APPLICATION OF THE THEORY OF NUMBERS TO THE MAGNETIC PROPERTIES OF A FREE ELECTRON GAS

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CHAPTER 1

INTRODUCTION

1.1 General Aspect of the Problem

The fundamental problem in applying statistical thermodynamics to the theory of metals is to find the proper energy level distribution function. Once this function has been found, the energy, entropy, heat capacity and magnetic moment can readily be determined. Many mathematical procedures have been used to compute distribution functions. In the final analysis they all strive to replace summations by integrals. In fact, advancements in the theory have been the result of more accurate replacement of sums by integrals.

1.2 Purpose of Present Work

There are two purposes for the present work. The first, and more general, objective is to propose a different mathematical method for getting distribution functions. The particular method to be used is often applied to the number theoretical problem of counting the lattice points within or on a closed surface. Subsequent chapters will deal with the correspondence between number theory and quantum mechanics. It is believed that the proposed method could be applied to a variety of problems in solid state physics and to studying statistical properties of nuclei. However, in this paper we will restrict our applications to the simple free electron theory of a metal.

Our second aim, therefore, is to apply number theoretical methods to the specific problem of the magnetic properties of a free electron gas. It would appear as though this particular problem is a guinea pig for new methods since Pauli's work (Ref. 7) on the "spin paramagnetism" of electrons was also the first application of Fermi-Dirac statistics to the theory of metals. In fact, another new idea was used in the same problem when Landau (Ref. 6) proved the existence of a diamagnetic effect caused by the discreteness of electronic levels in a magnetic field. Almost simultaneously with the theoretical work of Landau, de Haas and van Alphen (Ref. 4) found experimentally that at sufficiently low temperatures the diamagnetism of bismuth shows an anomalous dependence on magnetic field strength. The discovery of the de Haas-van Alphen effect [1] was an impetus to further theoretical work. Peierls (Ref. 8) was the first to show that the d-v-e could be explained quantum mechanically. His theory has subsequently been amplified by Blackman (Ref. 1) and Landau (Ref. 9) to include anisotropic media such as crystals of the bismuth type. Although we will be concerned with the d-v-e, our efforts will be restricted, as stated above, to the free electron concept of a metal.

The effect of using a finite container to hold the electron gas has been the subject of a number of recent papers. Since the results reported are widely divergent, it will be of interest to examine this aspect of the problem by the proposed method.

It is hoped that the method and applications to be given here may prove of heuristic value in furthering the theory of solids.

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[1] Throughout the remainder of this work de Haas-van Alphen effect will be designated by d-v-e.

CHAPTER 2

QUANTUM STATISTICAL FORMULAE AND THEIR RELATION TO THE THEORY OF NUMBERS

Since much of the material that follows will make use of formulae based on Fermi-Dirac statistics, it is convenient to discuss these relations before embarking upon the detailed calculations. Such discussion has the further advantage of introducing the correspondence between quantum statistics and the theory of numbers.

2.1 Free Energy

The free energy of a system of N non-interacting electrons (obeying Fermi-Dirac statistics) is

$$F = NE_o - kT\sum_i \log\left(1 + e^{(E_o - E_i)/kT}\right) \qquad (2\text{-}1)$$

where E_o is the Fermi energy; k is Boltzmann's constant; T is the absolute temperature; and E_i are the energy levels for any one of the electrons. E_o and N are related through the normalizing condition

$$N = \sum_i \frac{1}{1 + e^{(E_i - E_o)/kT}} \qquad (2\text{-}2)$$

Both (2-1) and (2-2) are derived[1] on the assumption that there are only electrons of one value of spin present in the system. When both values of spin are allowed all sums are multiplied by two if N still refers to

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[1] For details of the derivation of these relations see, for example, R. H. Fowler, Statistical Mechanics (Cambridge University Press, 1937).

the total number of electrons.[2]

If we now assume the existence of an energy distribution function $\left(\frac{dG(E)}{dE}\right) dE$, where $G(E)$ denotes the number of states having energies equal to or less than E, the summations in (2-1) and (2-2) can be replaced by integrals. The free energy can then be written

$$F = NE_o - kT \int_{E_L}^{\infty} \frac{dG(E)}{dE} \log\left(1 + e^{(E_o - E)/kT}\right) dE \qquad (2\text{-}3)$$

where E_L is the lowest energy level of the electron. Integrating once by parts gives

$$F = NE_o - kT \left[-G(E_L) \log\left(1 + e^{(E_o - E_L)/kT}\right) + \frac{1}{kT} \int_{E_L}^{\infty} G(E)\, f(E)\, dE \right] \qquad (2\text{-}4)$$

where $f(E)$ is the Fermi function, i.e.

$$f(E) = \frac{1}{1 + e^{(E - E_o)/kT}} \qquad (2\text{-}5)$$

2.2 Magnetic Moment

In all the work that follows the magnetic moment will be obtained from the formula

$$M = -\left(\frac{\partial F}{\partial H}\right)_{V,T} \qquad (2\text{-}6)$$

where M is the magnetic moment; H is the magnetic field intensity; and V is the volume. We shall consider only systems in which N is held constant so that E_o and H can be considered as the variables that determine M. Then (2-6) can be written as

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[2] This is true when the spin interaction with applied fields is not accounted for. When spin energy is included one has two independent sums to consider.

$$M = -\left(\frac{\partial F}{\partial H}\right)_{E_o} - \left(\frac{\partial F}{\partial E_o}\right)_H \frac{dE_o}{dH} \tag{2-7}$$

But from (2-1) and (2-2) we have

$$\left(\frac{\partial F}{\partial E_o}\right)_H = N - \sum_{i} \frac{1}{1 + e^{(E_i - E_o)/kT}} = 0 \tag{2-8}$$

so that

$$M = -\left(\frac{\partial F}{\partial H}\right)_{E_o} = -\left[\frac{\partial(F - NE_o)}{\partial H}\right]_{E_o} \tag{2-9}$$

2.3 Relation to the Theory of Numbers

From (2-9) it is clear that we must find F before computing M. But (2-4), which is the desired expression for F, shows that our immediate aim is to evaluate the function $G(E)$.

For the particular problem of the diamagnetism of free electrons Landau (Ref. 6) used the Euler-Maclaurin formula[3] for getting $G(E)$. In the course of repeating Landau's calculation the present author found that the results obtained by using the Euler-Maclaurin formula depended not only on the order of summation over quantum numbers but also on the particular form of the formula. Since it was believed that the theory of physical phenomena should be independent of order of summation, a detailed study was undertaken to resolve the difficulty. It was at this stage that the concepts of number theory were first employed.

Let us suppose that for a particular problem the solution of Schrodinger's equation gives rise to an eigenvalue relation in which the energy levels are expressed as explicit functions of quantum numbers.

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[3] For the derivation and application of the Euler-Maclaurin formula, see, for example, Whittaker and Robinson, Calculus of Observations (Blackie & Sons, London, 1932) p. 134

Then by fixing the energy parameter at E, the eigenvalue relation will describe some surface in quantum number space. Now the computation of G(E) resolves itself into the problem of counting the number of quantum states within or on the particular energy surface. This counting is completely analogous to the number theory problem of finding the number of lattice points within a closed surface located in a grid of discrete unit cells. (A lattice point is defined as a point having integers for coordinates.) The discreteness of the quantum numbers is sufficient to indicate that there will be corrections to the result obtained by merely computing the volume enclosed by the energy surface.

Lattice point problems have been considered in great detail by mathematicians. The lattice points of a circle have received particular attention since this problem is considered the most fundamental as well as the most interesting.[4] Generally, the mathematician is more concerned about finding the order of magnitude of the corrections to the number of lattice points than actually getting an explicit relation for the desired total number. Although order of magnitude relations are of value in solid state problems, it was felt more desirable to strive for explicit relations in all cases. Unfortunately, we shall see that even in relatively simple quantum mechanical problems the task of getting an explicit representation for G(E) becomes quite formidable.

Number theorists have used a variety of methods in solving lattice point problems. The particular procedure to be used throughout this paper follows closely the work of Kendall (Ref. 5) on the number of lattice points inside a random oval. Details of the method, as applied to quantum mechanics, will be given in the text that follows.

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[4] An interesting historical account of the lattice points of a circle is given by J. R. Wilton, Messenger of Math. **58**, 67 (1929)

CHAPTER 3

SPIN PARAMAGNETISM

3.1 Content

In this chapter we consider the application of number theory to the problem of spin paramagnetism. The principal value of this is to illustrate the use of existing results of number theory to a specific problem. From a physical point of view the development is wrong since we will be assuming plane waves for the electronic motion in a magnetic field. But the results obtained here can be compared to Pauli's work since he too assumed plane waves. Subsequent chapters will deal with the proper electronic wave functions in a magnetic field.

3.2 Schrodinger Equation

In the absence of a magnetic field the Schrodinger equation for an electron in a box of dimensions L_x, L_y, L_z, is

$$-\frac{\hbar^2}{2m}\nabla^2\psi + (\mathcal{U} - E)\psi = 0 \tag{3-1}$$

Here m is the mass of the electron; $\hbar$ is Planck's constant divided by 2π; ψ is the wave function; $\mathcal{U}$ is the potential energy; and E is the energy. If we assume $\mathcal{U} = 0$ inside the box, and $\mathcal{U} = \infty$ on the walls, the wave functions are

$$\psi = \sin\left(\frac{\pi n_1 x}{L_x}\right) \sin\left(\frac{\pi n_2 y}{L_y}\right) \sin\left(\frac{\pi n_3 z}{L_z}\right) \tag{3-2}$$

where n_1, n_2, n_3 are integers. This wave function satisfies the condition of vanishing at the walls. However, it is more convenient for the purposes of this chapter to take for the wave function

$$\psi = e^{2\pi i\left[\frac{n_1 x}{L_x} + \frac{n_2 y}{L_y} + \frac{n_3 z}{L_z}\right]} \tag{3-3}$$

which is periodic along the three axes with periods L_x, L_y, and L_z respectively. This wave function does not satisfy the boundary conditions, but simplifies the number theory problem by allowing positive or negative values for the integers n_1, n_2, n_3.

The energy levels obtained from (3-3) are

$$E = \frac{h^2}{2m}\left[\left(\frac{n_1}{L_x}\right)^2 + \left(\frac{n_2}{L_y}\right)^2 + \left(\frac{n_3}{L_z}\right)^2\right] \tag{3-4}$$

where n_1, n_2, n_3 can now take on all positive and negative integer values.

We now introduce the magnetic field H to this system of electrons. If we assume that H only acts on the spin of the electron (i.e. no effect on the spatial wave function) then the new energy levels will be

$$E = \frac{h^2}{2m}\left[\left(\frac{n_1}{L_x}\right)^2 + \left(\frac{n_2}{L_y}\right)^2 + \left(\frac{n_3}{L_z}\right)^2\right] \mp \beta H \tag{3-5}$$

where β is the Bohr magneton $\frac{e\hbar}{2mc}$.

3.3 Free Energy

In quantum number space (3-5) describes two ellipsoids when E is fixed. The calculation of G(E) is therefore equivalent to finding the number of lattice points of a three-dimensional allipsoid. Since we have two such ellipsoids G(E) can be written as

$$G(E) = G_+(E) + G_-(E) \tag{3-6}$$

corresponding to $\mp\beta H$ in (3-5). Introducing (3-6) and the proper lowest energy values into (2-4), the free energy is given by

$$F - NE_o = -\left[\int_{-\beta H}^{\infty} G_+(E) f(E)\, dE + \int_{\beta H}^{\infty} G_-(E) f(E)\, dE \right] \qquad (3\text{-}7)$$

since both $G_+(-\beta H)$ and $G_-(\beta H)$ are zero.

The lattice points of an ellipsoid is one of the classic problems in number theory. In fact it is one that has been solved explicitly. Consider the ellipsoid

$$\sum_{i=1}^{3} \left(\frac{n_i}{L_i} \right)^2 \leq \chi \qquad (3\text{-}8)$$

(which represents (3-5) when $\sqrt{x} = \frac{1}{h} \sqrt{2m(E \pm \beta H)}$)

It is shown[1] in number theory that the number of lattice points within or on this ellipsoid is

$$G(x) = \frac{4\pi\upsilon}{3} x^{3/2} + \upsilon x^{3/4} \sum_{n_1, n_2, n_3 = -\infty}^{\infty}{}' \frac{J_{3/2}\left[2\pi \chi^{1/2} \sqrt{\sum_{r=1}^{3} n_r^2 L_r^2} \right]}{\left[\sum_{r=1}^{3} n_r^2 L_r^2 \right]^{3/4}} \qquad (3\text{-}9)$$

where $J_{3/2}$ is the 3/2 order Bessel function of the first kind; $\upsilon = L_1 L_2 L_3$; and $\sum'$ means we do not count $n_1 = n_2 = n_3 = 0$. The first term in (3-9) is just the volume of the ellipsoid, while the terms that follow are the corrections which arise from the discreteness of the lattice. From the properties of Bessel functions it is clear that the correction terms are oscillatory functions of the parameter χ and the quantities L_i.

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[1] An explicit expression for the lattice points of an n-dimensional ellipsoid is given in Kendall's paper (Ref. 5)

3.4 Magnetic Moment

a. Non-oscillatory Term.

The total volume of both ellipsoids in quantum space gives rise to a non-oscillatory term in the magnetic moment. The calculation of this moment has been the subject of several papers even since the original work of Pauli (Ref. 7). It is sufficient to give the result here since the algebra involved can be found in great detail in several papers.[2] The result obtained here is in agreement with previously published results. To first approximation (neglecting temperature dependence) one finds that the non-oscillatory term (n. o.) is

$$M_{n.o.} = \frac{4\pi V}{h^3} (2m)^{3/2} \beta^2 E_o^{1/2} H \tag{3-10}$$

If the Fermi energy is assumed to be of the order of one electron volt, we get

$$\frac{M_{n.o.}}{V} \sim 10^{-6} H .$$

b. Oscillatory Terms.

The remaining question is How large are the oscillatory terms? Before answering this question we first need to estimate the effect of temperature on the amplitude of these oscillatory terms. Physically it seems reasonable to expect that as the temperature increases the amplitude of the oscillatory terms will decrease. This estimate is based on the fact that the Fermi distribution is smeared out with increasing temperature. It would then seem plausible that by estimating the oscillatory term at $T = 0°K$ we will have the maximum effect.

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[2] See, for example, the work of E. C. Stoner (Ref. 10)

Since we are concerned with an order of magnitude calculation it will be sufficient to consider only one term in the sum of (3-9). Setting $n_1 = 1$ and $n_2 = n_3 = 0$, the correction term in $G_+(E)$, designated by δG_+, is

$$\delta G_+ = \frac{V(2m)^{3/4}(E + \beta H)^{3/4}}{L_x^{3/2}\ h^{3/2}} \quad J_{3/2}\left[\frac{2\pi}{h}(2m)^{1/2} L_x (E + \beta H)^{1/2}\right] \tag{3-11}$$

Substituting (3-11) into (3-7) and designating this correction to $(F - NE_o)$ by $\delta_+ (F - NE_o)$, we have at $T = 0°K$

$$\delta_+ (F - NE_o) = -K \int_{-\beta H}^{E_o} (E + \beta H)^{3/4} \ J_{3/2}\left[\alpha(E + \beta H)^{1/2}\right] dE \tag{3-12}$$

where

$$K = \frac{V(2m)^{3/4}}{h^{3/2}\ L_x^{3/2}}$$

and

$$\alpha = \frac{2\pi}{h}(2m)^{1/2}\ L_x$$

By setting $\alpha(E + \beta H)^{1/2} = \phi$, (3-12) gives

$$\delta_+ (F - NE_o) = -\frac{2K}{\alpha^{7/2}} \int_0^{\alpha E_{o+}^{1/2}} \phi^{5/2}\ J_{3/2}(\phi)\ d\phi \tag{3-13}$$

where $E_{o+} = E_o + \beta H$. The value of the integral in (3-13) is given in Jahnke and Emde, Tables of Functions, p. 145. Therefore

$$\delta_+ (F - NE_o) = -\frac{2KE_{o+}^{5/4}}{\alpha}\ \ J_{5/2}\ (\alpha E_{o+}^{1/2}) \tag{3-14}$$

But since $\alpha E_{o+}^{1/2} >> 1$, we can use the asymptotic formula for

$J_{5/2}(\alpha E_{o+}^{1/2})$ to get (upon resubstituting the values of K and α)

$$\delta_+ (F - NE_o) \sim \frac{VE_{o+}}{\pi^2 L_x^3} \sin\left[2\pi (2m)^{1/2} \frac{L_x}{h} E_{o+}^{1/2}\right] \tag{3-15}$$

Introducing (3-15) into the expression (2-9) gives the correction to M designated by $\delta_+ M$. Neglecting higher order terms it is

$$\delta_+ M \sim - \frac{V(2m)^{1/2} \beta E_{o+}^{1/2}}{\pi L_x^2 h} \cos\left[2\pi (2m)^{1/2} \frac{L_x}{h} E_{o+}^{1/2}\right] \tag{3-16}$$

Considering the same correction ($n_1 = 1$ and $n_2 = n_3 = 0$) to $G_-(E)$, we have for $\delta_- M$, the value

$$\delta_- M \sim + \frac{V(2m)^{1/2} \beta E_{o-}^{1/2}}{\pi L_x^2 h} \cos\left[2\pi (2m)^{1/2} \frac{L_x}{h} E_{o-}^{1/2}\right] \tag{3-17}$$

where $E_{o-} = E_o - \beta H$. The net correction to M is the sum of (3-16) and (3-17). For $E_o >> \beta H$, it is found that

$$\delta M = \delta_+ M + \delta_- M$$

$$\sim \frac{2V(2m)^{1/2} \beta E_o^{1/2}}{\pi L_x^2 h} \sin\left[2\pi (2m)^{1/2} \frac{L_x}{h} E_o^{1/2}\right] \sin\left[\pi (2m)^{1/2} \frac{L_x}{h} \frac{\beta H}{E_o{}^{1/2}}\right] \tag{3-18}$$

In order of magnitude the amplitude of this correction is

$$\left|\frac{\delta M}{V}\right| \sim \frac{10^{-12}}{L_x^2}$$

Although it would appear that this correction might become comparable to the non-oscillatory term (3-10) at sufficiently low fields and small dimensions, it can be inferred that most likely the effect will be completely negligible. This inference is based on the fact that the argument of the first sine term in (3-18) is so large. Suppose there were an uncertainty of δL_x in the dimension L_x. How small must δL_x be in order that the term

$$\sin\left[2\pi(2m)^{1/2}\ \frac{L_x}{h}\ E_o^{1/2}\right]$$

have a definite value? A simple answer to this question is to require that the uncertainty δL_x should not change the phase of the term by more than $\pi/2$. This criterion imposes the condition

$$\delta L_x < \frac{h}{4(2m)^{1/2}\ E_o^{1/2}} \tag{3-19}$$

In terms of numbers this requires

$$\delta L_x \lesssim 10^{-8}\ \text{cm}.$$

This severe restriction on the accuracy with which L_x must be known is enough to assure that for all laboratory specimens the correction (3-18) will be negligible.

3.5 Summary

This treatment of spin paramagnetism by number theoretical methods has shown that there are corrections to the non-oscillatory term in M, but that from an experimental point of view these corrections are negligible. The principal value of this work has been to introduce the use of number theory in solving a relatively simple problem. In one of the following chapters we will deal with the effect of spin in a more rigorous manner.

CHAPTER 4

DIAMAGNETISM AND THE DE HAAS-VAN ALPHEN EFFECT FOR A SPINLESS ELECTRON GAS

4.1 Content

In this chapter we consider magnetic properties other than the spin paramagnetism. The effect of spin will be merely to introduce an additional degeneracy of two in the various energy levels. Number theory concepts will be used to compute the free energy and magnetic moment. We will restrict this development to such magnetic field strengths and dimensions of the container as to avoid, seemingly, the need for considering the effect of surface states. The latter will be treated in a later chapter.

4.2 Schrodinger Equation

The Hamiltonian function for an electron in a magnetic field is

$$\frac{1}{2m}\left[\left(p_x + \frac{e}{c} A_x\right)^2 + \left(p_y + \frac{e}{c} A_y\right)^2 + \left(p_z + \frac{e}{c} A_z\right)^2\right] + U \qquad (4\text{-}1)$$

where $\vec{A}$ is the vector potential defined so that

$$\vec{H} = \text{curl } \vec{A} \qquad (4\text{-}2)$$

In (4-1) e is the absolute value of the electronic charge. If the applied field $\vec{H}$ is along the z axis of our box containing the electrons, a suitable vector potential is

$$\vec{A} = (o, Hx, o) \qquad (4\text{-}3)$$

The potential energy, U, is set equal to zero within the box so that the Schrodinger equation is

$$\frac{1}{2m}\left[-\hbar^2\nabla^2 + \frac{e^2A_y^{\,2}}{c^2} - \frac{2e\hbar}{ci}A_y\frac{\partial}{\partial y}\right]\psi = E\psi \tag{4-4}$$

This equation can be separated into two ordinary differential equations if we assume a solution of the form

$$\psi = \phi(x)\,\zeta(z)\;e^{\frac{2\pi i n_y y}{L_y}} \tag{4-5}$$

Substituting (4-5) into (4-4) and introducing separation constants gives

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2}/\phi + \frac{1}{2m}\left(\frac{h\,n_y}{L_y} - \frac{e}{c}A_y\right)^2 = E_1 \tag{4-6}$$

and

$$-\frac{\hbar^2}{2m}\frac{d^2\zeta}{dz^2}/\zeta = E_2 \tag{4-7}$$

where $E = E_1 + E_2$. The motion in the direction of the field is clearly that of a free particle so that we can immediately write the eigenvalues as

$$E_2 = \frac{h^2 n_z^2}{2m L_z^2} \tag{4-8}$$

if we assume periodic boundary conditions in the z dimension. With this assumption the quantum number n_z takes on all positive and negative integer values (including zero).

We will now use the WKB approximation to solve for the eigenvalue E_1 since this is the method which will be subsequently applied to estimate the effect of surface states. However, in this chapter we will restrict our development to problems in which such surface effects are apparently negligible. Equation (4-6) is the Schrodinger equation of a one-dimensional system with a classical Hamiltonian of the form

$$\mathcal{H} = \frac{p^2}{2m} \qquad U = E_1 \tag{4-9}$$

where

$$U = \frac{1}{2m} \left(\frac{h n_y}{L_y} - \frac{e}{c} A_y \right)^2$$

Inserting the value of A_y given in (4-3) the classical turning points of the motion become

$$x = \frac{c h n_y}{eHL_y} \pm \frac{c}{eH} \sqrt{2mE_1} \tag{4-10}$$

(For symmetry it is convenient to set the origin of coordinates such that the walls are at $\pm Lx/2$.) Using these turning points in the WKB quantum condition

$$\oint p_x \, dx = (n + 1/2) h \tag{4-11}$$

leads to the eigenvalue relation

$$E_1 = 2 \beta H (n + 1/2) \tag{4-12}$$

These levels are recognized as the energy values of a simple harmonic oscillator having a frequency of $eH/2\pi mc$. From (4-10) we see that the equilibrium position of the oscillator (center of the orbit) is chn_y/eHL_y and the orbit radius is $\frac{c}{eH}\sqrt{2mE_1}$. The eigenvalues given by (4-12) are highly degenerate because of the multitude of n_y values that can be assigned in the orbit center (n_y takes on the same range of values as n_z). In fact the degeneracy will be fixed by the maximum value that can be assigned to n_y and still have the parabolic potential determine the turning points. For $|n_y|$ greater than this critical value (4-12) will no longer be applicable since one turning point will then be fixed at $\pm L_x/2$, where the potential is assumed to be infinite. We will now obtain an explicit expression for this degeneracy since this will clarify the approximations to be made. If we fix the value of E_1 the harmonic oscillator solution (4-12) will fail when the condition $U = E_1$ is satisfied simultaneously with the condition that one of the turning points is at $\pm L_x/2$. This leads to the restriction

$$|n_y| \leq \left| \frac{e H L_x L_y}{2 c h} - \frac{L_y}{h} \sqrt{2mE_1} \right|$$

on n_y. The total degeneracy of the level (4-12) is therefore

$$\frac{e H L_x L_y}{c h} - \frac{2 L_y}{h} \sqrt{2mE_1} \qquad (4-13)$$

If n_y is allowed to take on values outside of the above range we would have to obtain a new expression for the eigenvalues.[1] The states resulting from this extension in n_y are our so-called surface states. At this point we follow Landau (Ref. 6) in specifying that for sufficiently strong magnetic fields and/or large enough L_x we can neglect the second term in (4-13) and designate the degeneracy, D, of the level (4-12) by

$$D = \frac{e H L_x L_y}{c h} \qquad (4-14)$$

This specification is equivalent to saying that the orbit radius corresponding to energies of the order of the Fermi energy is small compared to the dimension L_x. When $E_1 \sim 1$ electron volt this requires

$$H L_x \gg \frac{2 c \sqrt{2mE_1}}{e} \sim 10$$

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[1] The quantum number n_y can actually take on all integer values in the range $|n_y| \leq \left| \frac{e H L_x L_y}{2 c h} + \frac{L_y}{h} \sqrt{2mE_1} \right|$. In Chapter 7 we deal with the complete range.

This condition is satisfied even for relatively low fields if we use macroscopic dimensions.

Before proceeding with the calculation of the free energy, it should be noted that in treating the magnetic susceptibility with a classical model omission of the surface states under any circumstances would lead to a huge diamagnetism.[2] The question therefore arises as to the legitimacy of our neglecting the surface states in the quantum mechanical case. At this stage we merely indicate that some compensation was made for omitting the surface states when we increased the degeneracy of the interior states from (4-13) to (4-14). If this compensation happens to restore the effects of the neglected states then we have justified the use of the increased degeneracy. Detailed calculations given in a later chapter will show that the compensation is fortuitously exact. But without such calculation it is not at all obvious that Landau's (Ref. 6) argument for neglecting the surface states is valid. An elaboration of this point was believed to be in place here since there has appeared in the literature[3] a somewhat misleading qualitative physical explanation to justify Landau's approximation.

4.3 Free Energy

Combining (4-8) and (4-12) gives

$$E = \frac{h^2 n_z^2}{2m L_z^2} + 2\beta H (n + 1/2) \tag{4-15}$$

This level is degenerate in the quantum number n_y to the extent D given in (4-14). Equations (4-15) and (4-14) describe a parabolic cylinder in

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[2] For a complete account of this development see, for example, J. H. Van Vleck, Theory of Electric and Magnetic Susceptibilities, (Oxford University Press, 1932) p. 100.

[3] See, for example, F. Seitz, Modern Theory of Solids, (McGraw-Hill, 1940) p. 585.

quantum number space. Our calculation of G(E) is therefore equivalent to the problem of finding the number of lattice points within such a cylinder bounded by the $n = 0$ plane. Since the degeneracy is independent of E we need only consider the two-dimensional lattice point problem in the n, n_z plane. In that plane (4-15) described a parabola which is cut off by the line $n = 0$. The particular number theory problem of computing the lattice points under such a curve had not been considered at the time this work was initiated. But following the work of Kendall (Ref. 5) it is possible to obtain here an explicit representation for the number of lattice points. A detailed account of this calculation is given below since the method employed may be of value in other problems.

Let us allow the parabola (4-15) in the n, n_z plane to be randomly located but with its axis parallel to the n axis. Then we can write the equation of the parabola as

$$E = A(n_z - \alpha_2)^2 + B(n + 1/2 - \alpha_1) \qquad (4\text{-}16)$$

where

$$A = h^2/2mL_z^2$$

$$B = 2\beta H$$

Now the number of lattice points under this parabola (cut off by the line $n = \alpha_1$) will be periodic in α_1 and α_2 with a periodicity of a single lattice spacing (unity) along either the n or n_z axes. We can therefore represent G(E) as a doubly-periodic function in a Fourier series,

$$G(E) = D \sum_{\kappa=-\infty}^{\infty} \sum_{\lambda=-\infty}^{\infty} a_{\kappa,\lambda} \; e^{2\pi i(\kappa\alpha_1 + \lambda\alpha_2)} \qquad (4\text{-}17)$$

The Fourier coefficients $a_{\kappa,\lambda}$ depend on the parameter E as well as the factors A and B. Before proceeding with the determination of $a_{\kappa,\lambda}$ we must examine the question of where the parabola should be cut off.

In the final analysis we must set $\alpha_1 = \alpha_2 = 0$ in order that the parabola (4-16) be correctly oriented in accordance with the quantum mechanical requirement (4-15). Further, the lowest value of n is supposed to be zero. However, by setting $\alpha_1 = 0$ and leaving the cut-off of the parabola at $n = 0$, the Fourier series will only count one-half of the states along the $n = 0$ line. This would be due to the large discontinuity experienced by the number of lattice points as one slides the parabola (along the n axis) so that the cut-off passes through an integer value of n. The Fourier series would then give the average of the two values on either side of the discontinuity. Since the discontinuity would correspond to the number of states along $n = 0$ we would be undercounting the states by one half the amount along that line. In order to avoid this difficulty and still maintain the requirement $\alpha_1 = \alpha_2 = 0$, it is convenient to move the cut-off from $n = 0$ to $n = -1/2$. This shift of the cut-off increases the area enclosed by our closed curve <u>but it does not change the number of lattice points</u>. The particular choice of $n = -1/2$ for the cut-off may appear to be arbitrary at this stage since we could have chosen any value in the range

$$-1 < n < 0$$

without changing the number of lattice points. We shall see that the value $n = -1/2$ simplifies the problem enormously.

Let G(E) also be represented by the sum

$$G(E) = D \sum_{n, n_z} C\,(n_z - \alpha_2,\ n + 1/2 - \alpha_1) \tag{4-18}$$

where C(u, v) is equal to unity or zero according as (u, v) does or does not fall in the range

$$A v^2 + B u \leq E, \quad u \geq 0 \tag{4-19}$$

The summation in (4-18) is extended over all lattice points but only a finite number of these contribute non-zero terms. From (4-17) and the periodicities in α_1 and α_2 it follows that

$$a_{\kappa,\lambda} = \int_0^1 \int_0^1 \frac{G(E)}{D} e^{-2\pi i(\kappa\alpha_1 + \lambda\alpha_2)} d\alpha_1 \, d\alpha_2 \tag{4-20}$$

If we now make the transformation

$$\begin{aligned} u &= n + 1/2 - \alpha_1 \\ v &= n_z - \alpha_2 \end{aligned} \tag{4-21}$$

and use (4-18) we get

$$a_{\kappa,\lambda} = \sum_{n,n_z} \int_{n_z}^{n_z - 1} \int_{n+\frac{1}{2}}^{n-\frac{1}{2}} C(u,v) \, e^{-i\kappa\pi} e^{2\pi i(\kappa u + \lambda v)} du \, dv$$

or

$$a_{\kappa,\lambda} = (-1)^{\kappa} \iint_{Av^2 + Bu \leq E} e^{2\pi i(\kappa u + \lambda v)} \, du \, dv \tag{4-22}$$

Since α_1 and α_2 will both be set to zero, and the cut-off will be at $n = -1/2$, it follows from (4-21) that the limits of integration in the u, v plane will be

u: from 0 to E/B
v: from $-(E/A)^{1/2}$ to $(E/A)^{1/2}$

From (4-22) we have $a_{\kappa,\lambda} = (a_{-\kappa,-\lambda})^*$, $a_{\kappa,-\lambda} = (a_{-\kappa,\lambda})^*$, and $a_{\kappa,\lambda} = a_{\kappa,-\lambda}$, so that G(E) can be written as

$$G(E) = D\sum_{\kappa,\lambda=-\infty}^{\infty} a_{\kappa,\lambda} = D\left[a_{0,0} + 2\sum_{\kappa=1}^{\infty} \mathrm{R}(a_{\kappa,0}) + 2\sum_{\lambda=1}^{\infty} \mathrm{R}(a_{0,\lambda}) + 4\sum_{\kappa,\lambda=1}^{\infty} \mathrm{R}(a_{\kappa,\lambda})\right]$$

(4-23)

(where $\mathcal{R}$ denotes "the real part of"). Utilizing the symmetry of our boundary curve with respect to v it follows from (4-22) that

$$\mathcal{R}\,(a_{\kappa,\lambda}) = (-1)^{\kappa} \iint\limits_{Av^2+Bu\leq E} \cos(2\pi\kappa u)\cos(2\pi\lambda v)\,du\,dv \tag{4-24}$$

The coefficient $a_{o,o}$, which corresponds to the area of the closed curve, is found to be simply

$$a_{o,o} = \frac{4\,E^{3/2}}{3\,B\,A^{1/2}} \tag{4-25}$$

(This is the first advantage of having chosen n = -1/2 as the cut-off.) The general coefficient $\mathcal{R}(a_{\kappa,\lambda})$ can be expressed as (for $\kappa \neq 0$)

$$\mathcal{R}\,(a_{\kappa,\lambda}) = (-1)^{\kappa}\, B^{1/2}\, U_{3/2}(w,y)/A^{1/2}\,\pi(2\kappa)^{3/2} \tag{4-26}$$

where

$$\begin{aligned} w &= \frac{4\pi\kappa E}{B} \\ y &= 2\pi\lambda\sqrt{E/A} \end{aligned} \tag{4-27}$$

and $U_{3/2}(w,y)$ is the 3/2 order Lommel function of two variables discussed by Watson (Ref. 11) in his Bessel function treatise. The Lommel function $U_\nu(w,y)$ is a series (of the Neumann type) defined by

$$U_\nu(w,y) = \sum_{m=o}^{\infty} (-1)^m \left(\frac{w}{y}\right)^{\nu+2m} J_{\nu+2m}(y) \tag{4-28}$$

Details of the evaluation of $\mathcal{R}(a_{\kappa,\lambda})$ in terms of Lommel functions are given in Appendix I.

From the results given above, G(E) is given explicitly by the expression

$$G(E) = \frac{4DE^{3/2}}{3BA^{1/2}} + \frac{2DB^{1/2}}{A^{1/2}\pi} \sum_{K=1}^{\infty} \frac{(-1)^K}{(2K)^{3/2}} \; U_{3/2}(w,o) + 2D \sum_{\lambda=1}^{\infty} R(a_{o,\lambda})$$

$$+ \frac{4DB^{1/2}}{A^{1/2}\pi} \sum_{K,\lambda=1}^{\infty} \frac{(-1)^K}{(2K)^{3/2}} \; U_{3/2}(w,y) \qquad (4\text{-}29)$$

The free energy can now be given formally by substituting (4-29) into (2-4). It is noted that by shifting the cut-off to $n = -1/2$ we have changed E_L from βH to zero. This is very convenient in (2-4) since $G(E_L)$ then becomes zero. In fact this is the second advantage of choosing $n = -1/2$ instead of some other values for the cut-off. If we now take into account the factor of two due to spin degeneracy we get

$$\begin{aligned} F - NE_o = & \frac{-8D}{3BA^{1/2}} \int_0^{\infty} E^{3/2} f(E)\, dE \\ & \frac{-4DB^{1/2}}{A^{1/2}\pi} \sum_{K=1}^{\infty} \int_0^{\infty} \frac{(-1)^K}{(2K)^{3/2}} \; U_{3/2}(w,o) f(E)\, dE \\ & -4D \sum_{\lambda=1}^{\infty} \int_0^{\infty} R(a_{o,\lambda}) f(E)\, dE \\ & \frac{-8DB^{1/2}}{A^{1/2}\pi} \sum_{K,\lambda=1}^{\infty} \int_0^{\infty} \frac{(-1)^K}{(2K)^{3/2}} \; U_{3/2}(w,y) f(E)\, dE \end{aligned} \qquad (4\text{-}30)$$

Before continuing with the evaluation of this expression it is possible to make some general statements concerning the nature of the result. The first integral in (4-30) is one which occurs frequently in applications of the Fermi-Dirac statistics. A detailed treatment of the evaluation of such integrals is given by Brillouin (Ref. 2). The important thing to note in this first term is that there is no explicit dependence on the magnetic field. In fact we shall show that it is identically the term which results from treating free electrons in a box in the absence of a magnetic field. On the other hand, the double sum and the single sum on κ in (4-30) are very definitely a function of the magnetic field. Further, from the oscillatory nature of the Lommel functions we can suspect that these terms may give rise to periodic (in magnetic field strength) fluctuations in the free energy. These general features will also describe the behavior of such properties as the heat capacity and the magnetic moment. In the case of magnetic moment the oscillatory terms can be plausibly identified with the experimentally observed d-v-e.

A. Non-oscillatory term ($\lambda = 0$, $\kappa = 0$)

Using the results given by Brillouin (Ref. 2) for Fermi-Dirac integrals at sufficiently low temperatures, the non-oscillatory term (n. o.) is found to be

$$(F - N E_o)_{n.o.} = \frac{-16 D E_o^{5/2}}{15 B A^{1/2}} \left[1 + \frac{5}{8} \pi^2 \left(\frac{kT}{E_o}\right)^2 \right] \tag{4-31}$$

The condition $E_o >> kT$ must be fulfilled for (4-31) to be valid. Inserting the values of D, B and A we can rewrite (4-31) as

$$(F - N E_o)_{n.o.} = -\frac{16\pi V (2m)^{3/2} E_o^{5/2}}{15 h^3} \left[1 + \frac{5}{8} \pi^2 \left(\frac{kT}{E_o}\right)^2 \right] \tag{4-32}$$

where $V = L_x L_y L_z$.

B. Oscillatory terms.

In general, the integrals appearing within the summations of (4-30) can not be evaluated in closed form. We shall now treat the summations individually since certain of the terms will not be of importance in determining the magnetic moment.

1. Terms with $\kappa = 0$, $\lambda \neq 0$.

Using the series representation of the Lommel function it can be shown that

$$\lim_{\kappa \to 0} \frac{(-1)^{\kappa}}{(2\kappa)^{3/2}} U_{3/2}(w, y) = \frac{E^{3/4} A^{3/4}}{\lambda^{3/2} B^{3/2}} J_{3/2}(y) \tag{4-33}$$

This expression corresponds to the value

$$\mathcal{R}(a_{o,\lambda}) = \frac{E^{3/4} A^{1/4}}{\pi B \lambda^{3/2}} J_{3/2}(y) \tag{4-34}$$

for the Fourier coefficients $a_{o,\lambda}$. It can also be shown by direct integration of (4-24) that this is the correct value of $\mathcal{R}(a_{o,\lambda})$. Details of such a calculation are given in Appendix II.

Thus $\kappa = 0$ gives rise to the infinity of terms

$$-\sum_{\lambda=1}^{\infty} \frac{4L_x L_y (2m)^{3/4}}{L_z^{1/2} h^{3/2} \lambda^{3/2}} \int_0^{\infty} E^{3/4} J_{3/2}\left(\frac{2\pi\lambda L_z}{h} \sqrt{2mE}\right) f(E)\, dE \tag{4-35}$$

in the value of $(F - NE_o)$. Since none of these terms contain the magnetic field explicitly there will be no need to carry out the integration in (4-35) if we restrict our attention to the evaluation of the magnetic moment.

2. Terms with $\kappa \neq 0$.

The terms with $\kappa \neq 0$ in the sums of (4-30) are all dependent on the magnetic field. In order to evaluate the magnetic moment we will need to transform these integrals. Integrating by parts gives

$$\int_0^\infty U_{3/2}(w,y)\, f(E)\, dE = \left[f(E) \int U_{3/2}(w,y)\, dE \right]_0^\infty - \int_0^\infty \left[\frac{df(E)}{dE} \int U_{3/2}(w,y)\, dE \right] dE \tag{4-36}$$

But it is shown in Appendix III that

$$\int U_{3/2}(w,y)\, dE = \frac{B}{2\pi\kappa}\, U_{5/2}(w,y) \tag{4-37}$$

Since $U_{5/2}(o,o) = 0$, the integrated part of (4-36) vanishes and we are left with

$$\int_0^\infty U_{3/2}(w,y)\, dE = -\frac{B}{2\pi\kappa} \int_0^\infty U_{5/2}(w,y)\, \frac{df(E)}{dE}\, dE \tag{4-38}$$

With this transformation the remaining terms in (4-30) become (in terms of our physical quantities)

$$\frac{2\, V\, e\, (2m)^{1/2} \beta^{3/2} H^{5/2}}{\pi^2 h^2 C} \sum_{\kappa=1}^{\infty} \frac{(-1)^\kappa}{\kappa^{5/2}} \int_0^\infty U_{5/2}(w,o)\, \frac{df(E)}{dE}\, dE$$

$$+\frac{4V\, e\, (2m)^{1/2} \beta^{3/2} H^{5/2}}{\pi^2 h^2 C} \sum_{\kappa,\lambda=1}^{\infty} \frac{(-1)^\kappa}{(\kappa)^{5/2}} \int_0^\infty U_{5/2}(w,y)\, \frac{df(E)}{dE}\, dE \tag{4-39}$$

For convenience in discussing the magnetic moment, the total expression for $(F - NE_o)$ is given below

$$F - NE_o = -\frac{16\pi V(2m)^{3/2} E_o^{5/2}}{15\,h^3}\left\{1 + \frac{5}{8}\pi^2 \left(\frac{kT}{E_o}\right)^2\right\}$$

$$- \sum_{\lambda=1}^{\infty} \frac{4 L_x L_y (2m)^{3/4}}{L_z^{1/2} h^{3/2} \lambda^{3/2}} \int_0^{\infty} E^{3/4} J_{3/2}\left(\frac{2\pi\lambda L_z}{h}\sqrt{2mE}\right) f(E)\,dE$$

$$+ \sum_{\substack{\kappa=1 \\ \lambda=0}} T_\lambda \frac{(-1)^{\kappa} 2Ve(2m^{1/2}\beta^{3/2} H^{5/2}}{\pi^2 h^2 C\,\kappa^{5/2}} \int_0^{\infty} U_{5/2}(w,y)\frac{df(E)}{dE}\,dE$$

(4-40)

where $T_\lambda = \begin{cases} 1 & \text{for } \lambda = 0 \\ 2 & \text{for } \lambda \neq 0 \end{cases}$.

4.4 Magnetic Moment

The magnetic moment is obtained by substituting (4-40) into (2-9) and carrying out the indicated differentiation. Since the integrated term and the single sum on λ in (4-40) do not contain H explicitly, they do not contribute anything to the magnetic moment. Differentiating the double sum gives

$$M = -\sum_{\substack{\kappa=1 \\ \lambda=0}}^{\infty} T_\lambda \frac{(-1)^{\kappa} 2Ve(2m)^{1/2}\beta^{3/2}}{\pi^2 h^2 C\,\kappa^{5/2}} \left\{ \begin{aligned} &\frac{5}{2} H^{3/2} \int_0^{\infty} U_{5/2}(w,y)\frac{df(E)}{dE}\,dE \\ &- \frac{\pi\kappa H^{1/2}}{\beta} \int_0^{\infty} U_{3/2}(w,y)\frac{df(E)}{dE}\,dE \\ &- \frac{\pi\lambda^2 \beta H^{5/2}}{\kappa A} \int_0^{\infty} U_{7/2}(w,y)\frac{df(E)}{dE}\,dE \end{aligned} \right\}$$

(4-41)

The last two integrals in (4-41) arise from the relation

$$\frac{\partial}{\partial H} U_{5/2}(w, y) = -\frac{\pi \kappa E}{\beta H^2} U_{3/2}(w, y) - \frac{\pi \lambda^2 \beta}{\kappa A} U_{7/2}(w, y) \qquad (4\text{-}42)$$

The proof of this identity is given in Appendix IV. Equation (4-41) is an exact representation of the magnetic moment. But in order to obtain an answer in integrated form we have to impose some restriction on the relative magnitudes of E and βH. In addition, we will limit ourselves to the low temperature region.

Case I: $E_o >> \beta H$

The first case we consider is for

$$E_o >> \beta H \qquad (4\text{-}43)$$

This requirement will allow us to use the asymptotic expansion of the Lommel function $U_\nu (w, y)$.

1. Terms with $\lambda = 0$.

For purposes of later discussion it is now again convenient to break up the sum of (4-41) into two parts, i.e. $\lambda = 0$ and $\lambda \neq 0$. For $\lambda = 0$ we have the asymptotic expansion

$$U_\nu (w, o) \sim \cos\left(\frac{1}{2} w - \frac{\nu \pi}{2}\right) + \sum_{p=o}^{\infty} \frac{(-1)^p}{\Gamma(\nu - 1 - 2p)(\frac{1}{2} w)^{2p-\nu+2}} \qquad (4\text{-}44)$$

for $|w|$ large. In our case (4-43) expresses the condition $|w|$ large. Since the series in (4-44) is rapidly convergent we need only retain the first term of the sum. Thus we have

$$U_\nu \left(\frac{4\pi\kappa E}{B}, o\right) \sim \cos\left(\frac{2\pi\kappa E}{B} - \frac{\nu\pi}{2}\right) + \frac{B^{2-\nu}}{\Gamma(\nu - 1)(2\pi\kappa E)^{2-\nu}} \qquad (4\text{-}45)$$

This gives rise to the sum

$$-\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} 2Ve(2m)^{1/2}\beta^{3/2}}{\pi^2 h^2 C \kappa^{5/2}} \left\{ \begin{aligned} &\frac{5}{2} H^{3/2} \int_0^{\infty} \cos\left(\frac{2\pi\kappa E}{B} - \frac{5\pi}{4}\right) \frac{df(E)}{dE}\, dE \\ &+ \frac{4\kappa^{1/2} H}{\beta^{1/2}} \int_0^{\infty} E^{1/2} \frac{df(E)}{dE}\, dE \\ &- \frac{\pi\kappa H^{1/2}}{\beta} \int_0^{\infty} \cos\left(\frac{2\pi\kappa E}{B} - \frac{3\pi}{4}\right) \frac{df(E)}{dE}\, E\,dE \end{aligned} \right\} \tag{4-46}$$

in the value of M. The second integral of (4-46) is a standard type Fermi-Dirac integral. At low temperatures we have

$$\int_0^{\infty} E^{1/2} \frac{df(E)}{dE}\, dE = -E_o^{1/2} \left\{ 1 - \frac{\pi^2}{24} \left(\frac{kT}{E_o}\right)^2 \right\} \tag{4-47}$$

so that this part of the sum becomes

$$+\frac{8Ve(2m)^{1/2}\beta H E_o^{1/2}}{\pi^2 h^2 C} \left\{ 1 - \frac{\pi^2}{24} \left(\frac{kT}{E_o}\right)^2 \right\} \sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa}}{\kappa^2} \tag{4-48}$$

But since

$$\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa}}{\kappa^2} = -\frac{\pi^2}{12} \tag{4-49}$$

(4-48) becomes

$$-\frac{2Ve(2m)^{1/2}\beta E_o^{1/2} H}{3 h^2 C} \left\{ 1 - \frac{\pi^2}{24} \left(\frac{kT}{E_o}\right)^2 \right\} \tag{4-50}$$

This part of the magnetic moment is not periodic in H. In fact it is identically the ordinary Landau (Ref. 6) diamagnetism with the correction due to temperature. The result obtained here agrees with the previous work of Stoner (Ref. 10), who investigated the temperature dependence of the Landau diamagnetism.[4]

The two other integrals of (4-46) give terms in M which are periodic functions of the magnetic field. Their contribution to M is

$$-\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} 2Ve(2m)^{1/2}\beta^{3/2}}{\pi^2 h^2 C \kappa^{5/2}} \left\{ \frac{5\pi^2 \kappa kTH^{1/2} \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{5\pi}{4}\right)}{2\beta^{1/2} \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)} - \frac{\pi^2 \kappa kTH^{1/2} \sin\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\beta \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)} + \frac{\pi^4 \kappa^2 (kT)^2 \cosh\left(\pi^2 \kappa \frac{kT}{\beta H}\right) \sin\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\beta^2 H^{1/2} \sinh^2\left(\pi^2 \kappa \frac{kT}{\beta H}\right)} - \frac{\pi^3 \kappa^2 kT E_o \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\beta^2 H^{1/2} \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)} \right\} \tag{4-51}$$

Details of the evaluation of the first and third integrals in (4-46) are given in Appendix V. If we invoke our conditions

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[4] It is noted that Stoner expresses his results in terms of ϵ_o, the Fermi energy at T = 0°K and H = 0, whereas the E_o used in the present work is a function of T and H. E_o can be expressed as a function of ϵ_o, T, H to bring the two results into coincidence.

$$E_o >> kT$$

and $$E_o >> \beta H$$

we can neglect the first three terms appearing in the brackets of (4-51) compared to the fourth. The significant contribution to M from the terms with $\lambda = 0$ therefore becomes (using the definition of β, the Bohr magneton, to transform the non-periodic term)

$$- \frac{4\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3} \left[1 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2 \right]$$
$$+ \sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa}\, 2\pi k T V e (2m)^{1/2}\, E_o \cos\left(\frac{\pi \kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2}\, h^2\, C\, \beta^{1/2}\, H^{1/2} \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)} \qquad (4\text{-}52)$$

2. Terms with $\lambda \neq 0$.

Before obtaining the contribution from the terms with $\lambda \neq 0$ we must examine the relative magnitudes of y and w appearing in the argument of the Lommel functions. For $\lambda \neq 0$ we find that $y \sim w$ when $E = E_o$ and $H > 10$ gauss (if L_z is of order cm). Therefore if we require $|w| >> 1$ in our asymptotic solution we must simultaneously require $|y| >> 1$. This situation arises from the physical parameters which determine the argument of the Lommel functions. Unfortunately, it also means that we cannot use (without caution) the asymptotic development for $U_\nu(w, y)$ given by Watson (Ref. 11), in which only $|w| >> 1$.

When both $|y| >> 1$ and $|w| >> 1$ we can use the method of critical points (see Appendix VI) to get the asymptotic development of $U_\nu(w, y)$. The result is dependent upon whether $y \lesseqgtr w$. The three expansions for $U_{3/2}(w, y)$ are given below.

$$U_{3/2}(w,y) \sim \begin{cases} \cos\left(\frac{w}{2} + \frac{y^2}{2w} - \frac{3\pi}{4}\right) + \left(\frac{2}{\pi}\right)^{1/2} \frac{w^{3/2}\cos y}{(w^2 - y^2)}, & y < w \\ \frac{1}{2}\cos\left(w - \frac{\pi}{4}\right) + \frac{\cos w}{2^{3/2}\pi^{1/2}w^{1/2}}, & y = w \\ \left(\frac{2}{\pi}\right)^{1/2} \frac{w^{3/2}\cos y}{(w^2 - y^2)}, & y > w \end{cases} \tag{4-53}$$

The singular case of $y = w$ is not of great physical significance since it only occurs at a specific value of H. We are more concerned with the cases $y \lessgtr w$ since there H can take on continuous values. Before proceeding to the moments resulting from $\lambda \neq 0$ we note that $y < w$ requires that (for $E = E_o$)

$$\lambda < \frac{\kappa\, h\, E_o^{1/2}}{L_z (2m)^{1/2} \beta H} \tag{4-54}$$

After carrying out the calculations to get the magnetic moment, it is found that only those terms arising from the condition $y < w$ are significant. The specific contribution to M from these terms is

$$\sum_{\lambda=1}^{\infty} \sum_{\kappa=\kappa_L(H,\lambda)}^{\infty} \left\{ \begin{array}{l} (-1)^{\kappa} \dfrac{4\pi k T V e (2m)^{1/2} \beta^{1/2} H^{3/2}}{\kappa^{3/2} h^2 C} \left(\dfrac{2\lambda^2 m L_z^2 \beta}{\kappa h^2} - \dfrac{\kappa E_o}{\beta H^2} \right) \\ \times \dfrac{\cos\left(\dfrac{\pi \kappa E_o}{\beta H} + \dfrac{2\pi\lambda^2 m \beta L_z^2 H}{\kappa h^2} - \dfrac{3\pi}{4} \right)}{\sinh\left(\pi^2 \kappa \dfrac{kT}{\beta H} \right)} \end{array} \right\} \tag{4-55}$$

where $\kappa_L(H,\lambda)$ is the integral part of

$$\frac{\lambda L_z (2m)^{1/2} \beta H}{h\, E_o^{1/2}}$$

3. Discussion of Magnetic Moment.

For the case $E_0 \gg \beta H$ the magnetic moment is the sum of (4-52) and (4-55). We have already discussed the non-periodic term. The remaining terms are all periodic functions of H. We shall separate the discussion of the single sum in (4-52) and the double sum in (4-55). But we identify the totality of these terms with the experimentally observed d-v-e.

Consider now the single sum on κ. If we express our result in terms of the magnetization, M/V, then both the amplitudes and frequencies of all the terms in this sum are independent of the dimensions of the box. These terms are identically those found by Landau (Ref. 9) in his theory of the d-v-e. Before going on to the other terms it must be reemphasized that the results given here are subject to the conditions $E_0 \gg kT$, $E_0 \gg \beta H$. There is no condition on the magnitude of kT relative to βH. The physical significance of these conditions will be discussed later in this chapter.

We now examine the double sum in (4-55). The fundamental difference between these terms and those of the single sum is that the amplitudes and frequencies are now functions of the dimension L_z. By invoking an argument similar to that used in Chapter 3 we shall show that the contribution of the double sum can be neglected. Suppose there is an uncertainty δL_z in the dimension L_z. Then in order for the cosine term to have a definite value (when H is fixed) we require that δL_z should not change the phase by more than $\pi/2$. This leads to the condition

$$\delta L_z < \frac{\kappa h^2}{8\lambda^2 m \beta L_z H} \tag{4-56}$$

If we set $\lambda = 1$ and κ equal to the lowest possible value compatible with (4-54) this becomes

$$\delta L_z < \frac{2^{1/2} h}{8 m^{1/2} E_o^{1/2}} \tag{4-57}$$

Using the free electron value for m and E_o as 1 ev this requires

$$\delta L_z < 3 \times 10^{-8} \text{ cm}$$

This severe restriction on the uncertainty in L_z cannot be met in a laboratory specimen. Therefore the cosine term in the double sum will average to very nearly zero. The next question to answer is "what happens to δL_z when κ becomes very large?" Certainly as κ grows the restriction on δL_z becomes less severe. In fact the above argument fails completely when $\kappa >> \lambda$. Under such circumstances we have another factor which will nullify the significance of the double sum. It is the damping factor

$$1 \,/\, \sinh \left(\pi^2 \kappa \frac{kT}{\beta H} \right)$$

For κ large the damping factor will make the amplitude of the oscillation negligible.

As a result of this analysis we can completely neglect the double sum given by (4-55). This is equivalent to saying that the "Landau" counting of states leads to no significant size effect in the magnetic moment.

We now consider the feasibility of experimentally observing the magnetic moment. Since the discussion above has indicated that the double sum can be neglected we are left with

$$M = -\frac{4\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3}\left[1 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2\right]$$

$$+ \sum_{K=1}^{\infty} \frac{(-1)^K\, 2\pi kTVe(2m)^{1/2}E_o}{K^{1/2}\, h^2\, C\, \beta^{1/2}\, H^{1/2}} \; \frac{\cos\left(\frac{\pi K E_o}{\beta H} - \frac{3\pi}{4}\right)}{\sinh\left(\pi^2 K \frac{kT}{\beta H}\right)}$$

(4-58)

At sufficiently low temperatures the non-periodic (n.p.) term will be

$$\left(\frac{M}{V}\right)_{n.p.} \sim -10^{-6} H \qquad (4\text{-}59)$$

if $E_o \sim 1$ electron volt.

In order to examine the periodic terms we need to specify the relative magnitude of kT to βH. Consider first the case where $kT > \beta H$. Then because of the damping factor

$$1 / \sinh\left(\pi^2 K \frac{kT}{\beta H}\right)$$

the amplitude of the second term in the sum will be less than 10^{-4} times the first term. Therefore we need only consider the $K = 1$ term in the sum. It then follows that

$$\left|\frac{M}{V}\right|_{p.} \lesssim \frac{T\left(10^{-2\left[2\frac{kT}{\beta H} - 1\right]}\right)}{H^{1/2}} \qquad (4\text{-}60)$$

Now we can compare the non-periodic and periodic terms as a function of temperature and field strength. Let us first take T = 4.2°K (normal boiling point of helium). Then for $H = 10^3$ gauss

$$\left|\frac{M}{V}\right|_{n.p.} \sim 10^{-3}$$

while

$$\left|\frac{M}{V}\right|_{p.} \lesssim 10^{-255}$$

The periodic term would be completely negligible. At T = 1°K and H = 1.5 x 10^4 gauss

$$\left|\frac{M}{V}\right|_{n.p.} \sim 10^{-2}$$

while

$$\left|\frac{M}{V}\right|_{p.} \lesssim 10^{-4}$$

Although the periodic term is again the smaller one it is apparent that at still lower temperatures there may be an inversion in the relative magnitudes. In fact going to the $\lim\limits_{T \to 0°K}$ we get from (4-58)

$$\lim_{T \to 0°K} \left(\frac{M}{V}\right) = -\frac{4\pi(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3} + \left\{\frac{2e(2m)^{1/2} E_o \beta^{1/2} H^{1/2}}{\pi h^2 C} \sum_{\kappa=1}^{\infty} \frac{(-1)^\kappa \cos\left(\frac{\pi \kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{3/2}}\right\} \qquad (4\text{-}61)$$

In this limit we have

$$\left|\frac{M}{V}\right|_{n.p.} \sim 10^{-6} H$$

while for the first term of the sum

$$\left|\frac{M}{V}\right|_{p.} \lesssim 10^{-3} H^{1/2}$$

So for $H \leqq 10^5$ gauss (limit of fields available in the laboratory) the amplitude of the periodic term will be greater than the non-periodic term.

The analysis given above applied to a free electron gas. However, since the alkali metal properties are described quite nicely by the free electron model these results can be used to indicate the conditions that may be needed to detect the d-v-e in a metal such as sodium. To minimize the effect of the strong damping term we can say quite generally that one would need very low temperatures and very high magnetic fields. Specifically, the theory suggests that for $T < 1°K$ and $H > 10^4$ gauss the d-v-e might be observed in sodium. Although such conditions are available in a number of cryogenic laboratories, the particular experiment with sodium has not yet been performed.[5]

Case II, E_o βH.

For strong fields βH approaches the order of magnitude of E_o. In this range of fields the magnetic moment given by (4-41) cannot be expressed in closed form. Numerical integration could be used to obtain M as a function of H.

We can, however, consider a particular set of conditions which will give a closed form for M. To simplify matters let us examine the magnetic moment of our system at the absolute zero of temperature for field strengths so high that

$$\beta H \leqq E_o < 3\beta H \tag{4-62}$$

The result we obtain here can then be compared to the magnetic moment

---

[5] The author has recently learned that D. Shoenberg of the Royal Society Mond Laboratory, Cambridge, is currently designing apparatus for the possible detection of the de Haas-van Alphen effect in sodium.

given by (4-61) for lower field strengths. We have chosen the condition (4-62) so that the quantum number n can then only take on the value zero (from a discrete point of view). It then follows from (4-15) that

$$E = \frac{h^2 n_z^2}{2mL_z^2} + \beta H \tag{4-63}$$

and that this level is still degenerate to the extent given by (4-14). Our number theory problem is now simplified to one dimension. In fact from (4-63) and (4-14) it follows immediately that

$$G(E) = \frac{2Ve(2m)^{1/2}H}{h^2 C} (E - \beta H)^{1/2} \qquad (4\text{-}64)^6$$

Since we assume T = 0°K (2-4) becomes

$$F - NE_o = \frac{2Ve(2m)^{1/2}H}{h^2 C} \int_{\beta H}^{E_o} (E - \beta H)^{1/2} \, dE \tag{4-65}$$

Carrying out the integration gives (accounting for the spin degeneracy of two)

$$F - NE_o = \frac{-8Ve(2m)^{1/2}H}{3h^2 C} (E_o - \beta H)^{3/2} \tag{4-66}$$

This leads to a magnetic moment

$$M = \frac{8Ve(2m)^{1/2}}{3h^2 C} (E_o - \beta H)^{1/2} \left(E_o - \frac{5}{2} \beta H\right) \tag{4-67}$$

---

[6] There is actually an uncertainty of $\pm \frac{2eHL_xL_y}{hC}$ in G(E) as expressed by (4-64). But the effect of this uncertainty on the magnetic moment is negligible.

We can put (4-67) into a more useful form by noting from (4-66) and (2-8) that

$$N = \frac{4Ve(2m)^{1/2}H\,(E_o - \beta H)^{1/2}}{h^2 C} \tag{4-68}$$

Solving this for E_o as a function of H gives

$$E_o = \beta H + \left(\frac{N h^2 C}{4Ve(2m)^{1/2}H}\right)^2 \tag{4-69}$$

With (4-68) and (4-69) we can express M as

$$M = -\beta N + \frac{N^3 h^4 C^2}{48V^2 e^2 m H^3} \tag{4-70}$$

It then follows that for very high fields M approaches the saturation value $-\beta N$. This result is in agreement with the work of Peierls (Ref. 8). It is noted that at such high fields the oscillatory character of M (as expressed by (4-61)) disappears.

CHAPTER 5

EFFECT OF SPIN ON THE MAGNETIC MOMENT OF AN ELECTRON GAS

5.1 Content

In Chapter 4 we accounted for the electron spin by merely introducing a degeneracy of two in the Fermi summations. Actually the spin will alter the eigenvalues, so that we now consider how this affects the magnetic moment. Number theory methods will be used for this calculation.

5.2 Eigenvalues

If we assume that the total wave function is separable into a product of a spin function and a spatial coordinate function, then the eigenvalues of our electron become[1]

$$E = A n_z^2 + B(n + 1/2) \pm \frac{B}{2} \tag{5-1}$$

This level is still degenerate to the extent D given in (4-14).

5.3 Distribution Function G(E)

Our function G(E) must now be written as

$$G(E) = G_+(E) + G_-(E) \tag{5-2}$$

where the $\pm$ subscripts refer to the eigenvalues obtained from (5-1) with $\pm \frac{B}{2}$ respectively.

---

[1] We assume all the conditions that exist in Chapter 4 except that now we include the spin energy.

1. $G_-(E)$

The eigenvalue relation for $-\frac{B}{2}$ is

$$E = An_z^2 + Bn \tag{5-3}$$

We now proceed to find $G_-(E)$ by the number theory method described in Chapter 4. The essential difference is that we shall leave the cut-off of this parabola at n = 0. It then follows from our previous discussion in Chapter 4 that the Fourier series will only count one-half the points along the cut-off. This is objectionable since the energies along this line correspond to n = 0, and so they will certainly[2] be filled states. But our computation of $G_+(E)$ will show how to overcome this under-counting of the number of states.

From this point on the calculation is similar to the previous one and leads to the result

$$G_-(E) = \mathcal{E}_- + D\left\{\frac{4E^{3/2}}{3BA^{1/2}} + 2\sum_{\substack{\kappa=1\\ \lambda=0}}^{\infty}\frac{T_\lambda B^{1/2}U_{3/2}(w,y)}{A^{1/2}(2\kappa)^{3/2}\pi} + 2\sum_{\lambda=1}^{\infty}\frac{E^{3/4}A^{1/4}}{\pi B\lambda^{3/2}} J_{3/2}(y)\right\} \tag{5-4}$$

where $\mathcal{E}_-$ is equal to one-half the number of points along the cut-off n = 0, and the remaining symbols have the same meaning as before.

2. $G_+(E)$

The eigenvalue relation for $+\frac{B}{2}$ is

$$E = An_z^2 + B(n+1) \tag{5-5}$$

To compute $G_+(E)$ we move the cut-off of this parabola from n = 0 to

[2] Rather than with a probability of 1/2 as our counting would indicate.

$n = -1$. Then the Fourier series will give a result which is greater than the correct number by exactly one-half the number of states along the cut-off $n = -1$.

It then follows from the calculations that

$$G_+(E) = -\mathcal{E}_+ + G_-(E) - \mathcal{E}_- \tag{5-6}$$

where $\mathcal{E}_+$ is equal to one-half the number of points along the cut-off $n = -1$.

But from (5-3) and (5-5) it follows that the length of the cut-off $n = 0$ for the $G_-(E)$ parabola is exactly equal to the length of the cut-off $n = -1$ for the $G_+(E)$ parabola. This immediately leads to the conclusion

$$\mathcal{E}_- = \mathcal{E}_+ \tag{5-7}$$

It is this fortuitous equality which allows us to compute the effect of spin by number theory. It is also noted that for both $G_-(E)$ and $G_+(E)$ the lowest energy level is set at zero by our choice of cut-offs. This allows us to add $G_-(E)$ and $G_+(E)$ for the entire range of energies.

From the relations found above we get

$$G(E) = D\left\{\frac{8E^{3/2}}{3BA^{1/2}} + 4\sum_{\substack{\kappa=1\\ \lambda=0}}^{\infty}\frac{T_\lambda B^{1/2}U_{3/2}(w,y)}{A^{1/2}(2\kappa)^{3/2}\pi} + 4\sum_{\lambda=1}^{\infty}\frac{E^{3/4}A^{1/4}}{\pi B\lambda^{3/2}}J_{3/2}(y)\right\} \tag{5-8}$$

This $G(E)$ differs from the one in Chapter 4 (4-24) by a factor of two and the absence of the alternating sign $(-1)^{\kappa}$.

5.4 Magnetic Moment

If we again restrict the magnetic field such that $E_o >> \beta H$, the magnetic moment resulting from (5-8) becomes

$$M = \frac{8\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3}\left(1 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2\right)$$

$$+ \sum_{\kappa=1}^{\infty} \frac{2\pi kTVe(2m)^{1/2}E_o \quad \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2}h^2C\beta^{1/2}H^{1/2} \quad \sinh\left(\pi^2\kappa\frac{kT}{\beta H}\right)} \tag{5-9}$$

The non-periodic term is now paramagnetic. It is numerically equal to the algebraic sum of the Pauli spin paramagnetism and the Landau diamagnetism. The periodic parts differ from the spinless case by having a phase difference of $\pm\pi$ for terms with κ odd. At finite temperatures we have shown that only the term $\kappa = 1$ is of importance, therefore the result obtained here will differ from the spinless case by the phase change $\pm\pi$.

Finally we consider the case of very strong fields at $T = 0°K$. By restricting the Fermi energy to the limits

$$0 \leqq E_o < 2\beta H \tag{5-10}$$

we get

$$G_-(E) = \frac{2Ve(2m)^{1/2}H E^{1/2}}{h^2 C}$$

$$G_+(E) = 0 \tag{5-11}$$

It then follows from (2-4) that

$$F - NE_o = -\frac{4Ve(2m)^{1/2}HE_o^{3/2}}{3h^2C} \tag{5-12}$$

This gives a magnetic moment

$$M = \frac{4Ve(2m)^{1/2}E_o^{3/2}}{3h^2C} \tag{5-13}$$

In order to show the explicit dependence of M on H we must obtain E_o as a function of H. This is readily accomplished from the normalizing condition (2-2). It leads to

$$E_o = \left(\frac{N\,h^2\,C}{2Ve(2m)^{1/2}H}\right)^2 \tag{5-14}$$

Now M can be expressed as

$$M = \frac{N^3\,h^4\,C^2}{24\,V^2\,e^2\,m\,H^3} \tag{5-15}$$

For very high fields M approaches the value zero.

CHAPTER 6

SIZE EFFECTS DUE TO A FINITE CONTAINER (SPINLESS ELECTRONS)

6.1 Content

The results obtained in previous chapters were all dependent on the use of an eigenvalue degeneracy given by (4-14). In Chapter 4 we indicated that there is no *a priori* reason for believing that this degeneracy takes proper account of the surface states in a finite container. The present chapter is concerned with an examination of this question in light of the WKB approximation and number theoretical methods.

6.2 Distribution Function G(E)

The method we shall follow here is different from that used in the earlier chapters. Previously we utilized an eigenvalue relation with an assumed degeneracy to compute G(E). To find the effect of the surface states using such a method would first require an appropriate eigenvalue relation. Although it is possible to accomplish this via the WKB approximation, the resulting expression does not give the energy as an explicit function of the three quantum numbers. Because of this difficulty it is easier to leave the quantum number n in phase integral form and express G(E) as a triply periodic Fourier series in the quantum numbers. We shall show that such a procedure will allow us to draw certain general conclusions about the magnetic moment of an electron gas in a finite container.

We start with the WKB quantum condition for the motion in the x direction

$$\oint p\,dx = (n + 1/2)h \qquad (6\text{-}1)$$

If we suppose x_1 and x_2 are the classical turning points for a given orbit with energy E_1 we have

$$n = \frac{2}{h}\int_{x_1}^{x_2} p\,dx - \frac{1}{2} \tag{6-2}$$

where for our problem[1]

$$E = \frac{h^2 n_z^2}{2mL_z^2} + E_1$$
$$p = \sqrt{2mE_1 - \left(\frac{hn_y}{L_y} - \frac{eHx}{C}\right)^2} \tag{6-3}$$

Our number theory problem is now to count the lattice points within or on the energy surface E in the three dimensional quantum number space. No assumption is made about a degeneracy. If the counting is done properly all questions of degeneracy will be automatically answered. Let G(E) be represented by a triply periodic Fourier series

$$G(E) = \sum_{\kappa}\sum_{\lambda}\sum_{\mu} a_{\kappa,\lambda,\mu}\, e^{2\pi i(\kappa\alpha_1+\lambda\alpha_2+\mu\alpha_3)} \tag{6-4}$$

where $\alpha_1, \alpha_2, \alpha_3$ correspond to translations along the n, n_y, n_z axes respectively. In order to avoid a discontinuity in G(E) when $\alpha_1, \alpha_2, \alpha_3$ are all set to zero we must move the lower limit of n from 0 to -1/2. This is done to count all the states in the n_z, n_y plane. Leaving the cut-off plane of the surface at n = 0 would result in counting only one-half the states in the n_z, n_y plane.

---

[1] See Chapter 4 for details. The notation here follows that used previously.

Following the method in Chapter 4 we find that

$$G(E) = a_{o,o,o} + 2\sum_{\kappa=1}^{\infty} R(a_{\kappa,o,o}) + 2\sum_{\lambda=1}^{\infty} R(a_{o,\lambda,o})$$
$$+ 2\sum_{\mu=1}^{\infty} R(a_{o,o,\mu}) + 8\sum_{\kappa,\lambda,\mu=1}^{\infty} R(a_{\kappa,\lambda,\mu}) + 4\sum_{\kappa,\lambda=1}^{\infty} R(a_{\kappa,\lambda,o})$$
$$+ 4\sum_{\lambda,\mu=1}^{\infty} R(a_{o,\lambda,\mu}) + 4\sum_{\kappa,\mu=1}^{\infty} R(a_{\kappa,o,\mu})$$

where

$$R(a_{\kappa,\lambda,\mu}) = (-1)^{\kappa} \iiint_{\mathcal{T}(p)} \cos(2\pi\kappa n)\cos(2\pi\lambda n_y)\cos(2\pi\mu n_z)\, dn\, dn_y\, dn_z \qquad (6\text{-}5)$$

and the integration is over the volume $\mathcal{T}(p)$ throughout which p is a real number.[2] This volume will include both the harmonic oscillator states of Chapter 4 and our surface states. Consider first the principal coefficient $a_{o,o,o}$ which corresponds to the volume of our energy surface. This coefficient will be, by far, the largest term in the expansion of G(E). The other terms will represent the number theory correction to the replacement of a sum by an integral.

1. The $a_{o,o,o}$ Term:

From (6-5) we have

$$a_{o,o,o} = R(a_{o,o,o}) = \iiint_{\mathcal{T}(p)} dn\, dn_y\, dn_z \qquad (6\text{-}6)$$

Integrating first over n, using the upper limit $\frac{2}{h}\int_{x_1}^{x_2} p\, dx$ and the lower limit zero gives

$$a_{o,o,o} = \frac{2}{h}\iiint_{\mathcal{T}'(p)} p\, dx\, dn_y\, dn_z \qquad (6\text{-}7)$$

[2] The lower limit for the n appearing in (6-5) is zero. This results from the shift in cut-off as explained in Chapter 4.

where $\mathcal{J}'(p)$ is the volume in x, n_y, n_z space throughout which p is real. It is now more convenient to integrate over n_y first. The limits on n_y are determined by the condition p = 0. This gives the upper (u) and lower (l) limits

$$
\begin{aligned}
(n_y)_u &= \frac{eHL_y x}{hC} + \frac{L_y}{h}\sqrt{2mE_1} \\
(n_y)_l &= \frac{eHL_y x}{hC} - \frac{L_y}{h}\sqrt{2mE_1}
\end{aligned}
\qquad (6\text{-}8)
$$

The limits on x are determined by the extreme values of the classical turning points. By assuming an infinite potential at the walls of the box these limits become

$$(x)_u = \frac{L_x}{2} \qquad (6\text{-}9)$$

$$(x)_l = -\frac{L_x}{2}$$

Finally, the limits on n_z are obtained directly from (6-3) with E_1 set to zero. This gives

$$
\begin{aligned}
(n_z)_u &= \frac{L_z}{h}\sqrt{2mE} \\
(n_z)_l &= -\frac{L_z}{h}\sqrt{2mE}
\end{aligned}
\qquad (6\text{-}10)
$$

Having thus defined $\mathcal{J}'(p)$ we carry out the integration of (6-7) in the order n_y, x, n_z. This gives

$$a_{o,o,o} = \frac{4\pi V(2mE)^{3/2}}{3h^3} \qquad (6\text{-}11)$$

which is exactly the number of states for free electrons in a box without a magnetic field. In fact, (6-11) is identical to the result obtained in Chapter 4 when we modified the degeneracy to eliminate (hopefully) the need for calculating the effect of surface states. To this extent the calculation given here is a justification of Landau's argument. From a physical point of view our calculation shows that Landau's overcounting of the harmonic oscillator states exactly compensates his neglecting the surface states.

2. The $a_{\kappa,o,o}$ Terms:

Although the two methods of counting give the same total volume term it is evident that the corrections will be different. The question that remains is how much of a change in the correction terms is brought about by the surface states? Qualitatively, the energy surface will approach that of Chapter 4 as H becomes large since the harmonic oscillator states then comprise the greatest part of the volume. Under such conditions it seems plausible to say that $G(E)$ would be given by (4-29) plus higher order corrections. This conclusion could be made still more plausible by allowing the dimension L_x to be large. However, the situation for low fields and finite L_x does not offer any obvious conclusions. Under such conditions the effect of the surface states is emphasized.

From the results given in Chapter 4 we know that to compute the magnetic moment we need only consider those correction terms in which the frequency of the oscillatory part is not a function of the dimensions of the box. In the present Fourier expansion this corresponds to using only the terms $R(a_{\kappa,o,o})$. Our immediate task is therefore to calculate those coefficients. It seems plausible that the results of Chapter 4 should be identifiable in such a calculation. In this sense we have some control on the validity of the analysis.

From (6-5) we have

$$R(a_{\kappa,o,o}) = (-1)^{\kappa} \iiint_{\mathcal{T}(p)} \cos(2\pi\kappa n)\, dn\, dn_y\, dn_z \tag{6-12}$$

Integrating first over n, and inserting the limits, gives

$$R(a_{\kappa,o,o}) = \frac{(-1)^{\kappa}}{2\pi\kappa} \iint_{\mathcal{T}'(p)} \sin\left(\frac{4\pi\kappa}{h} \int_{x_1}^{x_2} p\, dx\right) dn_y\, dn_z \tag{6-13}$$

Now we break the integral into two parts, corresponding to the oscillator states and the surface states. The division is determined by the value of n_y. In Chapter 4 we found that for

$$0 \leqq |n_y| \leqq \left| \frac{eHL_xL_y}{2hC} - \frac{L_y}{h}\sqrt{2mE_1} \right|$$

we had oscillator states, but for

$$\left| \frac{eHL_xL_y}{2hC} - \frac{L_y}{h}\sqrt{2mE_1} \right| \leqq |n_y| \leqq \left| \frac{eHL_xL_y}{2hC} + \frac{L_y}{h}\sqrt{2mE_1} \right|$$

we got surface states. For the oscillator states the turning points x_1, x_2 are given by the equations

$$x_1 = \frac{hCn_y}{eHL_y} - \frac{C}{eH}\sqrt{2mE_1}$$

$$x_2 = \frac{hCn_y}{eHL_y} + \frac{C}{eH}\sqrt{2mE_1}$$

For the surface states we have (the subscript s denotes surface)

$$x_{1,s} = \frac{hCn_y}{eHL_y} - \frac{C}{eH}\sqrt{2mE_1}$$

$$x_{2,s} = \frac{L_x}{2}$$

Thus (6-13) can be written as

$$R(a_{\kappa,o,o}) = \frac{4(-1)^{\kappa}}{2\pi\kappa} \int_0^{\frac{L_z}{h}\sqrt{2mE}} \left\{ \int_{n_y=0}^{\frac{eHL_xL_y}{2hC} - \frac{L_y}{h}\sqrt{2mE_1}} \sin\left(\frac{4\pi\kappa}{h}\int_{x_1}^{x_2} p\,dx\right) dn_y + \int_{\frac{eHL_xL_y}{2hC} - \frac{L_y}{h}\sqrt{2mE_1}}^{\frac{eHL_xL_y}{2hC} + \frac{L_y}{h}\sqrt{2mE_1}} \sin\left(\frac{4\pi\kappa}{h}\int_{x_{1,s}}^{x_{2,s}} p\,dx\right) dn_y \right\} dn_z$$

(6-14)[3]

If we now impose the restriction $E_o >> \beta H$, it is possible to obtain the asymptotic value of $R(a_{\kappa,o,o})$. The evaluation of (6-14) is dependent on the use of the Method of Critical Points recently introduced by van der Corput (Ref. 3). With a plausible interpretation of this method it is found that

$$R(a_{\kappa,o,o}) \sim \frac{(-1)^{\kappa} D B^{1/2} U_{3/2}(w,o)}{A^{1/2}\,\pi\,(2\kappa)^{3/2}} - \frac{(-1)^{\kappa} L_y L_z (2m) E^{1/2} B^{1/2}}{\pi\, 2^{1/2} \kappa^{3/2} h^2} \cos\left(\frac{w}{2} - \frac{3\pi}{4}\right)$$
$$+ \frac{(-1)\, L_y L_z 2m E^{1/3} B^{2/3}}{h^2\ \kappa^{5/3}} \left(\frac{\Gamma(5/3)\,\Gamma(11/12)\,\pi^{1/3}\, 3^{7/6}}{\Gamma(17/12)\ 4^{5/3}} \right)$$

(6-15)

---

[3] The factor of 4 appearing in (6-14) results from using the symmetry properties of the integral with respect to n_y and n_z to change the limits appropriately.

The symbols in (6-15) have the same values as in Chapter 4. Details on the use of the method of critical points for the evaluation of (6-14) are given in Appendix VI.

6.3 Magnetic Moment

With the restriction[4] $E_o \gg \beta H$ the magnetic moment resulting from $R(a_{\kappa,o,o})$ is

$$M = -\frac{4\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3}\left(1 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2\right)$$

$$+\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} 2\pi kTVe(2m)^{1/2} E_o \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2} h^2 C \beta^{1/2} H^{1/2} \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)}$$

$$-\sum_{\kappa=1}^{\infty} \frac{(-1)^{\kappa} 2\pi kTL_y L_z(2m) E_o^{3/2} \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2} h^2 \beta^{1/2} H^{3/2} \sinh\left(\pi^2 \kappa \frac{kT}{\beta H}\right)}$$

$$-\frac{L_y L_z(2m) E_o^{4/3} \beta^{2/3}\left(1 - \frac{2\pi^2}{27}\left(\frac{kT}{E_o}\right)^2\right)}{h^2 H^{1/3}}\left(\frac{\Gamma(\frac{5}{3})\,\Gamma(\frac{11}{12})\,\pi^{1/3}\,3^{7/6}\,\zeta(\frac{5}{3})\,(2^{2/3}-1)}{2^{7/3}\,\Gamma(\frac{17}{12})}\right)$$

(6-16)

where $\zeta(5/3)$ is the Riemann Zeta-Function of argument 5/3. The first and second terms of (6-16) give exactly the result obtained in Chapter 4.

---

[4] The condition $E_o \gg \beta H$ imposes an upper bound on the magnetic field strength. However, it must be emphasized that the result given by (6-16) is also dependent on H having a lower bound. Our use of the WKB approximation has not considered states which have turning points determined by the infinite potentials at both walls ($\pm L_x/2$) simultaneously. This imposes the restriction that $H > 2C\sqrt{2mE_o}/eL_x$ for the applicability of (6-16).

This identification serves to confirm our conjecture that the size effects might appear as a correction to the previous results. The third and fourth terms of (6-16) give the effect of the finite size of the box. It is seen that both the oscillatory and non-oscillatory parts of the moment are affected by size.

The two oscillatory parts of (6-16) become of the same order of magnitude when

$$H = H_c \sim \frac{2C\sqrt{2mE_0}}{eL_x} \tag{6-17}$$

(where H_c denotes the critical field strength). This is exactly the field condition below which our solution fails. An extension of these calculations to fields below H_c might reveal some interesting features in the size dependence of the magnetic moment.

The additional non-oscillatory correction is noteworthy since it varies as $H^{-1/3}$. It is a diamagnetic effect which (for specimen dimensions of the order of cm) is comparable to the Landau diamagnetism at fields below a thousand gauss. Further discussion of this term will be delayed until after we have considered the effect of electron spin in Chapter 7.

6.4 Summary

We have shown here that a finite container does introduce size effects in the magnetic moment of a spinless electron gas. The size effect of the d-v-e becomes comparable to the result found in Chapter 4 for low fields and specimens of small dimensions. There is also a size effect in the non-oscillatory part of the magnetic moment, but details of its behavior will be postponed until the next chapter.

CHAPTER 7

SIZE EFFECTS DUE TO A FINITE CONTAINER

(ELECTRONS WITH SPIN)

7.1 Content

In this chapter we complete the calculation by considering the effect of both the electron spin and a finite container.

7.2 Eigenvalues

Assuming that the total wave function is separable into a product of a spin function and a spatial coordinate function, we can write the electronic eigenvalues as

$$E = An_z^2 + E_1 \pm \beta H \tag{7-1}$$

7.3 Distribution Function G(E)

The function $G(E)$ must now be written as

$$G(E) = G_+(E) + G_-(E) \tag{7-2}$$

where the $\pm$ subscripts refer to the eigenvalues obtained from (7-1) with $\mp \beta H$ respectively.

1. $G_+(E)$.

If we move the cut-off plane to $n = -1/2$ (just as for the spinless case in Chapter 6) we get identically the number theory problem considered in Chapter 6 with E replaced by $(E + \beta H)$. By designating the spinless distribution function as $G_{n.s.}(E)$, we can write

$$G_+(E) = G_{n.s.}(E+\beta H) \tag{7-3}$$

where $G_{n.s.}(E)$ is given by (6-5). It must be noted that the minimum value of E for which (7-3) holds is $-\beta H$. In other words, $G\ (-\beta H) = 0$.

2. $G_-(E)$.

Following the above reasoning we can write

$$G_-(E) = G_{n.s.}(E-\beta H) \tag{7-4}$$

if we move the cut-off again to $n = -1/2$. In (7-4) the minimum value of E is βH since $G_-(\beta H) = 0$.

7.4 Free Energy

The free energy for this case is given by

$$(F - NE_o) = -\left(\int_{-\beta H}^{\infty} G_+(E)f(E)dE + \int_{\beta H}^{\infty} G_-(E)f(E)dE \right) \tag{7-5}$$

We transform the first integral by the substitution

$$E + \beta H = \mathcal{E}^+$$

and the second integral by the substitution

$$E - \beta H = \mathcal{E}^-$$

This gives

$$(F - NE_o) = -\left(\int_{o}^{\infty} G_+(\mathcal{E}^+ -\beta H)f(\mathcal{E}^+ -\beta H)d\mathcal{E}^+ + \int_{o}^{\infty} G_-(\mathcal{E}^- +\beta H)f(\mathcal{E}^- +\beta H)d\mathcal{E}^- \right)$$

(7-6)

However, from (7-3) and (7-4) we have

$$G_+(\mathcal{E}^+ - \beta H) = G_{n.s}(\mathcal{E}^+)$$

and

$$G_-(\mathcal{E}^- + \beta H) = G_{n.s.}(\mathcal{E}^-)$$

so that we can write

$$(F - NE_o) = -\left(\int_o^\infty G_{n.s.}(\mathcal{E}^+) f(\mathcal{E}^+ - \beta H) d\mathcal{E}^+ + \int_o^\infty G_{n.s.}(\mathcal{E}^-) f(\mathcal{E}^- + \beta H) d\mathcal{E}^- \right) \tag{7-7}$$

In (7-7) there is no need to distinguish between $\mathcal{E}^+$ and $\mathcal{E}^-$ since they are both integration variables. By setting

$$\mathcal{E}^+ = \mathcal{E}^- = \mathcal{E}$$

we have finally

$$(F - NE_o) = -\left(\int_o^\infty G_{n.s.}(\mathcal{E}) f(\mathcal{E} - \beta H) d\mathcal{E} + \int_o^\infty G_{n.s.}(\mathcal{E}) f(\mathcal{E} + \beta H) d\mathcal{E} \right) \tag{7-8}$$

If we again restrict our interest to the terms $a_{o,o,o}$ and $R(a_{\kappa,o,o})$ in $G_{n.s.}(E)$, the asymptotic value (when $E_o >> \beta H$) of (7-8) is found to be

$$
\begin{aligned}
(F-NE_o) = & -\frac{8\pi V(2m)^{3/2}}{15h^3}\left\{(E_o+\beta H)^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{E_o+\beta H}\right)^2\right]+(E_o-\beta H)^{5/2}\left[1+\frac{5\pi^2}{8}\left(\frac{kT}{E_o-\beta H}\right)^2\right]\right\} \\
& + \frac{\pi V(2m)^{3/2}\beta^2 H^2}{3h^3}\left\{(E_o+\beta H)^{1/2}\left[1-\frac{\pi^2}{24}\left(\frac{kT}{E_o+\beta H}\right)^2\right]+(E_o-\beta H)^{1/2}\left[1-\frac{\pi^2}{24}\left(\frac{kT}{E_o-\beta H}\right)^2\right]\right\} \\
& + \sum_{\kappa=1}^{\infty}\frac{VekT(2m)^{1/2}\beta^{1/2}H^{3/2}\ \sin\left(\frac{\pi\kappa E_o}{\beta H}-\frac{3\pi}{4}\right)}{\kappa^{3/2}h^2 C\ \sinh\left(\pi^2\kappa\frac{kT}{\beta H}\right)} \\
& - \sum_{\kappa=1}^{\infty}\frac{2L_yL_z(2m)\beta^{1/2}H^{1/2}kT\ \sin\left(\frac{\pi\kappa E_o}{\beta H}-\frac{3\pi}{4}\right)}{\kappa^{3/2}h^2\ \sinh\left(\pi^2\kappa\frac{kT}{\beta H}\right)}\left\{(E_o+\beta H)^{1/2}+(E_o-\beta H)^{1/2}\right\} \\
& + \frac{6L_yL_z(2m)\beta^{2/3}H^{2/3}}{2^{4/3}h^2}\ \frac{\Gamma\left(\frac{5}{3}\right)\Gamma\left(\frac{11}{12}\right)\pi^{1/3}3^{7/6}(2^{2/3}-1)\zeta\left(\frac{5}{3}\right)}{\Gamma\left(\frac{17}{12}\right)4^{5/3}\ 2^{2/3}} \\
& \times\left\{(E_o+\beta H)^{4/3}\left[1-\frac{2\pi^2}{27}\left(\frac{kT}{E_o+\beta H}\right)^2\right]+(E_o-\beta H)^{4/3}\left[1-\frac{2\pi^2}{27}\left(\frac{kT}{E_o-\beta H}\right)^2\right]\right\}
\end{aligned}
\tag{7-9}
$$

The methods used for evaluating (7-8) have been described in the previous chapters and appendices.

7.5 Magnetic Moment.

The magnetic moment for this system of electrons is obtained from the partial differentiation of (7-9) with respect to H. This leads to a complicated result which contains many factors of the form

$$(E_o \pm \beta H)^{\pm p/2}$$

where p takes on the values 1, 3, 5. These factors can all be expanded in power series with $\beta H/E_o$ as the variable since in our asymptotic region $\beta H/E_o \ll 1$.

After performing these expansions and combining terms, we find that the magnetic moment is

$$M = \frac{4\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{h^3}\left(1 - \frac{1}{24}\left(\frac{\beta H}{E_o}\right)^2 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2\right)$$

$$- \frac{4\pi V(2m)^{3/2}\beta^2 E_o^{1/2} H}{3h^3}\left(1 - \frac{\pi^2}{24}\left(\frac{kT}{E_o}\right)^2\right)$$

$$+ \sum_{\kappa=1}^{\infty} \frac{2\pi kT\, Ve(2m)^{1/2} E_o \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2} h^2 C \beta^{1/2} H^{1/2} \sinh\left(\pi^2\kappa \frac{kT}{\beta H}\right)}$$

$$- \sum_{\kappa=1}^{\infty} \frac{2\pi kT(2m) L_y L_z E_o^{3/2} \cos\left(\frac{\pi\kappa E_o}{\beta H} - \frac{3\pi}{4}\right)}{\kappa^{1/2} h^2 \beta^{1/2} H^{3/2} \sinh\left(\pi^2\kappa \frac{kT}{\beta H}\right)}$$

$$- \frac{L_y L_z (2m) E_o^{4/3} \beta^{2/3}}{h^2 H^{1/3}}\left(1 + \frac{8}{9}\left(\frac{\beta H}{E_o}\right)^2 - \frac{2\pi^2}{27}\left(\frac{kT}{E_o}\right)^2\right)$$

$$\times \frac{\Gamma\left(\frac{5}{3}\right)\Gamma\left(\frac{11}{12}\right)\pi^{1/3}\, 3^{7/6}\, \zeta\left(\frac{5}{3}\right)\left(2^{2/3} - 1\right)}{2^{7/3}\,\Gamma\left(\frac{17}{12}\right)} \qquad (7\text{-}10)$$

We shall now identify and discuss each of the five terms which comprise the magnetic moment (7-10).

1. The first term is the Pauli spin paramagnetism with higher order temperature and field corrections. (It is noted that the explicit dependence upon temperature and field could be obtained if E_o were given explicitly in the variables T and H. This could be accomplished through the use of the normalizing condition (2-2).).

2. The second term is the ordinary Landau diamagnetism with higher order corrections.

3. The third term is the usual d-v-e obtained when no surface effects are included. The same result was found and discussed in Chapter 5.

4. The fourth term is the surface state correction to the d-v-e. It differs from the corresponding term found in Chapter 6 by a phase difference of $\pm\pi$ when κ is odd. This correction becomes comparable to the usual d-v-e when

$$H = H_c \sim 2C\sqrt{2mE_o} \;/\; eL_x \qquad (7\text{-}11)$$

It is re-emphasized here that (7-11) expresses the field condition below which the entire solution fails.

5. The fifth term is a non-oscillatory diamagnetic effect arising from the surface states. Since it was also found in Chapter 6 we can say that this effect is independent of electron spin. In light of this circumstance we will now focus our attention on this "surface" diamagnetism. For a free electron gas with $E_o \sim 1$ ev, the surface (s) magnetization (M/V) is

$$\left(\frac{M}{V}\right)_s \sim -10^{-3}/L_x H^{1/3} \qquad (7\text{-}12)$$

while the remaining (r) non-oscillatory magnetization from the Pauli and Landau terms is

$$\left(\frac{M}{V}\right)_r \sim 10^{-6}\, H \qquad (7\text{-}13)$$

For the assumed value of E_o we also have

$$H_c \sim 10 \;/\; L_x \qquad (7\text{-}14)$$

From (7-12) and (7-13) we find that $|(M/V)_s|$ is about equal to $|(M/V)_r|$ when

$$H = H_o \sim 3 \times 10^2 / L_x^{3/4} \tag{7-15}$$

In order to comment on the feasibility of finding the surface diamagnetism experimentally, we shall now examine the above quantities for real specimens:

a) If L_x is of order cm, $H_c \sim 10$ and $H_o \sim 300$ gauss. For 1cc of material at 300 gauss we would have to be able to measure a magnetic moment of about 10^{-4} cgs units in order to observe the surface diamagnetism. Although this is experimentally feasible, it is not an easy task.

b) If L_x were of order 10^{-2} cm, $H_c \sim 10^3$ while $H_o \sim 6 \times 10^3$ gauss. Now we would need to measure moments of about 5×10^{-3} cgs units in order to observe the surface diamagnetism. Such moments can be measured accurately without elaborate arrangements.

The analysis given above suggests that experiments be performed to test the theoretical prediction of surface diamagnetism. It would be desirable to use a monovalent metal such as Cu, Ag, Na or Au for such an experiment since these metals are most closely represented by a free electron model. The specimen could be in powder form with individual particles (electrically insulated from one another) having dimensions of order 10^{-2} cm. Finally, the experiment could be performed at room temperature since even at T = 300°K the corrections to the moment are small compared to the temperature independent terms.

APPENDIX I

EVALUATION OF THE INTEGRAL:

$$\iint_{Av^2+Bu\leq E} \cos(2\pi\kappa u)\ \cos(2\pi\lambda v)\ du\ dv$$

The Fourier coefficient $R(a_{\kappa,\lambda})$ in Chapter 4 is

$$R(a_{\kappa,\lambda}) = (-1)^{\kappa} \iint_{Av^2+Bu\leq E} \cos(2\pi\kappa u)\ \cos(2\pi\lambda v)\ du\ dv \tag{I-1}$$

The lower limit of u in this integral is taken to be zero. We will show here that $R(a_{\kappa,\lambda})$ can be expressed in terms of Lommel functions.

Integrating first with respect to u gives

$$R(a_{\kappa,\lambda}) = \frac{(-1)^{\kappa}}{2\pi\kappa} \int_{-\sqrt{E/A}}^{\sqrt{E/A}} \cos(2\pi\lambda v) \Big[\sin 2\pi\kappa u\Big]_{0}^{(E-Av^2)/B} dv$$

or (I-2)

$$R(a_{\kappa,\lambda}) = \frac{2(-1)^{\kappa}}{2\pi\kappa} \int_{0}^{\sqrt{E/A}} \cos(2\pi\lambda v) \quad \sin\left[\frac{2\pi\kappa E}{B}\ (1-\frac{A}{E}v^2)\right] dv$$

Substituting

$$v = \sqrt{\frac{E}{A}}\ \sigma \tag{I-3}$$

transforms (I-2) into

$$R(a_{\kappa,\lambda}) = \frac{(-1)^{\kappa}\, 2\sqrt{\frac{E}{A}}}{2\pi\kappa} \int_{0}^{1} \cos(2\pi\lambda\sqrt{\frac{E}{A}}\sigma)\ \sin\left[\frac{2\pi\kappa E}{B}\ (1-\sigma^2)\right] d\sigma \tag{I-4}$$

But since

$$\cos \zeta = \left(\frac{\pi \zeta}{2}\right)^{1/2} J_{-1/2}(\zeta) \tag{I-5}$$

we can write

$$R(a_{\kappa,\lambda}) = \frac{(-1)^{\kappa}\left(\frac{\pi}{2}\right)^{1/2} 2\left(\frac{E}{A}\right)^{1/2}}{2\pi\kappa} \int_0^1 J_{-1/2}(y\sigma) \sin\left[\frac{w}{2}(1-\sigma^2)\right] (y\sigma)^{1/2}\, d\sigma \tag{I-6}$$

where

$$\begin{aligned} w &= 4\pi\kappa E/B \\ y &= 2\pi\lambda\left(\frac{E}{A}\right)^{1/2} \end{aligned} \tag{I-7}$$

But from page 540 of Watson's book

$$U_{\nu+1}(w,y) = \frac{w^{\nu}}{y^{\nu-1}} \int_0^1 J_{\nu-1}(y\sigma) \sin\left[\frac{w}{2}(1-\sigma^2)\right] \sigma^{\nu}\, d\sigma \tag{I-8}$$

where U_{ν} is the ν^{th} order Lommel function of two variables. The series representation of $U_{\nu}(w,y)$ is given in Chapter 4 (Eq. 4-28). From a comparison of (I-6) and (I-8), it follows that

$$R(a_{\kappa,\lambda}) = \frac{(-1)^{\kappa} B^{1/2}}{A^{1/2}(2\kappa)^{3/2}\pi} U_{3/2}(w,y) \tag{I-9}$$

This result was given in Eq. (4-26) of Chapter 4.

APPENDIX II

PROOF OF: $R(a_{o,\lambda}) = E^{3/4} A^{1/4} J_{3/2}(y)/\pi B\lambda^{3/2}$

With $\kappa = 0$ we get from (4-24)

$$R(a_{o,\lambda}) = \iint_{Av^2+Bu\leq E} \cos(2\pi\lambda v)\, du\, dv \qquad \text{(II-1)}$$

where the limits are the same as in Appendix I. Integrating first with respect to u, and substituting the limits, gives

$$R(a_{o,\lambda}) = 2 \int_0^{\sqrt{E/A}} \frac{(E - Av^2)}{B} \cos(2\pi\lambda V)\, dv \qquad \text{(II-2)}$$

Substituting

$$v = \left(\frac{E}{A}\right)^{1/2} \Omega \qquad \text{(II-3)}$$

transforms (II-2) into

$$R(a_{o,\lambda}) = \frac{2E^{3/2}}{BA^{1/2}} \int_0^1 (1 - \Omega^2) \cos\left[2\pi\lambda \left(\frac{E}{A}\right)^{1/2} \Omega\right] d\Omega \qquad \text{(II-4)}$$

But from page 48 of Watson's* book

$$J_\nu(y) = \frac{2\left(\frac{y}{2}\right)^\nu}{\pi^{1/2}\Gamma(\nu + 1/2)} \int_0^1 (1 - \sigma^2)^{\nu - 1/2} \cos(y\sigma)\, d\sigma \qquad \text{(II-5)}$$

provided $R(\nu) > -1/2$. From a comparison of (II-4) and (II-5) it follows that

$$R(a_{o,\lambda}) = E^{3/4} A^{1/4} J_{3/2}(y) / \pi B \lambda^{3/2} \tag{II-6}$$

where y is defined as in (I-7) of Appendix I. This calculation serves as a check on the result (4-33) obtained from the Lommel function in the $\lim_{\kappa \to 0}$.

APPENDIX III

PROOF OF: $\int U_{3/2}(w,y)\, dE = B\, U_{5/2}(w,y) / 2\pi\kappa$

From the series representation of a Lommel function it follows that

$$\int U_{3/2}(w,y)\, dE = \sum_{m=0}^{\infty} (-1)^m \int \left(\frac{w}{y}\right)^{3/2+2m} J_{3/2+2m}(y)\, dE \qquad \text{(III-1)}$$

In our problem w and yare defined by (I-7). The substitution

$$\phi = 2\pi\lambda \left(\frac{E}{A}\right)^{1/2}$$

transforms (III-1) into

$$\int U_{3/2}(w,y)\, dE = 2\sum_{m=0}^{\infty} (-1)^m \left(\frac{2\kappa A^{1/2}}{\lambda B}\right)^{\frac{3}{2}+2m} \left(\frac{A^{1/2}}{2\pi\lambda}\right)^{\frac{3}{2}+2m+1} \int \phi^{\frac{3}{2}+2m+1} J_{\frac{3}{2}+2m}(\phi)\, d\phi \qquad \text{(III-2)}$$

But since

$$\int \phi^{p+1} J_p(\phi)\, d\phi = \phi^{p+1} J_{p+1}(\phi)$$

we can write (in terms of w and y)

$$\int U_{3/2}(w,y)\, dE = \frac{B}{2\pi\kappa} \sum_{m=0}^{\infty} (-1)^m \left(\frac{w}{y}\right)^{\frac{5}{2}+2m} J_{\frac{5}{2}+2m}(y)$$

or (III-4)

$$\int U_{3/2}(w,y)\, dE = B\, U_{5/2}(w,y) / 2\pi\kappa$$

This result was given in (4-37) of Chapter 4.

APPENDIX IV

PROOF OF: $\frac{\partial}{\partial H} U_{5/2}(w,y) = -\frac{\pi \kappa E}{\beta H^2} U_{3/2}(w,y) - \frac{\pi \lambda^2 \beta}{\kappa A} U_{7/2}(w,y)$

From the series representation of a Lommel function we have

$$\frac{\partial}{\partial H} U_{5/2}(w,y) = \sum_{m=0}^{\infty} (-1)^m (\tfrac{5}{2} + 2m) (\tfrac{w}{y})^{\frac{5}{2} + 2m - 1} \frac{1}{y} \frac{\partial w}{\partial H} J_{\frac{5}{2}+2m}(y) \qquad \text{(IV-1)}$$

since $\frac{\partial y}{\partial H} = 0$. (w and y are the same quantities appearing in the previous Appendices.) Using the identity

$$J_{\frac{5}{2}+2m}(y) = \frac{y}{2(\frac{5}{2} + 2m)} \left(J_{\frac{7}{2}+2m}(y) + J_{\frac{3}{2}+2m}(y) \right) \qquad \text{(IV-2)}$$

and the value

$$\frac{\partial w}{\partial H} = -2\pi \kappa E/\beta H^2 \qquad \text{(IV-3)}$$

we get

$$\frac{\partial U_{5/2}(w,y)}{\partial H} = -\frac{\pi \kappa E}{\beta H^2} U_{3/2}(w,y) - \frac{\pi \lambda^2 \beta}{\kappa A} U_{7/2}(w,y) \qquad \text{(IV-4)}$$

This result was given in Eq. (4-42) of Chapter 4.

APPENDIX V

EVALUATION OF THE INTEGRALS:

$$1. \quad I_1 = \int_0^\infty \cos\left(\frac{2\pi K E}{B} - \frac{5\pi}{4}\right) \frac{df(E)}{dE}\, dE$$

$$2. \quad I_2 = \int_0^\infty \cos\left(\frac{2\pi K E}{B} - \frac{3\pi}{4}\right) \frac{df(E)}{dE}\, E\, dE$$

We can express the first integral as

$$I_1 = R\left[- \frac{e^{i\left(\frac{2\pi K E_o}{B} - \frac{5\pi}{4}\right)}}{kT} \int_0^\infty \frac{e^{i\frac{2\pi K}{B}(E-E_o)}\, dE}{\left(1+e^{(E-E_o)/kT}\right)\left(1+e^{-(E-E_o)/kT}\right)} \right] \tag{V-1}$$

where R denotes "the real part of". The substitution

$$\phi = (E - E_o)/kT$$

transforms I_1 to

$$R\left[- e^{i\left(\frac{2\pi K E_o}{B} - \frac{5\pi}{4}\right)} \int_{-E_o/kT}^{\infty} \frac{e^{i\alpha\phi}\, d\phi}{\left(1+e^{\phi}\right)\left(1+e^{-\phi}\right)} \right] \tag{V-2}$$

where α is a real number with the constant value

$$\alpha = 2\pi K kT/B$$

At sufficiently low temperatures ($E_o \gg kT$) the nature of the integrand permits us to replace the lower limit $-E_o/kT$ by $-\infty$ without introducing any significant error. Our problem is therefore to evaluate

$$\int_{-\infty}^{\infty} \frac{e^{i\alpha\phi}\, d\phi}{(1 + e^{\phi})(1 + e^{-\phi})} \tag{V-3}$$

This integration is most readily carried out in the complex plane. The poles of the integrand occur at

$$\phi_o = \pm \pi i(2p + 1) \tag{V-4}$$

where p = 0, 1, 2, . . . If we consider a contour consisting of the real axis and a semicircle of radius R in the upper half plane, only the poles in the upper half plane are included. By letting $R \longrightarrow \infty$ the contribution to the integral from the semicircle vanishes and we have from Cauchy's Theorem

$$\int_{-\infty}^{\infty} \frac{e^{i\alpha\phi}\, d\phi}{(1 + e^{\phi})(1 + e^{-\phi})} + \sum_{p=o}^{\infty} \oint_{C_p} \frac{e^{i\alpha\phi}\, d\phi}{(1 + e^{\phi})(1 + e^{-\phi})} = 0 \tag{V-5}$$

Expanding the numerator and denominator of the integral (under the summation sign) in Taylor series around $\phi = \phi_o$ and then dividing, gives

$$\int_{-\infty}^{\infty} \frac{e^{i\alpha\phi}\, d\phi}{(1 + e^{\phi})(1 + e^{-\phi})} + \sum_{p=o}^{\infty} \oint_{C_p} -e^{i\alpha\phi_o}\left[\frac{1}{(\phi - \phi_o)^2} + \frac{i\alpha}{(\phi - \phi_o)} - \frac{\alpha^2}{2} + . . \right] d\phi = 0$$

(V-6)

Since the integral under the summation is now in Laurent series form we can write

$$\int_{-\infty}^{\infty} = \sum_{p=o}^{\infty} 2\pi i(i\alpha e^{i\alpha\phi_o}) = -2\pi\alpha \sum_{p=o}^{\infty} e^{-\alpha\pi(2p+1)} \qquad \text{(V-7)}$$

The geometric series in (V-7) can be summed to give

$$\int_{-\infty}^{\infty} = \frac{-\pi\alpha}{\sinh(\pi\alpha)} \qquad \text{(V-8)}$$

It now follows that

$$I_1 = \frac{2\pi^2\kappa\, kT \quad \cos\left(\frac{2\pi\kappa E_o}{B} - \frac{5\pi}{4}\right)}{B \quad \sinh\,(2\pi^2\kappa\, kT/B)} \qquad \text{(V-9)}$$

Following the same procedure for the second integral gives

$$I_2 = \frac{\pi kT \sin\left(\frac{2\pi\kappa E_o}{B} - \frac{3\pi}{4}\right)}{\sinh\,(2\pi^2\kappa\, kT/B)}$$

$$- \frac{2\pi^3\kappa\,(kT)^2 \cosh\,(2\pi^2\kappa\, kT/B) \sin\left(\frac{2\pi\kappa E_o}{B} - \frac{3\pi}{4}\right)}{B \quad \sinh^2\,(2\pi^2\kappa\, kT/B)} \qquad \text{(V-10)}$$

$$+ \frac{2\pi^2\kappa\, kT \quad \cos\left(\frac{2\pi\kappa E_o}{B} - \frac{3\pi}{4}\right)}{B \quad \sinh\,(2\pi^2\kappa\, kT/B)}$$

APPENDIX VI

The Method of Critical Points

1. In this appendix we shall show how the method of critical points can be used to evaluate the coefficient $R(a_{\kappa,o,o})$, represented by Eq. (6-14) in Chapter 6.

We shall consider the two integrals of Eq. (6-14) separately, and designate by I_1 and I_2 the first and second integrals respectively. By substituting

$$\theta = \frac{hn_y}{L_y} - \frac{eHx}{C} \tag{VI-1}$$

in I_1 and carrying out the integrations over θ and n_y we get

$$I_1 = \frac{4(-1)^\kappa}{2\pi\kappa} \int_o^{\frac{L_z}{h}\sqrt{2mE}} \left(\frac{eHL_xL_y}{2hC} - \frac{L_y}{h}\sqrt{2mE_1}\right) \sin\left(\frac{2\pi\kappa E_1}{2\beta H}\right) dn_z \tag{VI-2}$$

Now consider the first part of this integral. Setting

$$\phi = \frac{h}{L_z\sqrt{2mE}} \; n_z \tag{VI-3}$$

transforms this part to

$$\frac{2(-1)^\kappa \, eHL_xL_yL_z\sqrt{2mE}}{2\pi\kappa h^2 C} \int_o^1 \sin\left[\frac{2\pi\kappa E}{2\beta H}\left(1 - \phi^2\right)\right] d\phi \tag{VI-4}$$

The integral in (VI-4) is a special case of the more general integral evaluated in Appendix I. Following the methods described there we get the result

$$(-1)^{\kappa} D B^{1/2} U_{3/2}(w, o) \,/\, A^{1/2} \pi (2\kappa)^{3/2} \tag{VI-5}$$

for (VI-4).

If we use the same substitution (VI-3), the second part of (VI-2) becomes

$$-\frac{4(-1)^{\kappa} L_y L_z (2mE)}{2\pi\kappa h^2} \int_0^1 (1-\phi^2)^{1/2} \sin\left[\frac{w}{2}(1-\phi^2)\right] d\phi \tag{VI-6}$$

The evaluation of this integral will require the use of the method of critical points.

I_2, the second part of Eq. (6-14), can be put into the form:

$$I_2 = \frac{4(-1)^{\kappa} L_y L_z (2mE)}{\pi\kappa h^2} \int_0^1 \int_0^1 (1-\phi^2)^{1/2} \sin\left[\frac{w}{4}(1-\phi^2)\right]$$

$$\cos\left[\frac{w}{2\pi}(1-\phi^2)\, f(\sigma)\right] d\sigma\, d\phi \tag{VI-7}$$

where

$$f(\sigma) = \sigma\sqrt{1-\sigma^2} + \sin^{-1}\sigma$$

This can be further transformed to give

$$I_2 = \frac{2(-1)^{\kappa} L_y L_z (2mE)}{\pi\kappa h^2} \left\{ \begin{aligned} &\int_0^1 \int_0^1 (1-\phi^2)^{1/2} \sin\left[\frac{w}{2\pi}(1-\phi^2)\left(\frac{\pi}{2} + f(\sigma)\right)\right] d\sigma\, d\phi \; + \\ &\int_0^1 \int_0^1 (1-\phi^2)^{1/2} \sin\left[\frac{w}{2\pi}(1-\phi^2)\left(\frac{\pi}{2} - f(\sigma)\right)\right] d\sigma\, d\phi \end{aligned} \right\} \tag{VI-8}$$

We shall use the method of critical points to evaluate both of the double integrals in (VI-8).

2. **Details of the method of critical points.** Consider the general integral

$$I = \int_a^b g(x)\, e^{iwf(x)}\, dx \tag{VI-9}$$

where a, b, f(x) and g(x) are independent of the parameter w. It is further assumed that f(x) and g(x) are infinitely often differentiable in the closed interval $a \leqq x \leqq b$. We seek the value of I for $|w| \gg 1$. Van der Corput (Ref. 3) asserts that the asymptotic character of I is completely determined if the behavior of f(x) and g(x) is given in the vicinity of the critical points.[1] These points are the end points a and b and the points between a and b where the phase wf(x) is stationary. The contribution of each critical point is called the residue at that point. The residue at a critical point ξ can be developed asymptotically in ascending powers of $1/w^{1/m}$, where m is the smallest positive integer such that the m^{th} derivative of f(x) at ξ is not zero. To establish the nature of the residue at ξ we expand g(x) and f(x) in Taylor series around ξ. The residue then becomes

$$\int_{\xi_-}^{\xi_+} \left[g(\xi) + g'(\xi)(x-\xi) + \ldots\right] e^{iw\left[f(\xi) + \frac{f^m(\xi)}{m!}(x-\xi)^m + \ldots\right]} dx \tag{VI-10}$$

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[1] This condition on f(x) and g(x) is weaker than the requirement that f(x) and g(x) be infinitely often differentiable in the closed interval $a \leqq x \leqq b$. In practice we use the weaker condition for evaluation of integrals.

If we make the substitution

$$(x - \xi) = \left(\frac{m!}{wf^m(\xi)}\right)^{1/m} y \qquad \text{(VI-11)}$$

the first integration of (VI-10) becomes

$$\frac{e^{iwf(\xi)}\, g(\xi)}{\left(\frac{wf^m(\xi)}{m!}\right)^{1/m}} \int_{o-}^{o+} e^{iy^m}\, e^{i\left[\frac{f^m(\xi)\, y^{m+1}}{(m+1)!\, w^{1/m}\left(\frac{f^m(\xi)}{m!}\right)^{1+\frac{1}{m}}} + \cdots\right]} dy \qquad \text{(VI-12)}$$

Since the major part of this integral is contributed at $y \sim 0$, we can safely extend the upper limit to ∞. Further, the exponent of the second exponential in the integrand will be small compared to the first in the region of importance so we may expand it as

$$e^{i\epsilon} \sim 1 + i\epsilon + \ldots \qquad \text{(VI-13)}$$

This leads to the value

$$e^{iwf(\xi)}\left[\frac{g(\xi)}{w^{1/m}\left(\frac{f^m(\xi)}{m!}\right)^{1/m}} \int_0^\infty e^{iy^m} dy + \frac{i\, g(\xi)\, f^{m+1}(\xi)}{w^{2/m}(m+1)!\left(\frac{f^m(\xi)}{m!}\right)^{1+2/m}} \times \int_0^\infty y^{m+1}\, e^{iy^m}\, dy\right] \qquad \text{(VI-14)}$$ [2]

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[2] In choosing the limits o to ∞ for the integrals in (VI-14), we have assumed that ξ is the lower bound of the interval. If ξ were an interior point the limits would be $-\infty$ to ∞. If ξ were the upper bound of the interval, the limits would be $-\infty$ to o.

for (VI-12). The integrals in (VI-14) are examples of the general type

$$\int_0^{\infty} e^{it^n}\ t^z\ dt = \frac{1}{(z+1)}\ \frac{\left(\frac{z+1}{n}\right)!}{(-i)^{(z+1)/n}} \tag{VI-15}$$

From (VI-14) and (VI-15) it follows that the contribution of the first integration of (VI-10) can be written as

$$e^{iwf(\xi)}\left[\frac{a_{1,1}}{w^{1/m}} + \frac{a_{2,1}}{w^{2/m}} + \ldots\right] \tag{VI-16}$$

where

$$a_{1,1} = \frac{g(\xi)\ \left(\frac{1}{m}\right)!}{\left(\frac{f^m(\xi)}{m!}\right)^{1/m} (-i)^{1/m}} \tag{VI-17}$$

and

$$a_{2,1} = \frac{i\, g(\xi)\, f^{m+1}(\xi)\ \left(\frac{m+2}{m}\right)!}{(m+1)!\left(\frac{f^m(\xi)}{m!}\right)^{1+2/m} (m+2)\, (-i)^{1+2/m}} \tag{VI-18}$$

The second integration of (VI-10) is carried out analogously and leads to the value

$$e^{iwf(\xi)}\left[\frac{a_{2,2}}{w^{2/m}} + \frac{a_{3,2}}{w^{3/m}} + \ldots\right] \tag{VI-19}$$

In order to be able to get the complete coefficient of the $1/w^{2/m}$ term we show the value of $a_{2,2}$. It is

$$a_{2,2} = \frac{g'(\xi)\ \left(\frac{2}{m}\right)!}{\left(\frac{f^m(\xi)}{m!}\right)^{2/m} 2\ (-i)^{2/m}} \qquad \text{(VI-20)}$$

Continuing this operation shows that the complete residue at ξ can be put into the form

$$e^{iwf(\xi)} \left[\frac{c_1}{w^{1/m}} + \frac{c_2}{w^{2/m}} + \frac{c_3}{w^{3/m}} \cdots + \frac{c_s}{w^{s/m}} + \cdots \right] \qquad \text{(VI-21)}$$[3]

where

$$c_1 = a_{1,1}$$

$$c_2 = a_{2,1} + a_{2,2}$$

$$c_3 = a_{3,1} + a_{3,2} + a_{3,3}$$

The general coefficient c_s is found to be

$$c_s = \frac{g^{s-1}(\xi)}{(s-1)!} \left(\frac{m!}{f^m(\xi)}\right)^{s/m} \frac{(s/m)!}{s(-i)^{s/m}}$$

$$+ \frac{i\left(\frac{m+s}{m}\right)!}{(m+s)\,(-i)^{(m+s)/m}} \left(\frac{m!}{f^m(\xi)}\right)^{\frac{m+s}{m}} \sum_{0<p<s} \frac{g^{p-1}(\xi)\, f^{m+s-p}(\xi)}{(p-1)!\,(m+s-p)!}$$

(VI-22)

3. Let us now apply this development to the integral $I_{1,2}$ appearing in (VI-6). To put it into the desired form we write

$$I_{1,2} = \gamma \ell \int_0^1 g(\phi)\ e^{iwf(\phi)}\ d\phi \qquad \text{(VI-23)}$$

[3] van der Corput gives this form for the residue without showing the explicit values of c_1, c_2, . . .

where

$$g(\phi) = (1 - \phi^2)^{1/2}$$

$$f(\phi) = (1/2)(1 - \phi^2)$$

The critical points are 0 and 1. The point 0 is a stationary phase point as well as an end point. After obtaining the Taylor expansions around the point 0 the residue (designated as Res) there is found to be

$$(\text{Res})_{\phi=0} = e^{i\frac{w}{2}} \left\{ \frac{(1/2)!\,(2!)^{1/2}}{w^{1/2}(-i)^{1/2}(-1)^{1/2}} - \frac{(2!)^{3/2}\,(3/2)!}{w^{3/2}(2)!\,(-1)^{3/2}\,3(-i)^{3/2}} \right\} \quad \text{(VI-24)}$$

Since the function $g(\phi)$ cannot be expanded into a Taylor series around the point 1 we must make an appropriate transformation to get the residue there. If we let

$$(1 - \phi^2)^{1/2} = Z \quad \text{(VI-25)}$$

we would require the residue at $Z = 0$. The transformed integral is

$$\int_0^1 \frac{Z^2}{(1 - Z^2)^{1/2}} \quad e^{i\frac{w}{2}Z^2} \; dZ \quad \text{(VI-26)}$$

so that we can now expand our functions around $Z = 0$. Carrying out the details of expansion leads to

$$(\text{Res})_{Z=0} = (\text{Res})_{\phi=1} = \frac{2(2!)^{3/2}\,(3/2)!}{w^{3/2}\,(2)!\,3(-i)^{3/2}} \quad \text{(VI-27)}$$

By neglecting the terms $O(\frac{1}{w^{3/2}})$ and taking the imaginary part of the residues, we get

$$I_{1,2} \sim \left(\frac{\pi}{2}\right)^{1/2} \frac{1}{w^{1/2}} \cos\left(\frac{w}{2} - \frac{3\pi}{4}\right) \qquad \text{(VI-28)}$$

4. We now consider the double integrals in (VI-8). The general philosophy in handling double integrals is to apply the previous development in succession. There are additional features which make the double integration more complicated, but rather than discuss them generally we shall note them in solving the specific examples. We designate by $I_{2,1}$ and $I_{2,2}$ the first and second double integrals in (VI-8). Then $I_{2,2}$ can be written as

$$I_{2,2} = \vartheta \int_0^1 \int_0^1 g(\phi, \sigma)\, e^{iwF(\phi,\sigma)}\, d\sigma\, d\phi \qquad \text{(VI-29)}$$

where

$$g(\phi,\sigma) = (1 - \phi^2)^{1/2}$$

$$F(\phi,\sigma) = \frac{(1-\phi^2)}{2\pi}\left(\frac{\pi}{2} - \sigma\sqrt{1-\sigma^2} - \sin^{-1}\sigma\right)$$

The critical points here are first the points within the region of integration where the phase $wF(\phi,\sigma)$ is stationary, i.e. where $\frac{\partial F}{\partial \phi} = \frac{\partial F}{\partial \sigma} = 0$; then the vertices of the boundary of the region; finally those boundary points are critical where $F(\phi,\sigma)$ taken along the boundary curve is stationary. For our integral $I_{2,2}$ the following points (infinite in number) are critical:

$$\phi = 0\ ;\ \sigma = 0$$

$$\phi = 1\ ;\ 0 \leqq \sigma \leqq 1$$

$$0 \leqq \phi \leqq 1\ ;\ \sigma = 1$$

To get the residue at the point (0, 0) we expand $g(\phi, \sigma)$ and $F(\phi, \sigma)$ in double Taylor series around that point. Substituting these expansions into the integrand gives

$$(\mathrm{Res})_{0,0} = e^{i\frac{w}{4}} \int_0^\infty \int_0^\infty \left(1 - \frac{\phi^2}{2} - \ldots\right) e^{iw\left(-\frac{\sigma}{\pi} - \frac{\phi^2}{4} + \ldots\right)} d\sigma\, d\phi \qquad \text{(VI-30)}$$

Integrating first on σ (holding ϕ fixed) and keeping only the largest term gives

$$(\mathrm{Res})_{0,0} = \frac{e^{i\frac{w}{4}}\pi}{iw} \int_0^\infty \left(1 - \frac{\phi^2}{2} - \ldots\right) e^{iw\left(-\frac{\phi^2}{4} - \ldots\right)} d\phi \qquad \text{(VI-31)}$$

We now integrate over ϕ to get

$$(\mathrm{Res})_{0,0} = \frac{e^{i\frac{w}{4}}\pi}{iw} \left(\frac{(1/2)!}{w^{1/2}(-1/4)^{1/2}(-i)^{1/2}} \right) \qquad \text{(VI-32)}$$

This residue is $O\left(\frac{1}{w^{3/2}}\right)$.

Next we consider the residue from the points $0 \leqq \phi \leqq 1$, $\sigma = 1$. The function $F(\phi, \sigma)$ cannot be expanded in a Taylor series around any point having $\sigma = 1$. Therefore we must resort to a suitable transformation (just as we did in the single integral case) to accomplish the calculation. If we let

$$\sin^{-1}\sigma = \theta \qquad \text{(VI-33)}$$

we would require the residue from the points

$$0 \leqq \phi \leqq 1 \; ; \quad \Theta = \pi/2$$

By expanding the functions in the integrand around $\Theta = \pi/2$ we can express the residue from this entire boundary (designated as $(\mathrm{Res})_{b_1}$) as

$$(\mathrm{Res})_{b_1} = \int_0^1 \int_0^\infty (1 - \phi^2)^{1/2} \left(\oplus - \frac{1}{3!} \oplus^3 - \ldots\right) e^{\, i \frac{w(1-\phi^2)}{2\pi} \left(\frac{4}{3!} \oplus^3 - \ldots\right)} d\oplus \, d\phi \tag{VI-34}$$

where

$$\oplus = -(\Theta - \pi/2)$$

The integration over $\oplus$ follows from the general development for single integrals. If we keep only the largest term of the resulting expansion, the residue is

$$(\mathrm{Res})_{b_1} = \frac{(2/3)! \; (3\pi)^{2/3}}{w^{2/3} \; 2(-i)^{2/3}} \int_0^1 \frac{d\phi}{(1 - \phi^2)^{1/6}} \tag{VI-35}$$

The integral in (VI-35) is a standard type, so that the final result can be written as

$$(\mathrm{Res})_{b_1} = \frac{(2/3)! \; (3\pi)^{2/3} \; \pi^{1/2} \, \Gamma(11/12)}{w^{2/3} \; (-i)^{2/3} \; 4 \; \Gamma(17/12)} \tag{VI-36}$$

This residue is $O\left(\frac{1}{w^{2/3}}\right)$.

Finally we have the boundary $\phi = 1;\ 0 \leqq \sigma \leqq 1$ to consider. Here we must again make the transformation

$$(1 - \phi^2)^{1/2} = Z$$

The integral itself then becomes

$$\nu \int_0^1 \int_0^1 \frac{Z^2}{(1 - Z^2)^{1/2}} e^{i \frac{wZ^2}{2\pi}\left(\frac{\pi}{2} - \sigma\sqrt{1 - \sigma^2} - \sin^{-1}\sigma\right)} d\sigma dZ \tag{VI-37}$$

After carrying out the σ integration completely we will be concerned with the residue from the point $Z = 0$. The σ integration is a single integral problem of the type considered previously. Its critical points are 0 and 1. However, we need only keep the residue from the point $\sigma = 0,\ Z = 0$ since the point $\sigma = 1,\ Z = 0$ corresponds to the point $\sigma = 1,\ \phi = 1$ and its residue is already included in $(\mathrm{Res})_{b_1}$ given by (VI-36). This calculation therefore reduces to the evaluation of the residue of (VI-37) at the point $Z = 0, \sigma = 0$. The result is

$$(\mathrm{Res})_{Z=0,\ =0} = \frac{2\pi\ (1/2)!}{w^{3/2}\ i\ (-i)^{1/2}} \tag{VI-38}$$

This residue is $O\left(\frac{1}{w^{3/2}}\right)$.

The complete evaluation shows that the largest term in $I_{2,2}$ is given by the imaginary part of (VI-36) which is $O\left(\frac{1}{w^{2/3}}\right)$.

The integral $I_{2,1}$ can be evaluated by the same procedure as given above. It is noted that two parts of $I_{2,1}$ exactly cancel the contributions (VI-32) and (VI-38) of $I_{2,2}$. The largest term in $I_{2,1}$ is $O\left(\frac{1}{w^{7/6}}\right)$.

Combining the results of the two integrations $I_{2,1}$ and $I_{2,2}$ we find that

$$I_2 \sim \frac{(3\pi)^{7/6}\,\Gamma(5/3)\,\Gamma(11/12)}{8\,\Gamma(17/12)\;w^{2/3}} \qquad \text{(VI-33)}$$

From (VI-5), (VI-28) and (VI-33), we get the value for $R(a_{\kappa,o,o})$ given by Eq. (6-15) in Chapter 6.

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