way as to give equivalent good fits to the very precise low energy Van de Graaff data. On the basis of this plot, and again assuming only central forces, our results appear to favor the Yukawa type potential. However, it should be pointed out that Jackson and Blatt have investigated the allowable uncertainties in cross-section and bombarding energy required to discriminate between the two shapes, and that our uncertainties are somewhat greater than those given by these authors.

An analysis of these data in terms of the *f* function of Breit, Condon, and Present<sup>14</sup> yields a value for this function, as determined from the  $57.8^{\circ}$  S wave phase shift, of  $15.7 \pm 0.5$ , which is in fair agreement with the

14 Breit, Condon, and Present, Phys. Rev. 50, 825 (1936).

value  $16.5 \pm 0.17$  predicted by Yovits, Smith, Hull, Bengston, and Breit<sup>15</sup> for the Yukawa well.

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Note added in proof:—The points at angles from 169.8° to 176.2°, inclusive, on Fig. 3E are plotted incorrectly. They should be lowered 5 to 10 percent to conform with the values given in Table I.

<sup>16</sup> Yovits, Smith, Hull, Bengston, and Breit, Phys. Rev. 85, 540 (1952).

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# Number Theory and the Magnetic Properties of an Electron Gas

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Theorems involving the correction terms of lattice point problems in the theory of numbers are interpreted to derive the orders of magnitude of the oscillatory (de Haas-van Alphen effect) and non-oscillatory (Landau and surface diamagnetism) terms in the magnetic moment of a Fermi gas in a finite cylindrical container. The results are valid for systems from atomic dimensions up, and all values of the magnetic field. The different types of moment are different from strong and weak fields, and may depend, for small particles, on the nature of the surface potential at the walls of the container. The applicability of the method to physical problems, and the difficulties associated with statistical mechanical problems involving magnetic fields are discussed.

## I. INTRODUCTION

HE problem of the diamagnetism of an electron gas was first examined from a fundamental standpoint by Bohr<sup>1</sup> and Van Leeuwen,<sup>2</sup> who showed for a rather general class of conditions that no magnetic properties whatever were to be found on the basis of classical statistics. Bohr, in particular, showed that this conclusion was a consequence of exact cancellation between the large diamagnetic properties of electrons whose orbits did not collide with the wall and the paramagnetic properties of those orbits which did collide with the walls. Landau<sup>3</sup> re-examined the problem on the basis of quantum statistics and showed that a small diamagnetism was to be expected when the levels were quantized on the basis of either Boltzmann or Fermi-Dirac statistics. However, it was not at all clear how the conclusions of Bohr were related to those of Landau via the correspondence principle. The reason for this was that Landau assumed a very strong magnetic field (orbit radius very much less than dimensions of the container) and did not attempt to satisfy the boundary conditions at the walls of the container, but merely

counted those quantum states which had the center of gravity of their probability distribution inside the container. If one attempts to follow the details of the Landau derivation, it appears that the results obtained are quite sensitive to such apparently trivial details as the order of integration over the different quantum numbers and of differentiation with respect to H to obtain the moment, the choice of origin for the energy level, and the choice of several possible forms for the Euler-McLaurin formula for replacing a sum by an integral.

Moreover, there is the added embarrassment that, if higher terms in the Euler-McLaurin formula are included, one may find infinite contributions to the moment because certain derivatives are infinite at the ends of the range of integration. Thus one can obtain the Landau result but one can also obtain quite different results which one has no a priori reason for rejecting.

The discrepancies can be roughly divided into two classes. First, a large difference in the moment per unit volume is computed by

 $M/V = kT(\partial/\partial H)\Sigma_i \log[1 + \exp(E_0 - E_i)/kT)]$ 

as opposed to  $M/V = -kT \Sigma_i (\partial E_i / \partial H) 1 / \{ \exp[(E_i - E_0) / kT] + 1 \};$ 

<sup>&</sup>lt;sup>1</sup> N. Bohr, unpublished dissertation, Copenhagen, 1911. For an account of this work, see reference 5, p. 97. <sup>2</sup> J. H. Van Leeuwen, J. phys. et radium 2, 361 (1921). <sup>3</sup> L. Landau, Z. Physik 64, 629 (1930).

that is, different order for summing and differentiating the partition function, the sum having been replaced by an integral over the density of states.

The second type of discrepancy arises as follows. One must remember that the sought-for Landau moment/cc is small, of order  $10^{-6}$  H. If one does not take the limit volume-infinity for the specimen, then small terms which are size-dependent arise, and contribute to the moment for macroscopic specimens (of order centimeter dimensions) amounts of the same order of magnitude as the Landau contribution. Moreover, these terms are different for different choices of all the apparently trivial details of calculations mentioned above.

Teller<sup>4</sup> and Van Vleck<sup>5</sup> attempted to clarify the first type of inconsistency which arises between differentiating with respect to the field before or after carrying out the sum over states. For example, Van Vleck, using a cylindrical container, attempted to show that the large contribution to the moment of electrons which do not encircle the origin nor collide with the walls just canceled, except for the Landau diamagnetism, the contribution of the electrons which do collide with the wall. However, if one includes the states of positive quantum number l (orbits which do encircle the origin which he, following Landau and Teller, excluded quite arbitrarily), the cancellation is completely destroyed for a container of finite macroscopic dimensions. One then finds a huge diamagnetic moment. It was this observation which led this writer<sup>6</sup> to conclude (also erroneously, as will be apparent from the subsequent discussion) that a gas of electrons in a finite container has a large diamagnetic moment.

The above discussion refers primarily to the strong fields (by definition orbit radius < specimen size) where the contradictory results associated with the small quantities involving dimensions (which did not give contributions to the moment small compared to the expected Landau result) were simply ignored or evaded by passing to the limit of infinitely large containers. In most statistical-mechanical problems such "surface terms" are indeed negligible.

For the case of weak fields (orbit radius > specimen size) or small containers, there is an equally great variety of conclusions. Van Vleck<sup>7</sup> suspected, on the basis of the principle of spectroscopic stability, that the susceptibility would be the same as for strong fields, an inference not borne out by the conclusions of this paper. Papaetrou<sup>8</sup> made a perturbation calculation of plane waves taking into account degeneracy and concluded to a strong diamagnetism for weak fields, and moreover concluded that the diamagnetism for very weak fields was different depending upon whether the ratio of the edge length for rectangular containers was

rational or not. He offered only a tentative explanation for this strange result. Slater<sup>9</sup> concluded to a strong diamagnetism for weak fields, whereas Welker<sup>10</sup> concluded there was none, but this method of calculation led Papapetrou<sup>11</sup> to interpret Welker's calculations as indicating a strong diamagnetism for adiabatic magnetization. Dingle<sup>12</sup> also concluded that for finite containers and weak fields a diamagnetism larger than the Landau value was to be expected.

In the low temperature region Shoenberg,<sup>13</sup> (quoting unpublished results of Landau), Blackman,14 and Peierls<sup>15</sup> derived expressions giving an oscillating moment (the de Haas-van Alphen effect) but they also used Landau-type wave functions which do not satisfy the boundary conditions at the walls of the container. Here also extreme care has to be taken in carrying out the necessary calculations in order to avoid, or rather, ignore inconsistencies of the type mentioned above.

This situation led Besden<sup>16</sup> to attack numerically the problem of a container of a specified volume containing a specified number ( $\sim 10^3$ ) of particles in order to solve exactly the problem of fitting the wave functions properly inside the container. He found a diamagnetic behavior suggestive of the de Haas-van Alphen effect, and possibly also of superconductivity.

The origin of these differences may be expressed most simply in the following way. Consider a finite Fermi-Dirac system in a magnetic field with discrete energy levels  $E_i = E_i(H, d, p)$ , where by d and p we refer explicitly to the dependence on dimensions of the container and physical constants. The total energy of this system is:

$$U = \sum_{i} E_{i} / \{ \exp[(E_{i} - E_{0})/kT] + 1 \}, \qquad (1)$$

where  $E_0$  is defined by the expression

$$N = \sum_{i} \frac{1}{\{\exp[(E_i - E_0)/kT] + 1\}}.$$
 (2)

N is the number of particles in the finite container, and N is finite and constant. The rate of change of the energy of the system with varying magnetic field is -M, the moment. For constant number of particles in the system it is:

$$-M = (\partial U/\partial H)_N = (\partial U/\partial H) E_0 + (\partial U/\partial E_0)_H (dE_0/dH)$$
  
=  $(\partial U/\partial H) E_0 - (\partial U/\partial E_0)_H (\partial N/\partial H) E_0/$   
 $(\partial N/\partial E_0)_H.$  (3)

Remembering that H appears explicitly only in  $E_i$ , then on differentiating there is considerable cancellation and

<sup>&</sup>lt;sup>4</sup> E. Teller, Z. Physik 67, 311 (1931).

<sup>&</sup>lt;sup>5</sup> J. H. Van Vleck, *The Theory of Electric and Magnetic Suscepti-bilities* (Oxford University Press, London, 1932), p. 356.

<sup>&</sup>lt;sup>6</sup> M. F. M. Osborne, Phys. Rev. 81, 147 (1951). <sup>7</sup> See reference 5, p. 354.

<sup>&</sup>lt;sup>8</sup> A. Papapetrou, Z. Physik 112, 587 (1939).
<sup>9</sup> J. C. Slater, Phys. Rev. 52, 214 (1937).
<sup>10</sup> H. Welker, Sitzber. bayer. Akad. 14, 115 (1938).
<sup>11</sup> Reference 8, p. 601.
<sup>12</sup> R. P. Dinck, Phys. Rev. 82, 666 (1951).

 <sup>&</sup>lt;sup>14</sup> R. B. Dingle, Phys. Rev. 82, 966 (1951).
 <sup>15</sup> R. B. Dingle, Phys. Rev. 82, 966 (1951).
 <sup>15</sup> D. Shoenberg, Proc. Roy. Soc. (London) A170, 341 (1939).
 <sup>14</sup> M. Blackman, Proc. Roy. Soc. (London) A166, 1 (1938).
 <sup>15</sup> R. Peierls, Z. Physik 81, 186 (1933).
 <sup>16</sup> D. J. Besden, Phys. Rev. 79, 417 (1950); unpublished thesis, Rice Institute (1950).



FIG. 1. Geometrical determination of Fourier coefficient  $a_{1,2}$ .

one finally obtains\* exactly

$$M = -\sum_{i} (\partial E_i / \partial H) / \{ \exp[(E_i - E_0) / kT] + 1 \}.$$
(4)

In this form, especially when one considers Fermi-Dirac statistics, it can be made evident why inconsistencies appear. If one takes as usually the case that the energy states whose classical orbits do not intersect the wall are as given by the energy states in free space, then all the contributions of these states to the sum in Eq. (4) are positive. This contribution alone leads naturally to a huge moment. If, nervertheless, the net result for the moment is to be small (see Bohr and Landau) this huge contribution must be almost exactly canceled by a contribution of equal magnitude but opposite sign by those states which do intersect the wall. If we ask : what are the orders of magnitude of the numbers of these two classes of states, those which do intersect the wall and those which do not?, and remember the very small (Landau) order of magnitude to which the two contributions to the moment must be equal, we see that the accuracy of the counting and the energy evaluation must be as good for the surface states as those in the interior, or the cancellation will be imperfect and a too-large absolute value for the moment is to be expected.

The average value of the energy is of order  $\frac{3}{5}$  the maximum energy  $E_0$ , i.e., most of the states have orbits whose dimensions are comparable to those at the top of the Fermi sea. It can be easily shown by considering the cross-sectional areas where the centers of orbits of different classes lie that the orders of magnitude of (1) the numbers of interior states, (2) the numbers of states which encircle the origin without intersecting the wall, and (3) the numbers of states which intersect the wall are like  $(1) \pi R^2 L_z k_0^3$ ,  $(2) \pi r_0^2 L_z k_0^3$ , and  $(3) 2\pi R r_0 L_z k_0^3$  or relatively like (1), 1,  $(2) r_0^2/R^2$ , and  $(3) r_0/R$ . Here  $r_0$  is the radius of the orbit for  $E = E_0$ , R,  $L_z$  are the dimensions of the container,  $k_0 = (2mE_0)^{\frac{1}{2}}/\hbar$ , and  $E_0$  is the Fermi energy.

If  $E_0$  is in volts, R,  $L_z$  in cms, H in gauss (along z), the relative numbers of states are approximately like 1,  $E_0^{\frac{1}{2}}/(HR)$ ,  $E_0/H^2R^2$ . The contributions to the moment

of the first and second classes of state are approximately where  $\mu = e\hbar/2mc$ :

Hence for the surface states, whose orbits do intersect the walls, the contribution  $M_s$  must be equal and opposite to the sum of the above to the order of magnitude of the Landau diamagnetism,  $M_L \sim 10^{-6} H R^2 L_z$ . Thus we see that for strong fields and macroscopic specimens, the contributions of the second and third classes of states are by no means negligible when one is looking for moments as small as the Landau moment. It is just the details of the delicate ways in which they *are* neglected which are responsible for the various inconsistencies mentioned previously.

Let us rewrite Eq. (4) as follows: Let 1(x) be the unit function

$$1(x) = 0, x < 0$$
  
=  $\frac{1}{2}, x = 0$   
= 1, x > 0

in such a way that

$$\int_{x<0}^{\infty} (d1/dx) dx = 1.$$

Then we can write Eq. (4) as:

$$M = -(\partial U/\partial H)_N = (\partial/\partial H) \int_0^\infty \Sigma_i 1(E - E_i) \times (1/\{\exp[(E - E_0)/kT] + 1\}) dE, \quad (5)$$

where the differentiation with respect to H is to be taken only where H appears explicitly, that is, in  $E_i = E_i(H, d, p)$  only. Now consider the expression  $\sum_i 1(E-E_i)$ . This is the number of states of energy  $E_i$ less than any chosen energy E, plus states of energy  $E_i = E$  counted as  $\frac{1}{2}$ . It is expressions of just this type which are given by solutions of lattice point problems in the theory of numbers, to which we now turn. It will be found that just the refinements of number theory give the information necessary to compute the magnetic moment.

#### **II. LATTICE POINT PROBLEMS OF NUMBER THEORY**

Kendall's<sup>17</sup> lattice point problem for the plane (we shall indicate the necessary generalizations for a threedimensional problem) consists of the following. Given a closed curve, everywhere convex, and with specified continuity conditions on its derivatives, how many points whose coordinates are integers lie inside or on the closed curve? The answer by definition is G(E)where by E we may here understand one or more parameters specifying the size and shape of the curve, such as the axes of an ellipse. G(E) is given by the area

<sup>\*</sup> Correction added in proof: This procedure gives the adiabatic moment. Equation (4) is the correct expression for the isothermal moment obtained from the free energy.

<sup>&</sup>lt;sup>17</sup> D. G. Kendall, Quart. J. Math. (Oxford) 19, 1 (1948).

plus a series of periodic correction terms. The area plus the correction terms can be shown to converge to the exact number of points inside the closed curve, plus those on the curve counted as  $\frac{1}{2}$ , i.e., to:

# [G(E+0)+G(E-0)]/2.

Kendall gives (his notation) the following asymptotic expression for the number of lattice points inside or on a closed centrally-symmetric oval, everywhere convex, with a finite second derivative of the curvature, and with no points of zero or infinite curvature: *O* denotes order of magnitude.

$$G(E) = \operatorname{area} + \sum_{n, m} a_{nm},$$
  

$$a_{nm} = (x^{\frac{1}{2}} \rho^{\frac{1}{2}} / \pi l^{\frac{3}{2}}) \cos(2\pi (lx)^{\frac{1}{2}} \rho - 3\pi/4) + O(x^{1/6}/l^{5/6}).$$
(6)

 $x^{\frac{1}{2}}$  is a parameter determining the size of the oval (Fig. 1). If we imagine n, m to specify a direction in the plane, then  $x^{\frac{1}{2}}\rho$  is the distance from the origin of a line perpendicular to the direction n, m and tangent to the oval.  $x^{\frac{1}{2}}\rho$  is the radius of curvature at the point of tangency and  $l^{\frac{1}{2}} = (m^2 + n^2)^{\frac{1}{2}}$  is the spacing of lattice points on the line through lattice points at right angles to the direction n, m, and  $1/l^{\frac{1}{2}}$  is the separation of successive lattice "lines" normal to the direction n, m. Unity, the spacing of the integers, is the unit of length.

Kendall shows that the error  $\sigma = (\sum_{n,m} |a_{nm}|^2)^{\frac{1}{2}}$  in taking the area of the oval as the number of lattice points is of order of the square root of the maximum radius of curvature. This has a geometrical interpretation as the maximum number of points just caught or just missed by an arc of unit sagitta, and  $\rho_{max}$  as radius of curvature. For a circle,  $(\text{chord})^2 = 8 \cdot (\text{radius curvature} \cdot \text{sagitta})$ , or

$$c = 2(2\rho s)^{\frac{1}{2}} \sim \rho^{\frac{1}{2}} \text{ for } s = 1.$$
 (7)

We wish to show that this geometrical interpretation of the total error as described by number theory can be extended to each one of the terms  $a_{mn}$ . Consider the oval (Fig. 1) as growing (increasing  $x^{\frac{1}{2}}$ ) and consider the number of points just caught or missed by the arc tangent to the lattice line, m, n, that is, perpendicular to the direction m, n. The increment will be periodic in the lattice spacing  $1/l^{\frac{1}{2}}$  for this lattice line, that is, of order  $A \sin[2\pi p x^{\frac{1}{2}}/(1/l^{\frac{1}{2}}) - \varphi]$ . The amplitude A will be the number of points on an arc of sagitta  $s=1/l^{\frac{1}{2}}$  and radius of curvature  $x^{\frac{1}{2}}\rho$ , and these points are  $l^{\frac{1}{2}}$  apart. Hence, chord length is approximately

$$(x^{\frac{1}{2}}\rho \cdot s)^{\frac{1}{2}} = [x^{\frac{1}{2}}\rho \cdot (1/l^{\frac{1}{2}})]^{\frac{1}{2}},$$

and the number of points on this length is  $(x^{\frac{1}{2}}\rho)^{\frac{1}{2}}/l^{\frac{3}{2}} = A$ . Hence, the fluctuation with growth of G(E) owing to the curve cutting this particular lattice line is

$$a_{mn} = O(x^{\frac{1}{2}} \rho^{\frac{1}{2}} / l^{\frac{3}{2}}) \sin[2\pi \rho (lx)^{\frac{1}{2}} - \varphi], \qquad (8)$$

which is just the form of the coefficient  $a_{mn}$ . This geometrical analysis is insufficient to give the exact amplitude  $x^{\frac{1}{2}}\rho^{\frac{3}{2}}/\pi l^{\frac{3}{2}}$  and the phase  $\varphi = 3\pi/4$ , nor does it give the residual  $O(x^{1/6}/l^{5/6})$ . It does give correctly the behavior of all the oscillatory terms required by number

theory, even though the above heuristic derivation is applicable only when m and n have no common factor.

For nonsymmetric ovals, Kendall shows that the coefficients  $a_{mn}$  are of the form Eq. (6) with imaginary exponentials instead of sines. However, on summation only the real part contributes to the real number of points within the oval.

One can also apply the above geometrical argument to curves with points of infinite radius of curvature. Kendall examines the oval  $u^2x+v^4 \le x^2$  which has infinite radius of curvature at  $u=\pm x^{\frac{3}{2}}$ , v=0. He shows for this oval that

$$a_{m,0} = 2\Gamma(5/4) J_{3/4}(2mx^{\frac{1}{2}}) x^{5/8} / \pi^{\frac{1}{4}} m^{\frac{3}{4}} = O[x^{3/8} \sin(2\pi mx^{\frac{1}{2}} - \varphi)], \quad x \gg 1,$$
(9)

from which he infers that the error  $\sigma = O(x^{3/8})$ . But this is just the order of magnitude of points just caught or missed by an arc (not approximable by a circle) of unit sagitta around the points  $(u, v) = \pm x^{\frac{1}{2}}$ , 0. At  $u = x^{\frac{1}{2}} - 1$ ,  $v \sim x^{3/8}$  and by the above geometrical interpretation of  $a_{m,0}$ 

$$v_{1,0} = O[x^{3/8} \sin(2\pi x^{\frac{1}{2}} - \varphi)]. \tag{10}$$

This is just the lowest and predominant frequency of the fluctuation in the number of points as the curve grows (increasing  $x^{\frac{1}{2}}$ ) in the direction 1, 0.

In the case of a right angle triangle, taken as the area between (u/a)+(v/b)=1 and  $u=-\frac{1}{2}$ ,  $v=-\frac{1}{2}$ , Fig. 2, the interpretation of the real part of the coefficient  $a_{mn}$ as the oscillating number of points just caught or missed as the figure changes its dimensions is also valid. We understand a, b both  $\gg 1$ . It can be easily verified, by evaluating the coefficient



FIG. 2. Number theory analysis for a triangular area. ODL for the case a=b; QCJ for the case  $a-b=\epsilon$ ; OBH for the case  $b\gg a$ .

that  $a_{11}$  is for b=a

$$a_{11} = [\exp(2\pi i a)a/2\pi i] + O(1).$$
 (12)

Here  $R(a_{11})$  in order of magnitude represents the fluctuating number of points along the hypotenuse, LD (Fig. 2). For  $a-b=\epsilon \ll a$ ,  $\epsilon \gg 1$ ,

$$a_{11} = \frac{-\left[a \exp(2\pi i(b+b/2_a)) - b \exp(2\pi i(a+a/2b))\right]}{4\pi^2(a-b)} + O(1). \quad (13)$$

 $R(a_{11})$  is here a fluctuation of the order of the number of points along the segments  $DE \sim CE$  and  $FJ \sim FK$  of Fig. 2.

For the case  $b \gg a$  of Fig. 2, it can be shown that  $a_{10}$  is  $a_{10} = \left[ \frac{(b+1)}{2\pi i} + \frac{b}{4\pi i} +$ 

$$\frac{10 - \lfloor (0 + \frac{1}{2})/2\pi i \rfloor + (0/4a\pi i) \exp[2\pi i (a + a/2b)]}{- \lfloor b/a(2\pi i)^2 \rfloor + b/(4a\pi i).$$
(14)

Here  $R(a_{10})$  is a fluctuation of the order of the number of points along  $GB \sim GA$ . In all cases the periodicity and



amplitude are correctly given in order of magnitude and the geometrical interpretation is valid.

For closed curves which are concave and have either cusps or inflection points, we make also the reasonable conjecture that the coefficient  $a_{mn}$  has this same interpretation, that is, as the number of points just caught or missed as a periodic function of the displacement of the periphery of the curve. We assume that it is periodic in the normal distance of the tangent line from the origin, with a period determined by the spacing of the lattice lines, and of amplitude determined by the radius of curvature at the point of tangency, and the spacing (sagitta) of the lattice lines, just as for Kendall's oval. If no tangent can be drawn perpendicular to the direction of interest, we expect the corresponding coefficient  $a_{mn}$  to be small (see Fig. 3) and, if this tangent falls near an influection point, a detailed analysis of the curve will be necessary to determine how many points are just caught or missed over a range of the normal distance corresponding to the spacing of the lattice lines, just as in the case of the oval  $u^2x + v^4 \le x^2$ .

There is another sort of conclusion which can be inferred from Kendall's arguments. Consider a closed curve one side of which is straight, of length c, and lies somewhere in the space between two principal lattice lines. Kendall's formula applied uncritically for the error  $\sigma$  of order  $\rho_{\max}^{\frac{1}{2}}$  would indicate an infinite error, but if we replace the straight portion by an arc slightly rounded at the ends to provide a closed continuous convex curve, this arc being at most of unit sagitta, then the modified oval fulfills the criteria which Kendall requires and contains exactly the same set of lattice points as the original curve. We now apply Kendall's argument to the modified oval, for which  $\rho_{\max}^{\frac{1}{2}} \sim c$ , that is, the length of the flat portion. Thus, for such flat-sided curves the maximum error is approximately the length of the flat side. This fits quite satisfactorily the interpretation of the error as the number of points just caught or missed. It is also the amplitude of the largest periodic coefficient  $a_{10}$  of the modified oval.

There is a particular circumstance for such flat-sided ovals, however, for which this oscillatory term and the corresponding contribution to the error can be removed. Let us suppose we are considering a particular class of flat-sided ovals where the flat side always bisects the space between two principal lattice lines. Then the number of points inside this curve is exactly one-half the number contained in the completely convex figure obtained by reflecting the given curve in its flat side. To this figure, we can then apply Kendall's arguments for the closed continuous convex curve, rounding off corners without loss of lattice points where necessary, and the large term previously given by the flat side will not appear. These different possibilities are illustrated in Fig. 3 by dotted lines.

There is yet another inference which can be drawn from Kendall's conclusions which we use in our discussion of the electron gas. Kendall shows that the error in using the area as an estimate of the number of lattice points inside a curve is of order  $\rho_{\max}^{\frac{1}{2}}$  and also of the order of the square root of the perimeter. From this we infer that, given a number of different closed curves, each enclosing exactly the same set of lattice points, the one whose perimeter and maximum radius of curvature is least has an area which is the best estimate of the number of points inside. This argument will be useful in deriving the order of magnitude of the Landau and other non-oscillatory terms in the diamagnetism.

Based on the above geometrical interpretation of the results of number theory for closed curves lying in a plane, one can easily give the generalization for a three-dimensional figure. The volume of a slab or segment of unit thickness is of order  $(\rho_1\rho_2)^{\frac{1}{2}}$  where  $\rho_1, \rho_2$  are the principal radii of curvature. Then the number of points just caught or just missed as the solid grows is of order  $(\rho_1\rho_2)^{\frac{1}{2}}$ . If the surface is developable, that is, one of the principal radii of curvature is infinite, the other  $\rho$  finite, the error is of order  $\rho^{\frac{1}{2}}$ . This simply

442

means the number of points in a slab of unit thickness and dimensions corresponding to the finite radius of curvature  $\rho$  and the length of the longest straight line c which can be drawn in the surface. This expression can be generalized for different directions exactly as in the case of the *mn*th coefficient in the plane. Similarly, when the enclosed surface is bounded by a plane (both radii of curvature infinite) we can take the number of points in this plane as the amplitude and the normal to the plane will determine the coefficient to which it applies and the periodicity, which is the spacing of lattice planes parallel to this plane face. Also, if it should happen that for a particular class of closed surfaces with flat sides, the flat side bisects the space between two principal lattice planes, we may close off the surface symmetrically with respect to this flat side and apply our arguments to the resulting volume and then take one-half the result, exactly as we did for the closed curve in two dimensions.

If we admit the conclusion (generalizing Kendall's conclusion for a plane curve) that the error is least when  $(\rho_1\rho_2)_{\max}$  or the area is least for different surfaces containing the same set of points, we may bevel off any edges which do not contain lattice points in order to improve the accuracy of using the enclosed volume as a measure of the number of points inside. It is important in this case that in beveling off we do not remove any lattice points in the process. It should also be noted that beveling only removes an appreciable volume for acute angle edges. For obtuse angles the requirement that  $\rho$  be finite and continuous means that not much volume can be removed. The beveling only occurs over unit distance at most.

A few remarks should be made here concerning the sense in which the correction to the area as a measure of the number of points inside is to be taken. The first sense is that in which the closed curve lies at random in the plane of the lattice points. The second is that to be taken when the closed curve is one in a family of different sizes and of fixed position and orientation in the lattice plane. The error is then taken in the sense of the average error as the parameters specifying the size and shape of the different members of the family are varied. It is in this second sense of the error that we are primarily interested. General conclusions, such as have been drawn above concerning the error and the periodicity, usually apply to both conceptions, at least this seems plausible.

It may be mentioned that the exact meaning of the order of magnitude from the number theory standpoint is a question of considerable subtlety and complexity. We shall use it in what follows in the conventional sense, since it seems to apply well to the "average" order of magnitude of the error when the number of points inside is very large. For a more precise discussion we refer to the literature,<sup>17</sup> as the problem, although it has received much attention, has not yet been solved. There is reason for believing that the square root of the

radius of curvature as a correction may be exceeded for a denumerably infinite set of closed curves in the family. This may imply that the fluctuations in the magnetic moment in the derivation which follows are, from a number theory standpoint, upper limits of the order of magnitude of the moment which may not be exceeded except at discrete values of the Fermi energy  $E_0$  and magnetic field H.<sup>18</sup> It is difficult to ascribe physical significance to such isolated values.

## III. THE ENERGY LEVEL DISTRIBUTION FOR A FINITE CONTAINER

We now have the problem of using the above considerations to determine the number of energy levels less than any arbitrary energy  $E_a$  for a charged particle in a finite cylindrical box in a uniform magnetic field. This number is essential to determining the thermodynamic properties, in particular the magnetic moment, of a gas of such particles according to Fermi statistics. The Schrödinger equation for this problem is <sup>19</sup>

$$-(\hbar^2/2m)(\partial^2\psi/\partial r^2 + \partial\psi/r\partial r + \partial^2\psi/r^2\partial\theta^2 + \partial^2\psi/\partial z^2) -(i\hbar eH/2mc)\partial\psi/\partial\theta + V(r, z) +(mr^2/2)(eH/2mc)^2\psi = E\psi, \quad (15)$$

where V(r, z) is the scalar potential of the box. For the present we shall take

$$V(r, z) = V_r(r) + V_z(z),$$

where  $V_z(z) = V_z(-z)$ , and introduce the notation

$$V_z(L_z(E_a)) = E_a$$
, or  $L_z(E_a) = V_z^{-1}(E_a)$ ,

and, similarly,

$$R(E_a) = V_r^{-1}(E_a)$$

to denote turning points determined by the scalar potential where the kinetic energy vanishes for some arbitrary energy  $E_a$ . Under the assumption

$$\psi = \rho(r) \exp(il\theta)\zeta(z),$$

the Schrödinger equation separates and we have

$$-(\hbar^{2}/2m)(\rho''/\rho+\rho'/r\rho-l^{2}/r^{2})+\hbar eHl/2mc +V_{r}(r)+(mr^{2}/2)(eH/2mc)^{2}=E_{r}, \quad (16) -(\hbar^{2}/2m)\zeta''/\zeta+V_{z}(z)=E_{z}.$$

By definition the eigenvalue for the energy is

$$E = E_r(l, n) + E_z(n_z) = E(l, n, n_z).$$

We will use the WKB approximation in solving these equations where the radial quantum number is n, taking on values  $0, +1, +2, \cdots$ , and the  $n_z$  quantum number is  $n_z=0, +1, +2\cdots$ . The orbital quantum number l ranges through all permissible integral (+, - and 0) values for which  $E = E(l, n, n_z) \leq E_a$ , and satisfies the requirement that the radial WKB integrand be real, and with real limits of integration. If we introduce the

<sup>&</sup>lt;sup>18</sup> There is a discussion of a class of these discrete values by M. C. Steele, following paper [Phys. Rev. **88**, 451 (1952)], Eq. (52).

<sup>&</sup>lt;sup>19</sup> C. G. Darwin, Proc. Cambridge Phil. Soc. 27, 86 (1931).

notation  $2mE(l, n, n_z)/\hbar^2 = k^2$ ,  $2mE_a/\hbar^2 = k_a^2$ ,  $2mE_0/\hbar^2$  $=k_0^2$ ,  $2mE_z(n_z)/\hbar^2 = k_z^2(n_z)$ ,  $L = (\hbar c/eH)^{\frac{1}{2}}$  (approximately the radius of the smallest quantized orbit in field H), and the radial equation can be written, substituting  $E_r = E(l, n, n_z) - E_z$ , and  $\rho(r) = u(r)/r^{\frac{1}{2}}$ ,

$$\frac{d^2u/dr^2 + (k^2 - 2mV_r(r)/\hbar^2 - k_z^2(n_z) - l^2/r^2}{-r^2/4L^4 - (l/L^2) + 1/4r^2}u = 0, \quad (17)$$

$$d^{2}\zeta/dz^{2} = -(k_{z}^{2}(n_{z}) - (\hbar^{2}/2m)V_{z})\zeta.$$
(18)

In accordance with the arguments of Kemble<sup>20</sup> and Kramers<sup>21</sup> in applying the WKB method in polar coordinates, one drops the  $1/4r^2$  term in Eq. (17) so that the radial quantum number is given by

$$n = (1/\pi) \int_{r_l}^{r_u} (k^2 - 2mV_r(r)/\hbar^2 - k_z^2(n_z)) - (l^2/r^2) - (r^2/4L^4) - l/L^2)^{\frac{1}{2}} dr - \frac{1}{2}, \quad (19)$$

and the z quantum number by [this determines  $k_z(n_z)$ ]

$$n_{z} = (1/\pi) \int_{z_{l}}^{z_{u}} (k_{z}^{2}(n_{z}) - \hbar^{2} V_{z}(z)/2m)^{\frac{1}{2}} dz - \frac{1}{2}, \quad (20)$$

where the subscripts u, l indicate the coordinates where the integrands of (19) or (20) vanish. We can solve for them explicitly when we know  $V_r(r)$  and  $V_z(z)$ .

We now have the problem of counting all the possible eigenvalues of  $E = E(l, n, n_z)$  (determined by combined solutions for E and  $E_z$  from Eqs. (19) and (20) less than some arbitrary  $E_a$ ). Since the quantum numbers  $n, l, n_z$  are integers, an estimate of this number of states according to number theory, is the volume in quantum number space  $(n, l, n_z \text{ considered as con-}$ tinuous variables) enclosed by the surface  $E(l, n, n_z) \leq E_a$ and the planes  $n_z = -\frac{1}{2}$  and  $n = -\frac{1}{2}$ . On these planes the upper and lower limits of coordinate integration in Eqs. (19) and (20) come together. According to our previous discussion, this is just one-quarter of the volume and encloses one-quarter of the points of a figure closed



FIG. 4. Strong field case.  $L^2k_a/R < 1$ . Region of integration where the radial WKB integrand is real for fixed  $n_s$ . Inner parabolas are for different  $n_z$  (dotted).

<sup>20</sup> E. C. Kemble, The Fundamental Principles of Quantum Mechanics (McGraw-Hill Book Company, Inc., New York, 1937), p. 107. <sup>21</sup> H. A. Kramers, Z. Physik **39**, 828 (1926).

symmetrically about these planes. Let us call this (quarter) volume in quantum number space  $V(E_a)$ . We may subsequently improve it as an estimate of  $G(E_a)$ , the number of *integer* coordinates n, l,  $n_z$  inside, by beveling off its sharp edges and subtracting the volume so removed from  $V(E_a)$ , and by adding periodic terms based on the dimensions and curvatures of the surface  $E(l, n, n_z) = E_a$ . So we have for  $V(E_a)$ ,

$$V(E_a) = \int_{n_x = -\frac{1}{2}}^{n_{xu}} \int_{l_1}^{l_u} \int_{n_z = -\frac{1}{2}}^{n_u} dn_z dl dn, \qquad (21)$$

where subscripts u, l refer to upper and lower limits. The question now is what are the limits of integration, which are not required to be integers. Being a volume integral, these limits will depend on the order of integration; however, if we integrate on n first, the upper limit on n is just Eq. (19) with k replaced by  $k_a$ . So integrating on dn in Eq. (21), we have, as the  $\frac{1}{2}$  terms cancel,

$$V(E_a) = \int_{n_a=-\frac{1}{2}}^{n_{zu}} \int_{l_l}^{l_u} \frac{1}{\pi} \int_{r_l}^{r_u} (-l^2/r^2 - r^2/4L^4 + k_a^2) \\ -2mV_r(r)/\hbar^2 - k_z^2(n_z) - l/L^2)^{\frac{1}{2}} dr. \quad (22)$$

To integrate further, as we still have a triple integral, we refer to Fig. 4, where the WKB integrand is plotted as a function of  $r^2$  and l. In the form given by Eq. (22) above, it is seen that  $V(E_a)$  is just the integral of the radial WKB integrand over all regions of r, l,  $n_z$  space where this integrand is real. The value of  $n+\frac{1}{2}$  corresponds to the integration on r along paths such as DB, FM, or HK in Fig. 4. The lower and the upper points of the curve correspond to  $r_l$ , and  $r_u$  of Eq. (19).

If we actually carry out the r integration, and compute  $n+\frac{1}{2}$  before proceeding with the  $n_z$ , *l* integrals, it will be necessary to divide the region of Fig. 4 into two parts, to the left and right of GL, corresponding to whether the upper limit of r is determined by the wall of the box [scalar potential  $V_r(r)$ ] or the vector potential of H. However, since the total expression Eq. (22) is still just a multiple intergal on r, l, and  $n_z$ , we may integrate in any order we like so long as we cover the same region, and we may write it as follows:

$$V(E_{a}) = \int_{n_{z}=-\frac{1}{2}}^{n_{zu}} dn_{z} \int_{r=0}^{V_{r}^{-1}[E_{a}-E_{z}(n_{z})]} dr \frac{1}{\pi} \\ \times \int_{l=-(r^{2}/2L^{2})}^{-(r^{2}/2L^{2})+r[k_{a}^{2}-(2mV_{r}(r)/\hbar^{2})-k_{z}^{2}(n_{z})]^{\frac{1}{2}}} Y dl, \qquad (23)$$
$$Y = (-(l^{2}/r^{2})-(r^{2}/4L^{4}) \\ +k_{a}^{2}-(2mV_{r}(r)/\hbar^{2})-k_{z}^{2}(n_{z})-(l/L^{2}))^{\frac{1}{2}}.$$

These lower and upper limits on l correspond in Fig. 4 to JLA and ACG, respectively,  $l = -r^2/2L^2$  corresponds to *IA*. Or, with  $l' = l + (r^2/2L^2)$ :

$$V(E_{a}) = \int_{n_{z}=-\frac{1}{2}}^{n_{zu}} dn_{z} \int_{r=0}^{V_{r}^{-1}[E_{a}-E_{z}(n_{z})]} dr$$

$$\times \int_{l'=-r[k_{a}^{2}-(2mV_{z}(z)/\hbar^{2})-k_{z}^{2}(n_{z})]^{\frac{1}{2}}} V'dl', \qquad (24)$$

$$V' = [k_{a}^{2}-(2mV_{r}(r)/\hbar^{2})-k_{z}^{2}(n_{z})-l'^{2}]^{\frac{1}{2}}/r.$$

With this order of integration,  $n_{zu}$  is given by the largest value it can obtain, for  $E_r = 0$ .

$$n_{zu} = \frac{1}{\pi} \int_{z = -V_z^{-1}(E_a)}^{+V_z^{-1}(E_a)} \left[ k_a^2 - (2mV_z(z)/\hbar^2) \right]^{\frac{1}{2}} dz - \frac{1}{2}.$$
 (25)

Integrating on  $n_z$  corresponds to adding the contributions of successively smaller parabolas (dotted) of Fig. 4.

All of this is independent of whether the field is strong or weak and whether the box is large or small, so long as the box potential is separable in r and z. Note, and this is the important point, that this  $V(E_a)$ , Eq. (24) or (26), is actually independent of the magnetic field. Hence, if used by itself as an estimate for  $G(E_a)$ , it will give no contribution to the magnetic moment (which involves a differentiation with respect to H) whatever. The only terms which can contribute to the moment will be oscillatory terms, depending on the curvatures of the energy surface or small corrections which may arise if we find we can snip off small edges of the "Fermi volume" without loss of quantum numbers, these oscillatory and subtractive terms being essentially the improvements on  $V(E_a)$  as an estimate of  $G(E_a)$ . It can be shown that this conclusion also holds using the higher corrections to the WKB approximation given by Dunham,<sup>22</sup> as the field dependent terms disappear with the same substitution  $l \rightarrow l'$  which removed them above.

From Eq. (24) we have

$$V(E_a) = \int_{n_z = -\frac{1}{2}}^{n_{zu}} dn_z \int_{r=0}^{V_r^{-1}[E_a - E_z(n_z)]} \times [k_a^2 - k_z^2(n_z) - 2mV_r(r)/\hbar^2] r dr. \quad (26)$$

We cannot proceed with our integral without definite assumptions concerning the potentials  $V_r(r)$ ,  $V_z(z)$ since  $k_z$  depends on  $n_z$  through Eq. (20). However, if we assume the simplest of all potentials, a simple well in r and z, so that

$$V_{r}(r) = 0, \quad r < R,$$
  
=  $M > E_{a}, \quad r > R;$   
 $V_{z}(z) = 0, \quad -L_{z}/2 < z < +L_{z}/2,$   
=  $M > E_{a}, \quad |z| > L_{z}/2;$ 

then, for all  $E_a < M$ , the turning points, when they



FIG. 5. Energy surface in quantum number space for strong fields.

occur at the walls, are constants, and we have<sup>23</sup>

$$k_{z}(n_{z}) = (n_{z} + \frac{1}{2})\pi/L_{z},$$

$$V(E_{a}) = \int_{n_{z} = -\frac{1}{2}}^{k_{a}L_{z}/\pi - \frac{1}{2}} (R^{2}/4) [k_{a}^{2} - (n_{z} + \frac{1}{2})^{2}\pi^{2}/L_{z}^{2}] dn_{z} \quad (27)$$

$$= (4\pi/3)(\pi R^{2}L_{z})(2mE_{a})^{\frac{1}{2}}/\hbar^{3}.$$

This is just the formula for the number of levels less than  $E_a$  in the absence of a magnetic field.

The disadvantage of integrating first on r and thus computing n directly is that it can be done exactly for paths BD or FM, but a series expansion which will depend on H is necessary to get it in a tractable form for subsequent integrations on l and  $n_z$  for paths such as HK. The paths DB, FM, HK correspond respectively to orbits which encircle the origin, interior orbits which do not encircle the origin, and surface states, or orbits which touch the wall. Hence, any errors committed by dropping terms in the expansion for the surface states will just appear as an H dependence of  $V(E_a)$  in the final result, which could be carried out exactly by integrating first on l and then on r.

It will be seen that it is essential to include the states of positive l to get a total  $V(E_a)$  independent of H, so that the calculations of Van Vleck,<sup>5</sup> who computed surface states but neglected the states of positive l, must have been in error by just an amount sufficient to compensate for the omission of positive l states. Similarly, this writer's calculations<sup>6</sup> were also in error.

In order to apply the corrections, both periodic and those due to edges and cusps in the surface, let us plot the energy surface in quantum number space. To do this it will only be necessary to represent specific regions of the surface accurately, since we know its overall volume, Eq. (27). This energy surface plot is given in Fig. 5. The portion of the surface MHDCB, which corresponds to integrating on r to compute n in

<sup>&</sup>lt;sup>22</sup> J. L. Dunham, Phys. Rev. 41, 713, 721 (1932).

<sup>&</sup>lt;sup>23</sup> The use of the WKB relation between  $n_z$  and  $E_z$  instead of an exact relation which could here be obtained will not alter any of the conclusions which follow.



FIG. 6. Energy surface in quantum number space for weak fields.

the region GLMACF of Fig. 4, can be expressed exactly and is

$$n = (1/\pi) \{ (L^2 k_a^2/2) - \pi^2 L^2 [(n_z + \frac{1}{2})^2/2L_z^2] - l - |l| \} - \frac{1}{2}.$$
(28)

This is valid for all l greater than the l coordinate of the line GM of Fig. 5, which is

$$\begin{split} l &= -R^2/2L^2 + R \big[ k_a^2 - (n_z + \frac{1}{2})^2 \pi^2/L_z^2 \big]^{\frac{1}{2}} \\ &- R^2/2L^2 \text{ is the ``length'' of } DH, \\ &\pm R \big[ k_a^2 - (n_z + \frac{1}{2})^2 \pi^2/L_z^2 \big]^{\frac{1}{2}} \end{split}$$

corresponds to MHL measured from a plane through OH perpendicular to the l axis. The cusp-shaped region MLH which corresponds to the region GLJ of Fig. 4, or surface states, is given approximately by

$$n \simeq \{ L^2 [k_a^2 - (n_z + \frac{1}{2})^2 \pi^2 / L_z^2] / 2\pi \} \times [x(1 - x^2)^{\frac{1}{2}} - \sin^{-1}x + \pi/2] + O(a) - \frac{1}{2}.$$
(29)

Here  $a = L^2 [k_a^2 - (n_z + \frac{1}{2})^2 \pi^2 / L_z^2] / R < 1$  for validity of approximations  $x = (l'' - a) / (1 - 2al'' + a^2)^{\frac{1}{2}}$ , where

$$\begin{split} l'' &= (l + R^2/2L^2)/R[k_a^2 - (n_z + \frac{1}{2})^2 \pi^2/L_z^2]^{\frac{1}{2}}, \\ &x \simeq (l - R^2/2L^2)/R[k_a^2 - (n_z + \frac{1}{2})^2 \pi^2/L_z^2]^{\frac{1}{2}} < 1. \end{split}$$

These are obtained by integrating Eq. (19) with  $r_u = R$ , and using the transformations of Eq. (29).

If we like, in order to justify applying our arguments to number theory, we may imagine Fig. 5 to be extended by reflection in the  $n = -\frac{1}{2}$  and  $n_z = -\frac{1}{2}$  plane. We can then expect that the largest periodic corrections arise from the ruled surfaces *BMHD* and *BDC* and that there will be nonperiodic corrections based on rounding off the edges *DH* and *HLDC*. There is no edge at all at *CBML* when reflection occurs at  $n_z = -\frac{1}{2}$ , and we cannot smooth off the edge *BD* without losing lattice points as the quantum states at l=0 are good quantum states.

Let us consider these various corrections. We shall compute them in order of magnitude only, although in most cases exact evaluation of the integrals gives a quite good estimate of the numerical coefficients required. Exact evaluation is best carried out by the number theory development of the correction terms as performed by Steele using the method of critical points.<sup>24</sup> In fact, the quantitative evaluations which follow can be regarded just as geometrical interpretations of the critical point method.

Consider first the edge *DH*. At this edge we may approximately subtract from the total volume without loss of lattice points a triangular prism of length  $DH = R^2/2L^2$ , of base  $EF = \frac{1}{2}$ , and of height

$$(dn_z/dn)_{n=0} \cdot (\Delta n = \frac{1}{2})$$

We say "approximately subtract" since the remaining figure must have a surface of continuous curvature, by our previous number theory discussion. Figure 5 for strong fields has  $(dn_z/dn)_{n=0}\gg1$ , so that this approximation is valid. As the field gets weaker the edge *DH* is less acute, and this approximation is less valid. When this edge approaches 90°, it may fail completely (Fig. 6). In so doing we improve the estimate of the volume as a measure of the total number of lattice points, since we reduce the total surface area and also the region removed is one of large radius of curvature (it increases with  $n_z$  on the Fermi surface). Thus the net volume removed is

$$\delta V_{-L} \sim -\frac{1}{2} (L_z/L^2 k_a) (R^2/2L^2)(\frac{1}{2}). \tag{30}$$

The corresponding contribution to the moment at  $T=0^{\circ}$  is, for  $E_0=$  Fermi energy,

$$M_{L} = (\partial/\partial H) \int_{0}^{E_{0}} \delta V_{-L}(E_{a}) dE_{a} \simeq -\pi R^{2} L_{z} E_{0}/L^{4} k_{0} H$$
$$= O[-\pi R^{2} L_{z} e^{2} H E_{0}^{\frac{1}{2}}/\hbar c m^{\frac{1}{2}}]. \quad (31)$$

This is the order of magnitude of the Landau moment and is diamagnetic.

Consider next the contribution of the surface states to the moment, which we may obtain by removing without loss of lattice points a thin strip of thickness  $\Delta n = \frac{1}{2}$  (from  $n = -\frac{1}{2}$  to n = 0) along the edge *HL*. In order to find its dimensions  $\Delta l$ , as a function of l and  $n_z$ (Fig. 5), we must find an expression for the quantum number *n*, valid for small ranges of *n*, that is  $(n+\frac{1}{2}) < \frac{1}{2}$ (near *J* of Fig. 4). This we may obtain from Eq. (19) (with r = R) as follows:

Let  $\Delta l$  be the distance in l from the line HL of Fig. 5, so that

$$l = (-R^2/2L^2) - R \lceil k_a^2 - (n_z + \frac{1}{2})^2 \pi^2 / L_z^2 \rceil^{\frac{1}{2}} + \Delta l. \quad (32)$$

If we substitute this expression for l in Eq. (19) and expand in terms of  $\Delta l$  keeping only the smallest powers, we find after considerable manipulation, and writing  $(n_z+\frac{1}{2})^2\pi^2/L_z^2 = k_z^2(n_z)$ , as for Eq. (27)

$$n = (1/\pi R^{\frac{3}{2}}) \{ L^2 [k_a^2 - k_z^2(n_z)] (2\Delta l)^{\frac{3}{2}} \} [1 + O(a)] - \frac{1}{2}.$$
(33)

This reaches the value n=0 at

$$\Delta l = O\{R/L^{4/3} [k_a^2 - k_z^2(n_z)]^{1/6}\}.$$
(34)

The length of the strip HL is  $\sim L_z k_a/\pi$  (largest  $n_z$ )  $\xrightarrow{^{24}$  J. G. van der Corput, Amsterdam Roy. Acad. Sci. 51, 650 (1948). value) so that the volume removed is of order

$$\delta V(E_a)_{\text{surf}} = -\int_{n_z = -\frac{1}{2}}^{L_z k_a / \pi - \frac{1}{2}} dn_z \int_{\Delta l = 0}^{\Delta l = \text{Eq. (34)}} d(\Delta l) \\ \times \int_{n = -\frac{1}{2}}^{n = \text{Eq. (33)}} dn \quad (35) \\ = -O(RL_z k_a^{2/3} / L^{4/3}),$$

and the contribution to the moment at  $T=0^{\circ}$  is of order

$$\begin{split} M &= (\partial/\partial H) \int_{0}^{E_{0}} \delta V(E_{a})_{\text{suri}} dE_{a} \\ &= O(RL_{z}k_{0}^{2/3}/L^{4/3})(E_{0}/H) \\ &= -O(\pi R^{2}L_{z} \cdot m^{1/3}e^{2/3}E_{0}^{4/3}/R\hbar^{4/3}c^{2/3}H^{1/3}), \end{split}$$
(36)

valid for  $k_0 L^2/R < 1$ . This is the order of magnitude of the surface diamagnetism previously reported,<sup>25</sup> and found by Steele using the method of critical points. Here again a numerical evaluation of the exact volume between  $n = -\frac{1}{2}$  and 0 and the limits on  $\Delta l$  in this edge would give a fair value of the numerical coefficient required in Eq. (36). It is considerably less than unity, as the edge HL is quite "thin," varying as  $(\Delta l)^{\frac{3}{2}}$ .

Finally we have the edge CD, which is actually a right angle in Fig. 5, completed by reflection in the plane  $n = -\frac{1}{2}$ . The maximum volume that could be removed along this edge without loss of lattice points is of order  $(\frac{1}{2})(L_z k_a/\pi)(\frac{1}{2})$ . This is independent of the magnetic field and hence can make no contribution to the moment, considered as a correction to  $V(E_a)$ .

We now have to consider periodic terms [see Eq. (6)] corresponding to the direction (1, 0, 0) in Fig. 5. Consider first a slab of unit sagitta as having a radius of curvature of order  $1/(d^2n/dn_z^2)n_z=0$ , of length  $BM = AO - OP = R^2/2L^2 - Rk_a$ . The distance of the tangent plane from the origin is  $AB = L^2k_a^2/2$ , so that

$$\delta V(E_a)_{1, 0, 0} \simeq (d^2 n/dn_z^2)_{n_z=0}^{-\frac{1}{2}} (R^2/2L^2 - Rk_a) \\ \times \cos 2\pi (k_a^2 L^2/2 - \varphi).$$

Using  $(d^2n/dn_z^2)_{n_z=0} = L_z/\pi L$ , and calculating the moments from  $\delta V(E_a)_{1,0,0}$  as in Eqs. (31), (35) we find at T=0

$$M_{1,0,0} \simeq (L_z/\pi L) (R^2/2L^2 - Rk_0) \cdot \{ [\partial (k_a^2 L^2/2) / \partial H] E_a = E_0 / [\partial (k_a^2 L^2/2) / \partial E_a] E_a = E_0 \} \cdot \cos 2\pi (k_0^2 L^2/2 - \varphi). \quad (37)$$

The expression in brackets implies the approximation that the last oscillation of the sinusoid determines its integral, and that the sinusoid contributes the major part of  $\partial/\partial H$ . In other words, this contribution to the moment is the effect of the Fermi surface just catching or missing a lattice plane in quantum number space. In

<sup>25</sup> M. F. M. Osborne and M. C. Steele, Phys. Rev. 86, 247 (1952).

terms of physical constants, Eq. (37) becomes

$$M_{1,0,0} = O(\pi R^2 L_z e^{\frac{3}{2}} H^{\frac{1}{2}} / c^{\frac{3}{2}} h^{\frac{3}{2}}) \cos(2\pi m E_0 c / \hbar e H - \varphi) - O(L_z R e^{\frac{1}{2}} m^{\frac{1}{2}} E_0^{\frac{3}{2}} / \hbar c^{\frac{1}{2}} H^{\frac{1}{2}}) \cos(2\pi m E_0 c / \hbar e H - \varphi).$$
(38)

This is just the order of magnitude of the leading term in the de Haas-van Alphen effect (1st term) and the surface correction (2nd term) thereto found by Steele.

In the direction (1, 1, 0), Fig. 5, the lattice planes are  $1/\sqrt{2}$  apart. The distance of the tangent plane (to ruled surface BCD) is  $BA/2^{\frac{1}{2}} = (\frac{1}{2}L^2k_a^2/\sqrt{2})$ . The radius of curvature in the section perpendicular to BC is  $\sim (d^2n/dn_z^2)_{n_z=0}^{-1}$  as before.  $BC = L^2k_a^2/\sqrt{2}$  so that the fluctuating correction to the volume  $V(E_a)$  is

$$\delta V(E_a)_{1,1,0} \sim (L_z/\pi L) (k_a^2 L^2/2^{\frac{3}{4}}) \\ \times \cos[2\pi (km^2 L^2/2)(\sqrt{2}/\sqrt{2}) - \varphi],$$

and the contribution to the moment at  $T=0^{\circ}$ ,

$$M_{1,1,0} = O(L_z m E_0^2 c^{\frac{1}{2}} / e^{\frac{1}{2}} \hbar^{\frac{3}{2}} H^{\frac{3}{2}}) \cos(2\pi m E_0 c / \hbar e H - \phi).$$
(39)

It will be seen that the terms contributing to the moment in Eqs. (38) and (39) are in relative order of magnitude like unity,  $L^2k_0/R$ ,  $L^4k_0^2/R^2$ . Thus, as the field gets weaker  $(L^2k_0/R\sim 5/HR)$  they approach the same order of magnitude, and are equal just when this description of the quantum states fails and we consider the field to be weak instead of strong.

Note that if we pick directions such as (1, 0, 1) in Fig. 5, where the slope  $dn_z/dn=1$  of the tangent plane is less than  $(dn_z/dn)_{n=0} \sim L_z/L^2k_a \sim L_zH/5$ , there is no tangent plane which can be drawn except at the artificially-rounded edge DH which contributed the Landau diamagnetism. This is to say the periodic correction terms corresponding to these directions are small in agreement with Steele's findings.<sup>18</sup>

In the direction (1, -1, 0) where the curve is both concave and convex, a detailed analysis of the region of the inflection points will be required. However, since MJL is a curve, it does not seem possible for the number of points just caught or missed to be as large as those on the straight edges BM or CB, evaluated above, hence the correction  $\delta V_{1,-1,0}(E_a)$  and the moment will be correspondingly smaller.

If we consider the shape which the Fermi surface obtains as the magnetic field weakens, it can be seen that the developable portion MBDH gets smaller while the region of surface states and those of positive l get larger until the turning points for orbits of energy  $E_0$ (at the top of the Fermi sea) are no longer determined



FIG. 7." Region for integration of the WKB radial integrand for weak fields.  $L^2k_a/R>1$ ,

by the vector potential but by the wall. The Fermi surface ultimately approaches that of Fig. 6. The diagram for the WKB integration corresponding to Fig. 6 is given in Fig. 7. There are two points to be noted, however. For small values of  $k_a^2 - k_z^2(n_z)$ , region QPRBA of Fig. 6 (see the dotted parabola of Fig. 7), the figure still preserves the character of the strong field surface. Second, surfaces interior to the given surface of Fig. 6 approach the shape of Fig. 5. This simply means that as the orbital component of energy and hence radius of orbit is small compared to the container dimensions, Fig. 5 still applies.

If we examine the Fermi surface shown in Fig. 6, we see along the edges KQ and HB volume may be removed without loss of lattice points. We can evaluate  $n+\frac{1}{2}<\frac{1}{2}$  for small powers of  $\Delta l$  using

$$l = -R^2/2L^2 \pm R[k_a^2 - k_z^2(n_z)]^{\frac{1}{2}} \mp \Delta l,$$

where  $\Delta l$  is the distance in *l* from the edges *KA* and *AH*. As before, to do this we write Eq. (19) in the form

$$n + \frac{1}{2} = (1/\pi) \int_{r_l}^{R} (1/r) [(r^2 - r_l^2)(r_u^2 - r^2)/4L^4]^{\frac{1}{2}} dr, \quad (40)$$

and denote by  $r_{u+}$ ,  $r_{l+}$ ,  $r_{-u}$ ,  $r_{l-}$  the roots of the integrand for positive and negative values of l, corresponding to paths JK and LM of Fig. 7 for small quantum numbers n. These are given in Eq. (41) in terms of

$$1/a = R/L^2 [k_a^2 - k_z^2(n_z)]^{\frac{1}{2}} < 1.$$

 $n_+$  and  $n_-$  indicate the values of *n* for these paths. In Eq. (42), as before, we have  $k_z(n_z) = (n_z + \frac{1}{2})\pi/L_z$  and also define  $\xi$  as  $k_a^2 - k_z^2(n_z)$ .

$$r_{u, l^{\mp}}^{2} = 4L^{4}\xi(1+1/4a^{2}\pm1/a\cdots),$$
  

$$r_{L, l^{\mp}}^{2} = R^{2}[1-(2\Delta l/\xi^{\frac{1}{2}}R)(1\pm1/a+1/a^{2}\cdots)].$$
(41)

Ultimately, we find for n in the neighborhood of the edges KO and RH

$$(n+\frac{1}{2})_{\pm} = n_{\pm}' = R^{-\frac{1}{2}} \xi^{-\frac{1}{4}} (\Delta l)^{\frac{3}{2}} (1 \pm 1/a + 1/a^2) / 3\pi.$$
(42)

If we integrate  $dnd(\Delta l)dn_z$  over values of n for which  $O < n + \frac{1}{2} < \frac{1}{2}$  and the corresponding values of  $\Delta l$  and  $n_z$  given by Eq. (42), we can find the net volumes  $\delta V(E_a)_{\pm}$  of the two edges. We indicate by  $\Delta l_{\pm \frac{1}{2}}$  the values of  $\Delta l$  for which  $n_{\pm}' = \frac{1}{2}$ , from Eq. (42).

$$-\delta V(E_a)_{\pm} = \int_{n_z = -\frac{1}{2}}^{n_z \lesssim L_z k_a/\pi - \frac{1}{2}} \int_{\Delta l = 0}^{\Delta l + \frac{1}{2}} \int_{n+'=0}^{n+'} dn_z d\Delta l dn_{+'} + \int_{n_z = -\frac{1}{2}}^{n_z \lesssim L_z k_a/\pi - \frac{1}{2}} \int_{\Delta l = 0}^{\Delta l - \frac{1}{2}} \int_{n-'=0}^{n-'} dn_z d\Delta l dn_{-'}.$$

On integrating and combining terms of the same order of magnitude, we find

$$-\delta V(E_a)_{\pm} = O(R^{1/3}R_a{}^{4/3}L_z) + O(R^{7/3}L_z/L^4k_a{}^{2/3}). \quad (43)$$

Note that the second term of Eq. (43) which is the

contribution of the term in  $1/a^2$  in Eq. (42) is the only term containing the magnetic field and hence the only part of the volume which can contribute to the moment; the terms in 1/a of Eq. (42) canceled out. If we evaluate the contribution to the moment at  $T=0^\circ$ , we have

$$\delta M_{\pm} = (\partial/\partial H) \int_{0}^{E_{0}} \delta V(E_{a})_{\pm} dE_{a}$$
$$= O(e^{2}R^{1/3}E_{0}^{2/3}H/h^{4/3}c^{2}n^{1/3}) \cdot \pi R^{2}L_{z}, \quad (44)$$

valid for  $k_0 L^2/R > 1$ . This is the order of magnitude of the Dingle diamagnetism.<sup>12</sup>

The derivation is valid to the extent that the energy surfaces  $(E_a)$  over which we integrated, Eq. (44), are represented by Fig. 6. Since interior surfaces approach Fig. 5, these would contribute a different moment corresponding to Eq. (36) with smaller effective  $E_0$ . If, for example,  $k_0L^2/R=2$ ,  $\frac{7}{8}$  of the volume is represented by energy surfaces like Fig. 6,  $\frac{1}{8}$  by Fig. 5, and Eq. (44) is valid to, say, 12 percent. For this reason the volume integral of Eq. (43) is carried out in order of magnitude only.

Exact evaluation will show that the numerical coefficient required in (44) is considerably less than 1, as the "edges" *BH* and *QK* are rather "thin" in the *n* direction, varying like  $(\Delta l)^{\frac{3}{2}}$ , as was also the case for the surface diamagnetism in the case of strong fields. As was previously reported,<sup>25</sup> the two types of moment go into each other as the field changes from strong to weak, as is indeed evident when we consider the regions of their origin in the Fermi volume. As before, in the case of strong fields, the edge *AL* at l=0 cannot be removed without loss of lattice points.

Although the analytic expression for surface in the region of the Landau edge AB is exactly the same as it was for the strong field case, we can no longer with certainty bevel off and conclude that there is also a term giving the Landau diamagnetism. The reason for this is that the Landau edge is now no longer an acute angle but a rather obtuse one, so that if we remember that we must bevel off to a surface which has a continuous radius of curvature not larger than the largest already present, not much volume can be removed. Surfaces considerably interior to that of Fig. 6, since they approach Fig. 5, would have an acute Landau edge, and these would contribute to a Landau-like term in the integral over  $dE_a$  giving the moment. In any event, the Landau diamagnetism is considerably smaller than that given by Eq. (44), and for some conditions<sup>24</sup> may be smaller than the surface diamagnetism of Eq. (36).

We would now like to estimate the order of magnitude of periodic terms corresponding to the directions (1, -1, 0) and (1, 1, 0), Fig. 6. Although the surface is saddle-shaped in these two directions, we still take, as was mentioned seemed plausible, the product of the square root of the two radii of curvature as an estimate of the number of points just caught or missed in these directions. Since the dimensions of the figure along the lines OH and OK are

$$Rk_{a}[1\pm O(R/L^{2}k_{a})], R/L^{2}k_{a}<1 \ (l, \text{ at } n-\frac{1}{2}),$$

whereas the distance OL is

$$Rk_a(1-O(R/L^2k_a)^2)$$
.  $(n+\frac{1}{2}, \text{ at } l=0),$ 

we can expect that the distance to the tangential plane in the direction 1, 1, 0, or 1, -1, 0 is in order of magnitude

$$(Rk_a/2^{\frac{1}{2}})[1\pm O(R/L^2k_a)].$$

The radii of curvature (one positive, one negative) are in order of magnitude  $(d^2n/dl^2)n_z=0^{-1}$  and either  $(d^2l/dn_z^2)n_z=0^{-1}$  or  $(d^2n/dn_z^2)n_z=0^{-1}$  which are, respectively,  $O(Rk_a)$  and  $O(L_z^2k_a/R)$ .

Hence, the periodic correction to V(E) is of the order of magnitude

$$\delta V(E_a) \sim (Rk_a)^{\frac{1}{2}} (L_z^2 k_a/R)^{\frac{1}{2}} \\ \times [\cos\{2\pi Rk_a(1 \pm R/L^2 k_a) - \varphi\}].$$
(45)

This contributes to the moment, for  $T=0^{\circ}$ ,

$$M = O(E_0 e/Rhc) \cos\{2\pi [R(2mE_0)^{\frac{1}{2}}/\hbar] \\ \times [1 \pm ReH/c(2mE_0)^{\frac{1}{2}}] - \varphi\} \cdot \pi R^2 L_z.$$
(46)

This is in agreement with the form and order of magnitude of periodic terms found by Dingle.<sup>26</sup> All the physical parameters appear correctly, but the period given by Dingle's leading term is three times as great. However, our analysis could not be expected to give this degree of accuracy. Note that in Eq. (46) if R is small, say 10<sup>-6</sup> cm, this term fluctuates so slowly with magnetic field that it might almost be interpreted as a constant moment of most uncertain sign.

We may also apply the above analysis to the parabolic potential given by Darwin.<sup>19</sup> The Fermi surface in Darwin's notation is shown in Fig. 8. If we identify as the "volume" of Darwin's parabolic well  $\pi R_0^2 L_z$ , where  $R_0$  is the radius at which the scalar potential of the wall is equal to the Fermi energy  $E_0$ , then it can easily be shown that the edge DK contributes a moment of the order of the Landau moment  $M_L$ . The nose KLM, which lies entirely between the planes  $n+\frac{1}{2}=0$ and  $n+\frac{1}{2}=\frac{1}{2}$ , contributes  $M_L \cdot 1/Lk_0 = M_L (eH/\hbar c)^{\frac{1}{2}}$  $(\hbar/(2mE_0)^{\frac{1}{2}})$ , i.e., considerably smaller, except for very large fields (in striking contrast to the contribution of the surface states for the cylindrical box.) The oscillatory terms corresponding to the directions 1, 1, 0 and 1, 0, 0 can easily be evaluated (see Fig. 2) and are smaller than their counterparts for the cylindrical box potential.

These differences between the box and parabolic well are not surprising, as all the states in a parabolic well potential are in a sense surface states to some degree, whereas for the box a significant distinction can be made between those states which do and those which



FIG. 8. Energy surface for the Darwin potential.

do not touch the wall. A 1/r or  $\exp(-kr)$  potential box (atomic system) might give still different results.

### IV. DISCUSSION

If we consider the application of these ideas to a real metal of shape other than a cylinder, it seems plausible to believe that expressions for the Landau diamagnetism, the de Haas-vanAlphen effect, and certainly the surface diamagnetism for strong fields will still apply. The surface diamagnetism is essentially a consequence of the quantization of orbits which intersect the wall, and if the radius of curvature of this orbit is small compared to the radius of curvature of the surface, it can be considered as plane, and Steele's result for the cubical box and the results of this paper for a cylindrical box are in agreement, so that one can expect that for any surface whose radius of curvature is large compared to that of the quantized orbits considered, the same result will apply.

Moreover, we can also expect that the introduction of a finite surface potential spread over a finite distance will not essentially alter these results, so long as the thickness of the surface layer is small compared to the radius of the orbit or the dimensions of the box. Since the thickness of the surface layer has been estimated at from  $10^{-6}$  to  $10^{-3}$  cm, one can expect that for most magnetic fields and particles not too small this can be regarded as a surface of zero thickness and the above results for a rectangular well potential will still apply.

It is evident from all of the foregoing discussion that the observed fluctuations in the magnetic moment according to the de Haas-van Alphen effect can always be interpreted as a Fermi surface just catching or just missing the lattice points or quantum states of a plane as the magnetic field changes the shape but not the volume of the Fermi surface. Moreover, the nonperiodic contributions to the magnetic moment follow from the fact that the Fermi surface can be shrunk, without loss of lattice points, into a figure of smaller surface area and smaller radius of curvature.

It should be possible to conclude from observation

<sup>&</sup>lt;sup>26</sup> R. B. Dingle, Proc. Roy. Soc. (London) A211, 500 (1952); 212, 38 (1952).

of the de Haas-van Alphen effect considerable information about the Fermi surface. However, such an interpetation would probably have to await a discussion by number theoretical methods of the problem of particles in a magnetic field and in a periodic instead of a box potential. Here it may be expected from the work of Steele that a considerable portion of the phenomena can be correctly represented by using Landau counting without explicitly taking into account the effect of surface states.

It might be appropriate to mentioned here the effect of a finite temperature and of collisions. If, instead of integrating  $\delta V(E_a)dE_a$  to a sharp cutoff at  $E_0$ , the Fermi energy, in the expression for the moment as given by Eqs. (31), (35) or (38), where  $\delta V(E_a)$  is one of the correction terms, we use the Fermi distribution for a finite temperature, this will have the general effect of "blurring" the cutoff. This has a negligible effect on the nonperiodic contributions to the moment, reducing them by a factor  $[1-O(kT/E_0)^2]$ . The oscillatory terms are not much affected so long as  $kT \ll e\hbar H/2mc = \mu H$ , since then the cutoff occurs over an energy range (kT) small compared to the spacing of the levels  $\mu H$ . On the other hand for  $kT > \mu H$  the oscillatory moment is damped out by a factor  $O(kT/\mu H)$  $\times (e^{-2\pi kT/\mu H})$  with respect to its T=0 value.

If the energy levels are blurred by collisions by an amount  $\epsilon$ , the above expressions with kT replaced by  $\epsilon$  will apply approximately, in order to estimate the collision damping. However, the damping of the oscillatory terms will depend to a considerable extent on the actual shape of the blurred level. The effect of collisions has been considered by Dingle in detail.<sup>26</sup> Kendall discusses the problem of lattice spots of finite size, but his development does not seem immediately applicable to the problem of collision damping.

The results of this paper apply for boxes ranging from atomic to astronomical dimensions, the definition of "strong" and "weak" fields being adjusted accordingly. The only restriction is that the number of electrons in the box be sufficiently greater than one (say ten or more) so that  $V(E_a)$  is a fair estimate of  $G(E_a)$ . If we try to find combinations of moment, field strength, and dimensions such that the moment per unit volume is >H, the applied field, we find that only for very small fields or small dimensions,  $HR < 10^{-5}$  gauss cm for the oscillatory moments, [Eq. (46)], or very large specimens<sup>12</sup> ( $R \sim km$ ) and very small fields ( $H < 10^{-9}$ ) for non-oscillatory moments [Eqs. (44) or (36)] is this possible. Adjusting the effective mass or the Fermi energy can modify these conclusions a little.<sup>27</sup>

These conclusions are in striking contradiction to those of Papapetrou and Slater, who concluded by perturbation arguments for weak fields or "small" boxes (Slater) that a strong diamagnetism was to be expected. If our conclusions from number theory are correct, it means that one must examine with great care any perturbation calculation in a magnetic field for statistical mechanical problems.<sup>28</sup> The conclusions of Welker, who found (neglecting  $H^2$  terms in the Hamiltonian) two huge susceptibilities which just canceled each other, are more in keeping with the results of this paper [see Eq. (27) for  $V(E_a)$ ].

There is a second point to be remembered in applying the conclusions of this paper to a physical problem. The perfect balance [Eq. (27)] insofar as magnetic properties are concerned, between interior and surface states, which is only altered by a consideration of number theory corrections, is only valid for the state of thermodynamic equilibrium. Be the departure from equilibrium ever so slight, this balance may be completely upset. This consideration is important in discussing the magnetic properties of the ionosphere, and may be significant in theories of superconductivity when it is recalled that multiply-connected bodies may not be in their lowest state of thermodynamic equilibrium when a magnetic field is present.

#### V. GENERALIZATION

It is interesting to consider the problem of generalizing to other quantum-mechanical problems the number theory point of view in computing the density of states. This aspect of a quantum-mechanical problem was first considered by Bohr and Kalckar.<sup>29</sup> Auluck and Kothari<sup>30</sup> have also considered an assembly of oscillators from this viewpoint.

It has been known for a long time that in the correspondence principle limit

$$V(E_a) = \int_{H(p, q) \leqslant E_a} dp_1 \cdots dq_3 / h^3 \tag{47}$$

is an estimate of the number of states (i.e., quantum cells) less than  $E_a$ . When this is applied to a Hamiltonian containing a vector potential where H = H(p + eA/c, q), it is immediately plausible why the result of Eq. (27) was obtained. A canonical transformation<sup>1</sup> of  $p + eA/c \rightarrow p'$ ,  $q \rightarrow q'$ , with unit Jacobian can always transform the six-dimensional volume integral of Eq. (47) to a form where the magnetic field does not appear either in the integrand or in the limits of integration, hence  $V(E_a)$  is independent of H.

The question now is: can we generalize the method of Eq. (47) to compute number theory correction terms to  $V(E_a)$  in order to calculate  $G(E_a)$ ? The number theory analog to Eq. (47) which agrees with it exactly is

$$V(E_a) = \int_{E(n_1, n_2, n_3) \leqslant E_a} dn_1 dn_2 dn_3.$$
(48)

 $E(n_1, n_2, n_l)$  are the eigenvalues of  $H(p, q)\psi = E\psi$ . The

<sup>&</sup>lt;sup>27</sup> J. Bardeen, Phys. Rev. 80, 567 (1950).

 <sup>&</sup>lt;sup>28</sup> See reference 5, p. 277 ff.
 <sup>29</sup> N. Bohr and F. Kalckar, Kgl. Danske. Videnskab. Selskab Mat.-fys. Medd. 14, No. 10 (1937).
 <sup>20</sup> F. G. Aviluet and D. S. Kotheri. Proc. Cambridge Phil. Soc.

<sup>&</sup>lt;sup>30</sup> F. C. Auluck and D. S. Kothari, Proc. Cambridge Phil. Soc. 42, 272 (1946).

number theory correction terms for Eq. (48) are

$$\delta V(E_{a})_{lmn} = R(a_{lmn})$$

$$= R \bigg( \int_{E(n_{1}, n_{2}, n_{3}) \leq E_{a}} \exp[2\pi i (ln_{1} + mn_{2} + nn_{3})] \times dn_{1} dn_{2} dn_{3} \bigg), \quad (49)$$

where the number of states less than  $E_a$  is  $G(E_a) = V(E_a)$  $+\Sigma_{l,m,n}a_{lmn}$ . It would appear that to compute Eq. (49) by analogy to Eq. (47) one might proceed as follows. In Eq. (49)  $dn_i$  is replaced by  $dp_i dq_i/h$  and  $n_i$  is replaced by

$$n_{i} = \int_{H(p, q) \leq E_{a}} dp_{i} dq_{i} / h = n_{i} (E_{a}, [p, q]_{i}), \quad (50)$$

i.e., by the area of the  $p_i q_i$  cross section of the surface  $H(pq) = E_a$  in phase space. ( $[p, q]_i$  means the set of p's and q's except  $p_i$ ,  $q_i$ .) Since this is subsequently to be integrated over all phase space by Eq. (49), in Eq. (50) when substituted into Eq. (49),  $E_a$  is again replaced by H(pq). Thus Eq. (49) becomes, computed in analogy to Eq. (47),

$$a_{lmn} = \int_{H(p, q) < E_a} \exp\{2\pi i (ln_1(H(p, q)[p, q]_1') + mn_2(H(p, q)[p, q]_2') + nn_3(H(p, q)[p, q]_3'))\} \cdot dp_1 \cdots dq_3/h^3, \quad (51)$$

where the  $n_i$  in the exponent are the cross sections as given by Eq. (50).

This scheme has been applied to give exact results for the simple problem of the particle in a box and the harmonic oscillator. Its success, or some modification of it, when applied to problems where the variables are not separable or there are several particles with interaction remains to be determined. One may expect that the critical point method, and the methods of combinatorial analysis will find application in such problems.

It is a pleasure to acknowledge the benefit of numerous discussions in the course of this work with M. C. Steele.

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# Application of the Theory of Numbers to the Magnetic Properties of a Free Electron Gas\*

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The methods of number theory are used to find the magnetic properties of a free electron gas. The mathematical procedure which connects number theory to quantum mechanics is given in detail since the same or a similar method may be useful in other problems of solid state and nuclear physics.

The magnetic moment calculation is given in three parts. For the case in which surface states are not considered the results obtained are in agreement with those of previous workers. But when the use of a finite container (rectangular box) to hold the electrons is considered, it is no longer possible to neglect surface states. Through the use of the WKB approximation it is found that the surface states give rise to new size-dependent terms in both the oscillatory and nonoscillatory parts of the magnetic

## I. INTRODUCTION

HE extension of Landau's<sup>1</sup> original work on the diamagnetism of free electrons has already been undertaken by several different methods. Landau<sup>2</sup> himself showed that in addition to the nonperiodic diamagnetic susceptibility the electron gas should exhibit the de Haas-van Alphen<sup>3</sup> effect. Sondheimer and

moment. The oscillatory corrections are generally negligible compared to the usual de Haas-van Alphen effect. However, the nonoscillatory correction, which is diamagnetic in character, can be larger than the Landau diamagnetism for properly chosen magnetic field strengths and containter sizes.

The calculation is concluded with a consideration of the effect of the electron spin. It is found, in agreement with other workers, that the only effect of spin on the oscillatory part of the magnetic moment is to introduce a phase change of  $\pm \pi$  in alternate terms. The "surface" diamagnetic correction due to a finite container is found to be independent of electron spin.

Details on the use of the method of critical points for evaluating integrals asymptotically are given in the appendix.

Wilson<sup>4</sup> have recently confirmed this result by an elegant use of the density matrix. However, neither of the above-mentioned papers attempted to find the effect brought about by using a finite container to hold the electrons. It is well known<sup>5</sup> that the absence of diamagnetism of free electrons in classical theory is dependent upon the behavior of the electrons on the surface of the container. The preceding paper in this

<sup>\*</sup> Based on a thesis presented for the degree of Doctor of Philosoph at the University of Maryland, June, 1952. <sup>1</sup>L. Landau, Z. Physik. **64**, 629 (1930).

<sup>&</sup>lt;sup>2</sup> D. Shoenberg, Proc. Roy. Soc. (London) A170, 341 (1939), (quoting L. Landau). \* W. J. de Haas and P. H. van Alphen, Proc. Acad. Sci. Amster-

dam 33, 1106 (1930).

<sup>&</sup>lt;sup>4</sup> E. H. Sondheimer and A. H. Wilson, Proc. Roy. Soc. (London) A208, 173 (1951).

<sup>&</sup>lt;sup>5</sup> See, for example, J. H. Van Vleck, *Theory of Electric and* Magnetic Susceptibilities (Oxford University Press, London, 1932), p. 100.