the chemical potential μ in the neighbourhood above the transition is given, at least qualitatively, by its value for a degenerate free electron gas :

$$\mu \equiv \frac{\hbar^2 k_o^2}{2m} \approx \frac{\hbar^2 k_F^2}{2m} \qquad (3.16)$$

with the Fermi wave-number k_F given by

$$\frac{N}{V} = \frac{k_F^3}{3\pi^2} \qquad (3.17)$$

Thus in the region of superconducting transition temperatures (i.e. $T_c \approx 3^{\circ}K$) the factor $\exp(2\alpha\mu)$, which appears in the above expression for the kernel, is an extremely large one:

$$e^{2\alpha\mu} \approx e^{2t^2 k_F^2} \approx e^{10^4} \qquad (3.18)$$

This factor is entirely compensated in the first term, (i), in the kernel $K(x,x')$, partly compensated in the term

(ii), and remains uncompensated in the remaining term (iii). Thus the last term, although small by powers of β, $(tk_F)^{-1}$ and λ/k_F (all of which are $\ll 1$), nevertheless dominates the kernel by virtue of the vast factor $\exp(2\alpha\mu)$.

That is to say, our prescription for calculating the matrix elements of $\widetilde{U}_2$ has the feature that small side-effects in the relative motion hamiltonian completely dominate in $\widetilde{U}_2$, while important effects are "quenched" out.

Physically, all effects should be quenched.

Once the above basic fact has been noted, the integral equation (3.13) may be solved, to get

$$\left.\begin{aligned} \gamma_M &= \frac{\sqrt{2\pi}}{5\pi}\beta^2\left(\frac{\lambda}{k_o}\right)^2 \frac{e^{2k_o^2t^2}}{(k_ot)^3}\left\{1+\mathcal{O}\left(\frac{\lambda}{k_o}\right)^2+\mathcal{O}\left(\frac{1}{\lambda t}\right)^2+\mathcal{O}(\beta)\right\}, t>\lambda^{-1} \\ &= \frac{4}{5}\beta^2\left(\frac{\lambda}{k_o}\right)^5 e^{2k_o^2t^2}\left\{1+\mathcal{O}\left(\frac{1}{tk_o}\right)^2+\mathcal{O}(t\lambda)+\mathcal{O}(\beta)\right\}, t<\lambda^{-1} \end{aligned}\right\} \quad (3.19)$$

There is therefore a positive eigenvalue greater than unity, and consequently a transition, for all temperatures less than the Fermi degeneracy temperature! (Unless the strength parameter β is less than 10^{-100} !)

(b) The Eckart Potential

The essential features of the above calculation are unchanged if we take quite different model potentials. As a further example, we quote the results obtained by using the Eckart (1930) potential,

$$V(\underset{\sim}{r}) = -\frac{2\hbar^2\lambda^2}{m} \times \beta \times \frac{e^{-\lambda r}}{(1+\beta e^{-\lambda r})^2} \qquad (3.20)$$

(This potential is qualitatively different from that considered above, in that it is non-singular at r = o). Then γ_M is found to be

$$\gamma_M = \frac{16\sqrt{2\pi}}{9\pi}\beta^2\left(\frac{\lambda}{k_o}\right)^6 \frac{e^{2k_o^2t^2}}{(k_o t)^3}\left\{1+\mathcal{O}\left(\frac{1}{tk_o}\right)^2 + \mathcal{O}\left(\frac{\lambda}{k_o}\right)^2 + \mathcal{O}(\beta)\right\} \qquad (3.21)$$

Furthermore, it may be shown that this result is not significantly altered by the introduction of an infinitely repulsive core (provided the radius of such a core is appreciably less than λ^{-1}).

4.4 : THE NEED FOR SELF-CONSISTENCY.

The results in section 4.3 have been seen to lead to completely unphysical results, since they imply that even for an extremely weak attraction, there exists a transition with $T_c \sim 10^4$ °K. Examining the mathematical properties of the kernel (2.8), (2.20) for the integral equation which gives γ_M, we can see that these unphysical results will arise so long as $\psi_1(K,k)$ [the $\underset{\sim}{k}$-space wave-function of the interaction hamiltonian, belonging to the energy value $\hbar^2K^2/m$] contains a component which is $>>$ $\exp(-k^2t^2)$ for $k >> K$. For if this is the case, then when the integral over K is performed (Eq (2.20)), such a component gives rise to a term in which the factor $\exp(2k_o^2t^2)$ is not compensated.

Since the wave-functions for unquenched electron pairs will in general contain such a (finite) term in the limit $k>>K$, we conclude that any approach which first computes the unquenched matrix U_2, and finally finds $\widetilde{U}_2$, is beset with the difficulty that features which dominate the interaction hamiltonian, H, will be quenched out, while small subsidiary effects in H play a dominant role, leading to nonsensical results. These difficulties, with their attendant unphysical results, will not be removed by a relaxation of all the assumptions which have been made for the sake of simplicity (e.g. the assumption that

max $\left[u_S(\underset{\sim}{K})\right]$ is achieved for $\underset{\sim}{K} = 0$, and that the screened Coulomb plus Fröhlich hamiltonian may be replaced by models which contain the basic features).

What is needed is a completely new prescription for finding the eigenvalue spectrum of the "quenched 2-particle correlation matrix" — such a prescription will be required to be self-consistent in the sense that it <u>at no stage refers to "unquenched" electrons.</u>

Formally such a prescription is obtained by first writing the density matrix $\mathcal{U}_N$ for the system of N particles as a product of single-particle and two-particle density matrices $\overline{\mathcal{U}}_1$ and $\overline{\mathcal{U}}_2$ (where statistical effects are accounted for in $\overline{\mathcal{U}}_1$ and $\overline{\mathcal{U}}_2$).

$$\mathcal{U}_N = \sum_{P(k_1 \ldots k_N)} \sum_{M} \overline{\mathcal{U}}_1^{N-2M} \times \overline{\mathcal{U}}_2^{M} \qquad (4.1)$$

The sum $\sum_P$ is extended over all assignments of the factors $\overline{\mathcal{U}}_1$, $\overline{\mathcal{U}}_2$ to the N states k_1 , k_2 , ... , k_N. Self-consistent matrices $\overline{\mathcal{U}}_1$ and $\overline{\mathcal{U}}_2$ may now be chosen from a variation principle :-

$$\text{Trace} \left(\mathcal{U}_N \ \ln \ \mathcal{U}_N \right) = \text{maximum} \qquad (4.2)$$

subject to

$$\text{Trace} \left(H_N \, \mathcal{U}_N \right) = E \qquad (4.3)$$

If we assume $\bar{u}_2 \equiv 0$, the above equations may be solved to get the Husimi (1940) solution for $\bar{u}_1$: the extension of such a calculation to include $\bar{u}_2$ appears to be very difficult.

It is worth remarking that the first step in the semi-classical approximation to $\tilde{U}_2$ (Wigner 1932, Mayer and Band 1947), which replaces $\left(e^{+1/2\alpha H_o} e^{-\alpha H} e^{+1/2\,\alpha H_o}\right)$ by $e^{-\alpha V}$, is of interest because it satisfies the requirements of self-consistency to a large extent. Quantitatively this approximation is a poor one, because it converges in powers of $(t\lambda)^2$ — λ^{-1} being the range of $V(\underset{\sim}{r})$, t defined by (2.12) — which is a large factor in the region of superconducting temperatures. However, due to the degree of self-consistency introduced by eliminating the term H_o for unquenched electrons, the results for γ_M are no longer physically unreasonable: the transition temperature in this approximation is given by

$$kT_c \approx \beta \frac{\hbar^2\lambda^2}{m} \qquad (4.4)$$

with β, λ^{-1} the strength and range parameters for our model potentials.

In conclusion, it is to be observed that, although the quasichemical equilibrium approach describes the qualitative features of superconductivity satisfactorily, two significant problems must be overcome before a quantitative theory is possible on this basis. Firstly, in order to study the nature of the transition, and the thermodynamic properties below such a transition, it is necessary to evaluate the correct expression for the partition function of the system below T_c. Secondly, before any expressions for Ω can be put to quantitative use, a self-consistent

method for computing the eigenvalue spectrum of the quenched pair correlation matrix must be provided.

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