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Theory of the Diamagnetic Interactions among the Conduction Electrons in Metals*

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The thermodynamic potential of a metal in the presence of a weakly nonuniform magnetic field of induction $B(r)$ is evaluated. The calculation is a mean-field theory for the interaction between the magnetization at different points in the metal, and is restricted to magnetic field strengths for which the Fermi energy is large compared to the separation between Landau levels. An integral equation for the spatially varying part of the magnetic induction is obtained by minimizing the appropriate thermodynamic potential of the system. The solution of this integral equation is studied. Both domain-type and magnetization-density-wave solutions can be obtained for appropriate Fermi surfaces. The nature of each of these solutions as discussed.

I. INTRODUCTION

There has been considerable interest recently in the effect of the magnetic interactions among the conduction electrons on diamagnetism in metals. This problem first arose with the study by Shoenberg[1] of the wave shape of de Haas–van Alphen oscillations in silver. Shoenberg suggested that the magnetization M of the real metal as a function of the magnetic field strength H could be approximated by the magnetization of a system of noninteracting electrons in the presence of the field $\vec{B} = \vec{H} + 4\pi\vec{M}$. This conjecture agrees with a simple self-consistent-field calculation of the magnetization.[2] Pippard[3] showed that this prescription for determining the magnetization could lead to a multiple-valued function $M(H)$, and he investigated the thermodynamic behavior of the system as a function of H. He found that the path of minimum free energy led to an abrupt jump in the magnetization in the region where $M(H)$ is multiple valued. In Pippard's work, the sample was implicitly assumed to be a long thin rod oriented parallel to the applied magnetic field. A very interesting situation, first pointed out by Condon,[4] arises when the sample has a finite demagnetizing factor. In that case, there can exist a region of applied magnetic field strength in which no portion of the $H-B$ isotherm is thermodynamically stable. As shown by Condon, the sample must in this case spontaneously divide into regions with different values of the magnetization, and a domain structure results. The domains are regions in which the magnetization is uniform; in the domain walls the magnetization changes smoothly from its value in one domain to its value in the neighboring domain. The behavior of the system is analogous to the condensation of a gas, with the two different states of magnetization playing the roles of the liquid and gas phases.

Another interesting possibility, the magnetization-density-wave (MDW) state was first suggested by the study of the wave-number-dependent susceptibility[5] $\chi(q)$. If we define $\chi(q) = dM(q)/dB(q)$, then the wave-number-dependent permeability $\mu(q) = dB(q)/dH(q)$ is equal to $[1 - 4\pi\chi(q)]^{-1}$. When $4\pi\chi(q)$ becomes equal to unity, $\mu(q)$ diverges. This implies that the system is capable of sustaining a nonvanishing spatially varying magnetic induction dB_q without any driving force dH_q. For the free-electron model[6] $\chi(q)$ is given by

$$(\partial M_0/\partial B_0)[2J_1(qr_c)/qr_c]^2,$$

where M_0 and B_0 are the spatially uniform magnetization and induction and r_c is the cyclotron radius of the extremal orbit on the Fermi surface. $J_1(x)$ is the Bessel function of order unity. In

Ref. 6 it was noted that $|\chi(q)|$ is always largest for q equal to zero. This means that $1-4\pi\chi(q)$ will first become negative at q equal to zero, and leads automatically to the domain state proposed by Condon.[4] It was also noted in Ref. 6 that $\chi(q)$ displays geometric resonances associated with matching an integral number of wavelengths $2\pi/q$ to the orbit diameter $2r_c$. Azbel'[7,8] pointed out that with more than one extremal orbit, it is possible for the geometric resonances from each orbit to so interfere with one another that $4\pi\chi(q)$ can first become equal to unity at a finite value of q, instead of at q equal to zero. In that case, the MDW state proposed by Quinn[5] will occur. The MDW state has been studied by Azbel'[7,8] and by the present authors.[9,10] The results in Refs. 7–9 are largely restricted to one-dimensional variations of the magnetization. The solution of the two-dimensional case was briefly sketched in Ref. 10.

The purpose of this paper is to present a more detailed discussion of the ideas introduced in Ref. 10, and to investigate the boundary conditions more carefully. The entire calculation is in the spirit of mean-field theory[11,24] (also referred to as molecular-field theory). In Sec. II, we consider a spatially varying magnetic induction $\vec{B}(\vec{r})=\vec{B}_0+\vec{B}_1(\vec{r})$, where $|\vec{B}_0|\gg|\vec{B}_1|$. We evaluate the energy levels of a system of Bloch electrons to first order in B_1. These energy levels are then used to evaluate the thermodynamic potential of the noninteracting electrons as a functional of $\vec{B}(\vec{r})$. In Sec. III, we obtain an integral equation for the function $\vec{B}_1(\vec{r})$ by minimizing the appropriate thermodynamic potential for the system. The solution of the integral equation is discussed in Sec. IV for the situation in which $4\pi\chi(q)$ exceeds unity by a very small amount. Several different cases seem possible and the transition can be either of first or second order. In Sec. V, we investigate the validity of the mean-field-theory approach to the present problem. In Sec. VI, we present the results of some numerical calculations for a simple Fermi-surface model.

II. EVALUATION OF THERMODYNAMIC POTENTIAL

Following the usual procedure of molecular-field theory, we first replace the interaction between the magnetization at different points by the interaction of the magnetization with a self-consistent magnetic induction $\vec{B}(\vec{r})$ in the sample. Since the chemical potential μ is a function of the magnetic field, the spatial variation of $\vec{B}$ will then lead to a spatially varying electric field. However, it can be easily shown that the effect of this electric field on the field energy and the quantization of the energy level of the electrons is negligible compared with the effect of the spatial variation of the field $\vec{B}(\vec{r})$. This is true only if the Landau-level spacing $\hbar\omega_c$ is much smaller than the Fermi energy E_F (which we will assume throughout this paper). We assume that the magnetic induction has only a very small spatially varying part

$$\vec{B}(\vec{r})=\vec{B}_0+\vec{B}_1(\vec{r}), \tag{2.1}$$

where

$$|\vec{B}_0|\gg|\vec{B}_1|.$$

We shall leave the value of B_0 unspecified for the moment, but assume that it is along a principal axis of symmetry. In this case, the magnetization $\vec{M}(\vec{r})$ and $\vec{B}(\vec{r})$ are aligned along the same direction, which we choose as the z axis. For the band structure of the conduction electrons we assume a many-valley model. Interband and intervalley effects are neglected, since they are not expected to affect the essential features of the phase transition. With this assumption, the single-particle effective Hamiltonian for the electrons in a particular valley can be written as

$$H=\epsilon[-i\vec{\nabla}+(e/c)\vec{A}], \tag{2.2}$$

where $\vec{A}$ is the vector potential for the magnetic induction $\vec{B}(\vec{r})$, and $\vec{\epsilon}(\vec{k})$ describes the energy dispersion law for the electrons in this valley in the absence of magnetic field. We take $-e$ as the electronic charge and use units in which $\hbar$ is equal to unity. The vector potential consists of two parts:

$$\vec{A}=\vec{A}_0+\vec{A}_1. \tag{2.3}$$

For A_0, we use the usual Landau gauge

$$\vec{A}_0=(0,\ B_0x,\ 0), \tag{2.4}$$

and we take A_1 to be of the form

$$\vec{A}_1=(A_1(x,y),0,0). \tag{2.5}$$

In the absence of the inhomogeneous field $\vec{B}_1$, the the eigenfunctions and eigenvalues of the Hamiltonian in Eq. (2.2) are well known. They are described by three quantum numbers $(n,\ k_y,\ k_z)$, and can be written in the form

$$\Phi_{nk_yk_z}(\vec{r})=(L_yL_z)^{-1/2}e^{ik_yy+ik_zz}\phi_{nk_z}(x+\alpha k_y). \tag{2.6}$$

The corresponding eigenvalue

$$E_0(n,k_z)=(n+\gamma)\hbar\omega_c(k_z)+\epsilon(k_z) \tag{2.7}$$

is independent of k_y. We have introduced the quantity $\alpha\equiv c/eB_0$ and the functions $\phi_{nk_z}(x)$ which are the solutions of the differential equation

$$\left[\epsilon\left(-i\frac{\partial}{\partial x},\ x\alpha^{-1},\ k_z\right)-E_{nk_z}\right]\phi_{nk_z}(x)=0. \tag{2.8}$$

When a small inhomogeneous field is present, we can expand the Hamiltonian in powers of B_1 and obtain

$$H = H_0 + H_1\,, \tag{2.9}$$

where

$$H_0 = \epsilon[-i\vec{\nabla} + (e/c)\vec{A}_0] \tag{2.10}$$

and

$$H_1 = (e/c)v_x A_1(\vec{r})\,. \tag{2.11}$$

In Eq. (2.11), we have neglected the noncommutativity of $v_x A_1(\vec{r})$, since we are only interested in quasiclassical regime. We now assume that $|\vec{B}_1|$ satisfies the criterion

$$|B_1/B_0|\,(E_F/\hbar\omega_c) < 1. \tag{2.12}$$

It is easily seen that in this case the energy shift due to H_1 is small compared with the Landau-level spacing, and hence perturbation theory can be applied. In the absence of A_1, all levels with the same value of n and k_z are degenerate. According to standard degenerate perturbation theory, the correct zeroth-order eigenfunctions are given by the combination

$$\psi^{(0)}_{n,k_z,l}(\vec{r}) = \sum_{k_y} C_l(k_y)\phi_{n,k_z,k_y}(\vec{r})\,, \tag{2.13}$$

with energy

$$E_{n,k_z,l} = E^0_{n,k_z} + \epsilon_{l,n,k_z}\,, \tag{2.14}$$

where l denotes a new set of quantum numbers. C_{l,n,k_z} and ϵ_{l,n,k_z} satisfy the equation

$$\sum_{k'_y} C_l(k'_y)\langle n, k_y, k_z|H_1|n, k'_y, k_z\rangle = \epsilon_l C_l(k_y), \tag{2.15}$$

where we have dropped the indices $\{n, k_z\}$ on C_l and ϵ_l for simplicity. Now we write $k'_y = k_y + q_y$. The functions $\phi_{n,k_z}(x + \alpha k_y)$, introduced in Eq. (2.6) with different values of k_y, are related by a translational operator

$$\phi_{n,k_z}(x, \alpha k'_y) = e^{i\alpha q_y p_x}\phi_{n,k_z}(x + \alpha k_y). \tag{2.16}$$

We also introduce the Fourier transform of a function $f(x, y)$ with respect to y as follows:

$$f(x,y) = (1/L)\int dy\, f(x,y)\, e^{iq_y y} \tag{2.17}$$

and

$$f(x,q) = \sum_{q_y} f(x, q_y)\, e^{-iq_y y}\,.$$

With the help of Eqs. (2.16) and (2.17), we can express the matrix element appearing in Eq. (2.15) in the form

$$\langle n, k_y, k_z|H_1|n, k'_y k_z\rangle = \int dx\, \phi_{n,k_z}(x + \alpha k_y)\,(e/c) \times A_1(x, q_y)\, v_x\, e^{i\alpha q_y p_x}\phi_{n,k_z}(x + \alpha k_y)\,. \tag{2.18}$$

From Eq. (2.18), we can see that the problem of evaluating the matrix element in Eq. (2.15) reduces to finding diagonal matrix elements in a one-dimensional case. In the semiclassical regime, these one-dimensional elements can be evaluated following a method due to Landau.[12] According to this scheme, the matrix element can be replaced by a time average over the classical orbit with all the operators replaced by their classical value. Thus Eq. (2.18) becomes

$$\langle n, k_y, k_z|H_1|n, k'_y, k_z\rangle = (1/T)\oint dt\,(e/c)A_1(x(t), q_y) \times v_x(t)\, e^{i\alpha q_y p_x(t)}\,. \tag{2.19}$$

We now make use of the equation $\dot{\vec{p}} = -(e/c)\,\vec{v}\times\vec{B}_0$ to express $v_x(t)\,dt$ as αdp_y and $x(t)$ as $\alpha(p_y - k_y)$. Then Eq. (2.10) takes the form of an integral over the classical orbit in $\vec{p}$ space:

$$\langle n, k_y, k_z|H_1|n, k'_y, k_z\rangle (\alpha e/cT) \times \oint dp_y\, A_1(\alpha p_y - \alpha k_y, q_y)e^{i\alpha q_y p_x}. \tag{2.20}$$

Here T is the period of the orbit in $\vec{p}$ space defined by

$$\epsilon(p_x, p_y, k_z) = E_0(n, k_z). \tag{2.21}$$

Substitution of Eq. (2.20) into Eq. (2.15) then gives an equation for the coefficents $C_l(k_y)$:

$$\sum_{q_y} C_l(k_y + q_y)(\alpha e/cT) \times \oint dp_y\, A_1(\alpha p_y - \alpha k_y, q_y)\, e^{i\alpha q_y p_x} = \epsilon_l C_l(k_y). \tag{2.22}$$

The exact solution of this equation is difficult. However, for our present purpose, we can introduce the following trial function with two parameters x_0 and y_0:

$$C_{x_0, y_0}(k_y) = e^{-iy_0 k_y}F(k_y, x_0)\,, \tag{2.23}$$

where $F(k_y, x_0)$ is a function of k_y with the property that it is very small outside a region of width Δ centered about the value $k_y = -x_0/\alpha$, and is large and roughly constant inside that region. The height of the peak is of course determined by normalization. Substitution of Eq. (2.23) into Eq. (2.22) then gives

$$\epsilon_{x_0, y_0}F(k_y, x_0) = \sum_{q_y} e^{-iy_0 q_y}(\alpha e/cT)\oint dp_y A_1(\alpha p_y - \alpha k_y, q_y) \times e^{i\alpha q_y p_x}F(k_y + q_y, x_0). \tag{2.24}$$

It is expected that the dominant terms in the sum over q_y on the left-hand side of Eq. (2.24) come from values of q_y such that $|q_y| < 1/r_c$, where r_c is a typical cyclotron radius. (This is verified by the final expression of A_1 in the subsequent calculation.) In this case, it is not difficult to see that for

$$1/r_c \ll \Delta \ll r_c/\alpha; \tag{2.25a}$$

that is,

$$1/r_c \ll \Delta \ll (E_F/\omega_c)(1/r_c), \tag{2.25b}$$

$C_{x_0,y_0}(k_y)$ is an approximate eigenfunction of Eq. (2.22) with eigenvalue $\epsilon(x_0, y_0)$:

$$\epsilon(x_0, y_0) \approx (\alpha e/cT) \oint dp_y\, A_1(\alpha p_y + x_0, y_0 - \alpha p_x). \tag{2.26}$$

The physical significance of the parameters x_0 and y_0 in the function ϵ can be seen by writing down the corresponding wave function

$$\psi^{(0)}_{n,k_z,x_0,y_0}(\vec{r}) = (L_y L_z)^{-1/2} e^{ik_z z} \times \int (dk_y/2\pi)\, e^{ik_y(y-y_0)} F(k_y, x_0)\, \phi_{nk_z}(x + \alpha k_y). \tag{2.27}$$

From the property of the function $F(k_y, x_0)$ and the criteria in Eq. (2.25), it can be seen that the wave function $\psi^{(0)}_{n,k_z,x_0,y_0}(\vec{r})$ has the property of being localized around the point (x_0, y_0) in real space. The approximate nature of our solution arises from the fact that quantum mechanically the two coordinates of the center cannot be specified with infinite accuracy. In fact, according to the definition of Roth[13] and of Kubo *et al.*[14] for x_0 and y_0 as operators, they obey the commutation relation

$$[\hat{x}_0, \hat{y}_0] = ic/|e|\, B_0 = i\alpha.$$

When ω_c/E_F tends to zero, the commutator $[x_0/r_c, y_0/r_c]$ also tends to zero. Hence in our present approximation where $\omega_c/E_F \ll 1$, treating x_0 and y_0 both as good quantum numbers is a reasonable approximation.

When reduced to a one-dimensional case, the result in Eq. (2.26) is in complete agreement with that obtained from the method of semiclassical quantization. The present approach seems superior because the validity of the semiclassical quantization for a two-dimensional variation of the field is rather doubtful.

Now we come to the evaluation of the thermodynamic potential. For the case of uniform magnetic field, the problem was solved in a classical paper by Lifshitz and Kosevich.[15] The central step in their calculation is a knowledge of a function $n(E, k_z)$. For every valley in reciprocal space the function $n(E, k_z)$ is obtained by inverting $E(n, k_z)$ when both n and E are regarded as continuous variables and k_z is regarded as a parameter. In the presence of the inhomogeneous field, inverting the function $E(n, k_z, x_0, y_0)$ gives us then

$$n(x_0, y_0, E, k_z) = n_0(E, k_z) + \frac{\partial n_0}{\partial E}\, \epsilon(x_0, y_0). \tag{2.28}$$

If we now introduce a function

$$S(E, k_z, x_0, y_0) \equiv (2\pi/\alpha)\, n(x_0, y_0, E, k_z),$$

then S can be written as

$$S(x_0, y_0, E, k_z) = S^0(1 + \delta S), \tag{2.29a}$$

where

$$S^0 = (2\pi/\alpha)\, n_0(E, k_z) \tag{2.29b}$$

and

$$\delta S = (-e/S^0 c) \oint dp_y\, A_1(x_0 + \alpha p_y, y_0 - \alpha p_x). \tag{2.29c}$$

The integral here is taken over the path defined by

$$\epsilon(p_x, p_y, k_z) = E.$$

Comparing with Ref. 15, we see that $S^0(E_F, k_z)$ is just the cross-sectional area bounded by the Fermi surface and the plane k_z = a constant. Equipped with a knowledge of $S(x_0, y_0, E, k_z)$, we can then follow the calculation of Ref. 15 step by step and obtain an expression for the thermodynamic potential density $\Omega_{\mathrm{LK}}(x_0, y_0)$. We omit the detailed steps and simply give the result[16]:

$$\Omega_{\mathrm{LK}}(x_0, y_0) = \pi^{-2}(2\pi)^{-1/2}\left(\frac{eB_0}{c}\right)^{5/2} \sum_m \left|\frac{\partial^2 S^0_m}{\partial k_z^2}\right|^{-1/2} \times \left(\frac{\partial S^0_m}{\partial \epsilon}\right)^{-1} \sum_{\nu=1}^{\infty} \frac{\psi(\lambda\nu)}{\nu^{5/2}} \cos\left(\frac{\nu}{2m_0}\,\frac{\partial S^m_0}{\partial \epsilon_F}\right) \cdot \times \cos[(\nu/eB_0)\, S^m(x_0, y_0) - 2\pi\nu\gamma \mp \tfrac{1}{4}\pi]. \tag{2.30}$$

The notation here is the same as in Ref. 10. S^0_m indicates the extremal value of $S(\epsilon, k_z)$ as a function of k_z. The sum over m runs through all the extremal areas of the Fermi surface. Only the oscillatory part of the thermodynamic potential is included, since only this part will be of importance in our subsequent discussions. In Eq. (2.30), $S_m(x_0, y_0)$ has been replaced by S^0_m everywhere except in the phase of the second cosine factor where $B_1(\vec{r})$ has a dominant effect. We have seen in Eq. (2.12) that for perturbation theory to be valid, $(B_1/B_0)(E_F/\omega_c)$ has to be smaller than unity. When this condition is satisfied, the second cosine factor in Eq. (2.30) can be expanded term by term in powers of B_1/B_0. Here a question may be raised as to why is it enough to keep only terms to order B_1/B_0 in the change in individual energy level to arrive at an infinite power-series expansion of $\Omega_{\mathrm{LK}}(x_0, y_0)$. The reason for this is that when we investigate the nth-order term in B_1 of the expansion of $\Omega_{\mathrm{LK}}(x_0, y_0)$, the contribution of a first-order shift in energy has a factor of $(E_F/\hbar\omega_c)^n$, whereas the contributions from higher-order changes in energy will only be multiplied by a factor $(E_F/\hbar\omega_c)^m$, with $m < n$. Hence in the limit $E_F/\hbar\omega_c \gg 1$, Eq. (2.30) is equivalent to a partial sum of the dominant terms for every order in a perturbative calculation of the thermodynamic potential. Before we write down the expansion of Ω_{LK}, we note that by introducing a function

$$\mathcal{S}_m(q_x, q_y) \equiv (-i/\alpha S_0 q_y) \oint_m dp_y\, e^{i\alpha(q_y p_x - q_x p_y)}, \quad (2.31)$$

Eq. (2.29) can be written as

$$\delta S_m(x_0, y_0) = -(1/B_0) \int d\vec{r}\, B_1(\vec{r}) \times \sum_{\vec{q}} e^{i\vec{q}\cdot(\vec{r}-\vec{r}_0)}\, \mathcal{S}_m(q_x, q_y), \quad (2.32)$$

where

$$\vec{r} = (x, y)$$

and

$$\vec{r}_0 = (x_0, y_0).$$

For an elliptical cross section given by $\alpha_1 p_x^2 + \alpha_2 p_y^2 = p_m^2$, the function $\mathcal{S}(q_x, q_y)$ can be easily evaluated and has the value

$$\mathcal{S}(q_x, q_y) = \frac{2J_1[(\alpha_2^{-1} Q_x^2 + \alpha_1^{-1} Q_y^2)^{1/2}]}{(\alpha_2^{-1} Q_x^2 + \alpha_1^{-1} Q_y^2)^{1/2}}, \quad (2.33)$$

where $\vec{Q} = \alpha p_m \vec{q}$. With the help of the function $\mathcal{S}_m(q_x, q_y)$, the expression for the thermodynamic potential can be finally written in a compact way as

$$\begin{aligned}\Omega_{\mathrm{LK}} &\equiv \int \Omega_{\mathrm{LK}}(x_0, y_0)\, d\vec{r}_0 \\ &= \Omega_0 - (1/4\pi) \int d\vec{r}_1\, B_1(\vec{r}_1)\, g_1 - \cdots \\ &\quad - (1/4\pi n) \int d\vec{r}_1 \int d\vec{r}_2 \cdots \\ &\quad \times \int d\vec{r}_n\, B_1(\vec{r}_1) \cdots B_1(\vec{r}_n) g_n(\vec{r}_{12}, \ldots, \vec{r}_{1n}),\end{aligned} \quad (2.34)$$

where

$$\vec{r}_{1n} = \vec{r}_1 - \vec{r}_n,$$

and

$$g_n(\vec{r}_{12}, \ldots, \vec{r}_{1n}) = \textstyle\sum_m g_n^m(\vec{r}_{12}, \ldots, \vec{r}_{1n})$$

is a sum of terms from different extremal areas of the Fermi surface. The Fourier transforms of the functions g_n^m are given by

$$\begin{aligned}g_{n+1}^m(\vec{q}_1, \ldots, \vec{q}_n) &= \frac{4\pi}{n!} \frac{\partial^n M_0^m}{\partial B_0^n}\, \mathcal{S}_m(\vec{q}_1)\, \mathcal{S}_m(\vec{q}_2) \cdots \\ &\quad \times \mathcal{S}_m(\vec{q}_n)\, \mathcal{S}_m(\vec{q}_1 + \vec{q}_2 + \cdots + \vec{q}_n).\end{aligned} \quad (2.35)$$

Here $M_0^{(m)}$ is the contribution of the mth extremal orbit to the uniform magnetization and $g_1^m = 4\pi M_0^m$.

III. INTEGRAL EQUATION FOR $B_1(\vec{r})$

Having obtained the expression for the thermodynamic potential Ω_{LK} of a system of electrons in a self-consistent field, we now proceed to investigate its physical meaning. This question has been looked at by Pippard,[3] by Condon,[4] and by Azbel'.[7] We will follow a slightly different line of approach. First, we notice that the thermodynamic potential calculated in Sec. II only includes the kinetic-energy part of the electrons. The total thermodynamic potential Ω_{tot} should include also the field energy. Hence, we have

$$\Omega_{\mathrm{tot}} = \Omega_{\mathrm{LK}} + \int [B^2(\vec{r})/8\pi]\, d^3r. \quad (3.1)$$

At fixed temperature, the variation of the thermodynamic potential is given by[17]

$$\delta\Omega_{\mathrm{tot}} = (1/4\pi) \int \vec{H}(\vec{r}) \cdot \delta\vec{B}(\vec{r})\, d^3r. \quad (3.2)$$

Comparing Eqs. (3.1) and (3.2), we obtain the relation between Ω_{LK} and the magnetization $M(r)$:

$$\delta\Omega_{\mathrm{LK}} = -\int \vec{M}(\vec{r}) \cdot \delta\vec{B}(\vec{r})\, d^3r$$

or

$$\vec{M}(\vec{r}) = -\delta\Omega_{\mathrm{LK}}/\delta\vec{B}(\vec{r}). \quad (3.3)$$

When the values of $\vec{B}(\vec{r})$ at each point $\vec{r}$, and the temperature T, are fixed, the equilibrium state corresponds to the minimum of Ω_{tot}. However, this is not the situation under consideration. The quantities fixed here are the temperature, the current $\vec{j}_{\mathrm{ext}}$ in the coils of the magnet, and the main magnetic field B_0 yet to be defined. Following de Gennes,[18] we can construct a thermodynamic potential adapted to this situation. Define the function G as

$$G = \Omega_{\mathrm{tot}} - \int \frac{\vec{B}_1(\vec{r}) \cdot \vec{H}}{4\pi}\, d^3r; \quad (3.4)$$

then

$$\delta G = -\int \frac{\vec{B}_1(\vec{r})}{4\pi} \cdot \delta\vec{H}\, d^3r. \quad (3.5)$$

In Eq. (3.5), the variation is performed under fixed temperature T and main field B_0. Since $\mathrm{div}\vec{B}_1 = 0$, we can set $\vec{B}_1 = \mathrm{curl}\vec{A}_1$ and integrate by parts:

$$\delta G = \frac{1}{4\pi} \int (\vec{\nabla} \times \vec{A}_1) \cdot \delta\vec{H}\, d^3r = \frac{1}{c} \int \vec{A}_1 \cdot \delta\vec{j}_{\mathrm{ext}}\, d^3r. \quad (3.6)$$

Thus for fixed T and B_0, δG vanishes when $\vec{j}_{\mathrm{ext}}$ is fixed. The equilibrium state under this condition then corresponds to the mininum of G. We can also write Eq. (3.4) in the form

$$G = \Omega_{\mathrm{LK}} + \frac{B_0^2}{8\pi} + \int \frac{B_1^2}{8\pi}\, d^3r + \int \vec{M}_0 \cdot \vec{B}_1\, d^3r. \quad (3.7)$$

To determine the form of $\vec{B}_1(\vec{r})$, we need another relation between $\vec{M}$ and $\vec{B}_1$. It is here that the sample shape factor comes into play. For simplicity, we shall assume that both the external field and the magnetization are directed along a principal axis of an elliposidal sample. The average of the field and the induction must obey the usual boundary condition[17]

$$4\pi n_{zz}\langle M\rangle = H_0 - H. \quad (3.8)$$

Here n_{zz} is the demagnetization factor of the ellipsoid along the z direction, H is constant over the whole sample, since both its curl and divergence vanish, and $\langle M\rangle$ denotes the spatial average of the magnetization.

Now we choose the value of B_0 to be that which would exist in the sample if the magnetization were uniform. The boundary condition that gives the value of B_0 is determined by

$$B_0 - 4\pi(1-n_{zz})M_0(B_0) = H_0 . \tag{3.9}$$

Here H_0 is the value of the magnetic field if the sample were absent. Equation (3.9) will admit a unique solution for B_0 only when the condition $4\pi \times (1-n_{zz})\,dM_0/dB_0 < 1$ is satisfied. This is one of the conditions that has to be kept in mind in subsequent discussions. Making use of Eqs. (3.8) and (3.9), the relation between B_1 and m can be written as

$$B_1 = 4\pi\{M(r) - M_0(B_0) - n_{zz}\langle M - M_0(B_0)\rangle\}. \tag{3.10}$$

To determine B_1, there exist two approaches. The first is to minimize the thermodynamic potential subject to the restriction on B_1 owing to the boundary conditions. The second approach, which proves to be much more convenient, makes use of the relation between Ω_{LK} and the magnetization. Substitution of Eq. (3.10) into Eq. (3.3) gives

$$B_1/4\pi = n_{zz}\langle \delta\Omega_{\mathrm{LK}}/\delta B_1 + M_0(B_0)\rangle - \delta\Omega_{\mathrm{LK}}/\delta B_1 - M_0(B_0). \tag{3.11}$$

Writing Eq. (3.11) explicitly in terms of B_1, we finally obtain an integral equation

$$B_1(\vec{r}_1) = \int d\vec{r}_2\, B_1(\vec{r}_2)\,\tilde{g}_2(\vec{r}_{12}) + \cdots + \int d\vec{r}_2\cdots d\vec{r}_n \times B_1(\vec{r}_2)\cdots B_1(\vec{r}_n)\tilde{g}_n(\vec{r}_{12},\cdots,\vec{r}_{1n}). \tag{3.12}$$

In Eq. (3.12), $\vec{r}_{1n}$ stands for $\vec{r}_1 - \vec{r}_n$. The functions $\tilde{g}_n$, etc., are very similar to the functions g_n introduced in Sec. II. They are defined by

$$\tilde{g}_n = g_n - n_{zz}(1/\Omega)\int d\vec{r}_1\, g_n(\vec{r}_{n1},\cdots,\vec{r}_{21}). \tag{3.13}$$

The Fourier transform of Eq. (3.12) can be written as

$$\begin{aligned} B_1(\vec{q}_1)\{1-\tilde{g}_2(\vec{q}_1)\} = \sum_{\vec{q}_2,\vec{q}_3} & B_1(\vec{q}_2)\,B_1(\vec{q}_3)\,\tilde{g}_3(\vec{q}_2,\vec{q}_3) \\ & \times \delta(\vec{q}_1-\vec{q}_2-\vec{q}_3) + \cdots \\ & + \sum_{\vec{q}_1\cdots\vec{q}_n} B_1(\vec{q}_2)\cdots B_1(\vec{q}_n) \\ & \times \tilde{g}_n(\vec{q}_2,\cdots,\vec{q}_n)\,\delta(\vec{q}_1-\vec{q}_2-\cdots-\vec{q}_n). \end{aligned} \tag{3.14}$$

Equation (3.12) naturally allows many classes of solution. To find out which solution corresponds to the equilibrium situation, it is necessary to substitute the function $B_1(\vec{r})$ obtained from Eq. (3.12) into the thermodynamic potential G expressed as a functional of $B_1(\vec{r})$. We see readily from Eqs. (3.7) and (3.11) that this functional can be written as[19]

$$\begin{aligned} G = \Omega_{\mathrm{LK}} + \int \frac{B_1^2\,d^3r}{8\pi} - \int n_{zz}\left\langle \frac{\partial\Omega_{\mathrm{LK}}}{\partial B_1}\right\rangle B_1\,d^3r + \frac{B_0^2}{8\pi} \\ + \int \vec{M}_0(B_0)\cdot\vec{B}_1(r)\,d^3r\,(1-n_{zz}). \end{aligned} \tag{3.15}$$

The equilibrium value of $B_1(\vec{r})$ then corresponds to the solution of Eq. (3.12) which renders G a minimum.

IV. SOLUTION OF INTEGRAL EQUATION

One can notice by inspection that $B_1 \equiv 0$ is a trivial solution of Eq. (3.12) corresponding to the state of spatially uniform magnetization. This solution need not, however, correspond to the state of minimum thermodynamic potential. To see this, it is sufficient to write out the leading terms in the expansion of G in powers of $B_1(q)$, the Fourier components of $B_1(r)$: For $n_{zz}=0$ we have

$$\begin{aligned} G &= \Omega_0 + \frac{B_0^2}{8\pi} + \sum_{\vec{q}} \frac{B_1^2(\vec{q})}{8\pi}\,[1-g_2(\vec{q})] + \cdots \\ &= \Omega_0 + \frac{B_0^2}{8\pi} + \sum_{\vec{q}}\,[1-4\pi\chi(\vec{q})]\,\frac{B_1^2(\vec{q})}{8\pi} + \cdots . \end{aligned} \tag{4.1}$$

From the form of Eq. (4.1) it is obvious that if the factor $1-4\pi\chi(\vec{q})$ becomes negative at some value of $\vec{q}$, it is energetically more favorable for the corresponding Fourier component $B_1(\vec{q})$ to assume a finite value than to vanish identically. If the Fermi-surface structure of the metal is such that there exists only one extreme cross section at the particular orientation of the magnetic field, then the expression for $g_2(\vec{q})$ in Eq. (2.35) shows that $|g_2|$ will always have its maximum at $q=0$. In other words, the quantity $1-4\pi\chi(\vec{q})$ will first vanish at $q=0$. The system is then thermodynamically unstable and will either jump to a new uniform state or break into domains depending on the demagnetizing factor of the sample. The boundary condition used in Sec. III is no longer applicable for this situation. Let us consider a disk-shaped sample. What happens in this case is that the internal field stays at a fixed value H for which $4\pi\chi(0)$ exceeds the value unity. Domains are formed, in each of which the local magnetization assumes a value which minimizes the thermodynamic potential. The appropriate choice for the value of induction B_0 is now $B_0 = H$, resulting in the relation $M = B_1/4\pi$. Equation (3.12) still enables us to find the value of magnetization in each domain. In particular, if the domain width is much larger than that of the transition layer, the structure of the transition layer can also be obtained with the help of the same equation. For explicit results we refer the reader to Ref. 9.

We will now concentrate our attention on the situation where $1-4\pi\chi(\vec{q})$ is negative at a finite wave number $\vec{q}$, but positive at $q=0$. In a subsequent section, we present some numerical calculations for a system with more than one extremal area to show that this is indeed a possible situation. In this instance, the system is stable against domain formation,[20] but unstable against the formation of a magnetization density wave. Suppose the condition $|1-4\pi\chi(\vec{\kappa})| \ll 1$ is satisfied, $\vec{\kappa}$ being the value of $\vec{q}$ which $4\pi\chi(\vec{q})$ assumes its maximum value with respect to $\vec{q}$. Later we will specify more clearly as to how small $|1-4\pi\chi(\vec{\kappa})|$ has to be. Then the form of G as in Eq. (4.1) suggests that the dominant Fourier component of the solution $B_1(\vec{r})$ is that with $\vec{q}=\vec{\kappa}$. In general, there may be several equivalent κ's, depending on the symmetry of the sample. Let us consider a material which has a twofold axis of symmetry such that $g_2(\vec{q})$ has maxima greater than unity at $\vec{q}=(0, \pm\kappa)$. The situation could arise, for example, in a hexagonal crystal with $\vec{B}$ perpendicular to the c axis. In this case, we can try a solution of the form[7]

$$B_1(\vec{r}) = A(\vec{r})\, e^{-i\vec{\kappa}\cdot\vec{r}} + A^*(\vec{r})\, e^{i\vec{\kappa}\cdot\vec{r}} + C(\vec{r}). \qquad (4.2)$$

Here $A(\vec{r})$ will be a slowly varying function of $\vec{r}$, and $C(\vec{r})$ will be of higher than first order in $A(\vec{r})$. By substituting Eq. (4.2) into Eq. (3.12), one can readily show that $C(\vec{r})$ must assume the form

$$C(\vec{r}) = C_0 + C_{2\vec{\kappa}}\, e^{-2i\vec{\kappa}\cdot\vec{r}} + C^*_{2\vec{\kappa}}\, e^{2i\vec{\kappa}\cdot\vec{r}}, \qquad (4.3)$$

where

$$C_0 = 2|A|^2 g_3(\vec{\kappa}, -\vec{\kappa})/[1-g_2(0)]$$

and

$$C_{2\vec{\kappa}} = |A|^2 g_3(\vec{\kappa}, \vec{\kappa})/[1-g_2(2\vec{\kappa})]. \qquad (4.4)$$

Now we make use of the fact that $A(\vec{r})$ varies very slowly in space, so that expressions like $A(\vec{r}+\Delta\vec{r})$ can be expanded as

$$A(\vec{r}+\Delta\vec{r}) \approx A(\vec{r}) + \sum_{i=1,2} \frac{\partial A}{\partial x_i}\Delta x_i + \frac{1}{2} \times \sum_{i,j=1,2} \frac{\partial^2 A}{\partial x_i\, \partial x_j}\Delta x_i\, \Delta x_j. \qquad (4.5)$$

Making use of Eqs. (4.2)–(4.5), we can finally convert the integral equation (3.12) into a differential equation for the function $A(r)$,[21]

$$-\frac{1}{2}\sum_{i=1,2}\frac{\partial^2 g^2(\vec{\kappa})}{\partial \kappa_i^2}\frac{\partial^2 A}{\partial x_i^2} + [g_2(\vec{\kappa})-1]A + \left(\frac{4g_3(\vec{\kappa}, -\vec{\kappa})\, g_3(\vec{\kappa}, 0)}{1-g_2(0)} + \frac{2g_3(\vec{\kappa}, \vec{\kappa})\, g_3(\vec{\kappa}, -2\vec{\kappa})}{1-g_2(2\vec{\kappa})} + 3g_4(\vec{\kappa}, \vec{\kappa}, -\vec{\kappa})\right)|A|^2 A = 0. \qquad (4.6)$$

Note that if $A(x,y)$ is independent of x, then Eq. (4.6) reduces to the one-dimensional equation given by Ying and Quinn.[9]

Equation (4.6) is identical in form to the Ginzburg-Landau equation for a superconductor in zero field, with $A(\vec{r})$ playing the role of the order paramater. This resemblance is brought out more clearly if we express the thermodynamic potential in terms of $A(\vec{r})$. Substitution of Eqs. (4.2) and (4.4) into Eq. (4.1) gives

$$G = \Omega_0 + \frac{B_0^2}{8\pi} + a\int A^2\, d\vec{r} + b\int A^4\, d\vec{r} + c\int (\nabla A)^2\, d\vec{r}, \qquad (4.7)$$

where

$$a = (1/4\pi)[1-g_2(\kappa)], \quad c = -(1/8\pi)\nabla_k^2 g_2(\kappa),$$

and

$$b = -\frac{1}{4\pi}\left(\frac{2g_3^2(\kappa, -\kappa)}{1-g_2(0)} + \frac{g_3^2(\kappa, \kappa)}{1-g_2(2\kappa)} + \tfrac{3}{2}g_4(\kappa, \kappa, -\kappa)\right). \qquad (4.8)$$

This is of course the standard form of the expression for the free energy[22] in the Landau theory of second-order phase transitions,[11] provided the sign of b is positive. In this case, the transition point occurs at $1-4\pi\chi(\vec{\kappa})=0$. Below the transition point $1-4\pi\chi(\vec{\kappa})<0$ and $A(\vec{r})$ is nonzero. $A(\vec{r})$ tends toward zero as the transition point is approached, and $A(\vec{r})=0$ above the transition point. It is not difficult to see from the form of G in Eq. (4.7) and the equation for A, in Eq. (4.6), that the spatially varying solution is energetically less favorable than the uniform solution given by[23]

$$A = (-a/2b)^{1/2}. \qquad (4.9)$$

Hence the MDW has the form

$$B_1(r) = 2(-a/2b)^{1/2}\cos\kappa(y-y_0). \qquad (4.10)$$

For the situation where b is negative, a first-order transition occurs at a negative value of $g_2(\kappa)-1$. In the case where $g_2(\vec{\kappa})$ has threefold symmetry, a first-order phase transition always occurs because the maximum of $g_2(\vec{\kappa})$ appears at values $\vec{\kappa}$ such that $\sum_i \kappa_i = 0$, and the cubic term in Eq. (4.6) is important.

V. VALIDITY OF MOLECULAR-FIELD THEORY

Now we come to the question of the validity of mean-field theory as applied to the present problem. As is well known, for any kind of second-order phase transition, fluctuations play a dominant role near the critical point.[24] These gigantic fluctuations cause the molecular-field theory to fail in the immediate neighborhood of the critical point. Hence, it is important to know in what physical region the results presented in the preceding sections are valid. For our present problem the transition point can be reached by varying the temperature at fixed H_0, or varying H_0 at fixed temperature. The quantities

$$\epsilon_T \equiv (T - T_c)/T_c, \quad \epsilon_H \equiv (H_0 - H_c)/H_c \tag{5.1}$$

are a measure of how close we are to the transition point in each case. In Ref. 24, it was shown that the Landau theory can be used to estimate the fluctuation itself. Suppose we define the correlation $g(\vec{r}, \vec{r}\,')$ as given by

$$g(\vec{r}, \vec{r}\,') = \langle [A(\vec{r}) - \langle A(\vec{r})\rangle] [A(\vec{r}\,') - \langle A(\vec{r}\,')\rangle] \rangle. \tag{5.2}$$

Here $\langle\ \rangle$ has the meaning of a statistical average instead of a spatial one. In Landau's theory, $g(\vec{r}, \vec{r}\,')$ is given by

$$g(\vec{r}, \vec{r}\,') = (\vec{r} - \vec{r}\,')^{-1} \exp(-|\vec{r} - \vec{r}\,'|/\xi) \frac{k_B T}{8\pi c}, \tag{5.3}$$

where ξ is the coherence length. The coherence length is given by

$$\xi(T) = c^{1/2} \left(\frac{\partial a}{\partial T}\right)_{T_c}^{-1/2} (T - T_c)^{-1/2} \quad \text{for } T > T_c$$

$$= \left(\frac{1}{2} C\right)^{1/2} \left(\frac{\partial a}{\partial T}\right)_{T_c}^{-1/2} (T_c - T)^{-1/2} \quad \text{for } T < T_c. \tag{5.4a}$$

We can also think of ξ as function of magnetic field H_0, in which case it is given by

$$\xi(H_0) = c^{1/2} \left(\frac{\partial a}{\partial H_0}\right)_{H_c}^{-1/2} (H_0 - H_c)^{-1/2} \quad \text{for } H_0 > H_c$$

$$= (\tfrac{1}{2} c)^{1/2} \left(\frac{\partial a}{\partial H_0}\right)_{H_c}^{-1/2} (H_c - H_0)^{-1/2} \quad \text{for } H_0 < H_c. \tag{5.4b}$$

In Eqs. (5.4) we have assumed for simplicity that $\partial^2 g_2/\partial\kappa_x^2 = \partial^2 g_2/\partial\kappa_y^2 \equiv -4\pi c$. According to Kadanoff *et al.*,[24] the criteria for the Landau theory to be valid are that fluctuations in the order parameter over distances comparable with ξ must be relatively small. In particular, they must be small in comparison with the order parameter itself. Therefore we must have

$$\langle [A(r) - \langle A\rangle][A(r') - \langle A\rangle] \rangle \ll \langle A\rangle^2, \; |r - r'| \sim \xi. \tag{5.5}$$

Here $\langle A\rangle$ is the value of the order parameter corresponding to the solution of Eq. (4.6), namely, $\langle A\rangle = (-a/2b)^{1/2}$. From Eqs. (5.5) and (5.3) we must then have

$$k_B T_c / 4\pi e c \xi(T) \ll -a/b$$

or (5.6)

$$k_B T / 4\pi e c \xi(H_0) \ll -a/b$$

for the validity of the mean-field theory. If we now define ϵ_c as the lower bound for values of ϵ satisfying Eq. (5.6), we readily obtain

$$(\epsilon_T)_c \approx 10^{-14}, \quad (\epsilon_H)_c \approx 10^{-17} \tag{5.7}$$

for a field strength $H_0 \sim 30$ kG, $T \sim 1$ °K, the ratio $E_F/\hbar\omega_c \sim 10^3$, and $r_c \sim 10^{-4}$ cm. Thus, the mean-field theory will be valid for

$$10^{-14} \ll \left|\frac{T - T_c}{T_c}\right| \ll 1, \quad 10^{-17} \ll \left|\frac{H - H_c}{H_c}\right| \ll 1. \tag{5.8}$$

These very small values of ϵ_c arise because of the long-range nature of the magnetic interactions. It indicates that we can neglect the effect of fluctuations in almost all practical situations. The transition from the normal state to the MDW state has the typical form of a second-order phase transition. According to mean-field theory, the second derivatives of the thermodynamic potential will exhibit discontinuities at the transition point. In particular, the susceptibility, regarded either as a function of temperature at constant magnetic field or a function of magnetic field at constant temperature, will have a discontinuous jump across the transition point. Here we will follow Landau's approach to calculate the jump in the susceptibility as the external magnetic field H_0 approaches the critical value H_c. For simplicity, we shall limit ourself to the case where n_{zz} is zero so that $H \equiv H_0$. It has been shown in Sec. IV that near the critical point the thermodynamic potential of the system can be written as

$$G = \Omega_0 + B_0^2/8\pi + a(H, T) A^2 + b(H, T) A^4 \tag{5.9}$$

for a unit volume where a and b are given in Eq. (4.8). Near the transition point where $H \approx H_c$, we can use the following approximation for a and b:

$$a \approx \left(\frac{\partial a}{\partial H}\right)_{H_c} (H_0 - H_c), \quad b \approx b(H_c). \tag{5.10}$$

We now recall the result

$$\delta G = -(1/4\pi) \int \vec{B}_1(r) \cdot \delta\vec{H}\, dr$$

given in Eq. (3.5). Together with the relation between B_1 and $M(r)$ given in Eq. (3.10), this yields

$$-\delta G/\delta H = \langle M\rangle - M_0(B_0). \tag{5.11}$$

Here a unit volume is assumed. If we now define a quantity M_0 such that

$$M_0 = M_0(B_0) - \frac{\partial}{\partial H} \left(\Omega_0 + \frac{B_0^2}{8\pi}\right), \tag{5.12}$$

then we have

$$\langle M\rangle = M_0 - \frac{\partial a}{\partial H} A^2$$

to lowest order in A^2. For the normal phase $A = 0$, so that the susceptibility is given by

$$\chi_N \equiv \frac{\partial\langle M\rangle}{\partial H} = \chi_0 . \tag{5.13}$$

In the MDW phase, A is given by the value corresponding to the minimum of G. It is given in Eq. (5. 9) as

$$A^2 = -\frac{a}{2b} \approx \left(\frac{\partial a}{\partial H}\bigg|_{H_c} (H - H_c)\right)\Big/ 2b(H_c) . \tag{5.14}$$

Hence the susceptibility in the MDW phase is given by

$$\chi_{\mathrm{MDW}} = \chi_0 + \left(\frac{\partial a}{\partial H}\right)^2_{H_c} \Big/ 2b(H_c) , \tag{5.15}$$

and the discontinuity in the susceptibility is

$$\Delta\chi = \left(\frac{\partial a}{\partial H}\right)^2_{H_c} \Big/ 2b(H_c) . \tag{5.16}$$

If we make use of the expressions in Eq. (5. 10) for a and b, it is not difficult to obtain an estimate for the order of magnitude of $\Delta\chi$. We will adopt a model in which one of the extremal cross sections of the Fermi surface gives the major contribution to $g_2, \cdots, g_n$, etc., at the wave number $q = \kappa$ of the MDW. We also assume this extremal area to be circular. In this case, the function $\mathcal{S}$ introduced in Sec. II becomes

$$\mathcal{S}(k_x, k_y) = 2J_1(kr_c)/kr_c \approx 1 \tag{5.17}$$

for this particular cross section, and approximately equal to zero for all other cross sections. According to Eq. (2. 35), the susceptibility when $|\vec{\mathrm{q}}| \approx |\vec{\kappa}|$ then becomes

$$4\pi\chi(\kappa) = g_2 \approx K\cos(cS_m/eB_0 \mp \tfrac{1}{4}\pi), \tag{5.18}$$

where K is a constant of the order of unity. Thus we obtain

$$\left(\frac{\partial a}{\partial H}\right)^2 \approx \left(\frac{\partial g_2}{\partial B_0}\right)^2 \approx \frac{K^2}{B_0^2}\left(\frac{E_F}{\hbar\omega_c}\right)^2 . \tag{5.19}$$

The order of magnitude of b is easily seen to be

$$|b| \approx |g_4(\kappa, \kappa, -\kappa)| \approx (|K|/B_0^2)(E_F/\hbar\omega_c)^2 . \tag{5.20}$$

Hence $|\Delta\chi/\chi_0| \sim 1$.[25] Since $\Delta\chi$ is of considerable magnitude, it should be readily observable experimentally. We can also do an exactly similar calculation for the discontinuity in the specific heat.

VI. MODEL CALCULATION

The possibility of a MDW state and the type of transition to that state will depend upon the coefficients a and b in Eq. (4. 7). We have seen that if $a > 0$ and $b > 0$, the trivial solution $A = 0$ minimizes the thermodynamic potential, while for $b < 0$ there is no minimum in the thermodynamic potential in the regime of infinitesimal A. This indicates that the transition is to a state of finite A and therefore first order. When $a < 0$ and $b > 0$, the MDW state of constant amplitude $A = (-a/2b)^{1/2}$ has the lowest free energy and the transition is second order as seen from Eq. (4. 7).

It seems worthwhile to investigate a simple model to see which of these conditions is realizable. We consider a Fermi surface with two extremal cross sections of elliptical shape, and take the magnetization M_0 to be of the form

$$M_0 = \alpha_1 \sin(2\pi f_1/B_0 + \delta_1) + \alpha_2 \sin(2\pi f_2/B_0 + \delta_2). \tag{6.1}$$

The frequencies f_1 and f_2 are proportional to the areas of the two extremal orbits; we define their ratio by the parameter $\eta = f_2/f_1$. The phase factors δ_1 are independent of magnetic field. By using Eqs. (6. 1) and (2. 35) we can obtain an explicit expression for the function $g_2(q)$:

$$\begin{aligned} g_2(q) = 4\pi\chi(q) &\approx a_1 \cos(2\pi f_1/B_0 + \delta_1)\, \mathcal{S}_1^2(q) \\ &\quad + a_2 \cos(2\pi f_1 \eta/B_0 + \delta_2)\, \mathcal{S}_2^2(q) . \end{aligned} \tag{6.2}$$

Here $a_i = -2\pi f_i \alpha_i/B_0^2$, and the functions $\mathcal{S}_i(q)$ are defined in terms of an integral over the orbit by Eq. (2. 33). For the present case of elliptical cross sections the functions $\mathcal{S}_i(q)$ are quite simple:

$$\mathcal{S}_i(q) = 2J_1(\vec{\mathrm{q}} \cdot \vec{\mathrm{r}}_{ci})\alpha/\vec{\mathrm{q}} \cdot \vec{\mathrm{r}}_{ci}) , \tag{6.3}$$

where $\vec{\mathrm{r}}_{ci}$ is the radius vector from the center to a point on the ith orbit. The procedure to be followed in looking at various instabilities is to plot $g_2(q)$ as a function of q_x, q_y, and B_0 for some fixed value of the temperature. Regions in which g_2 exceeds unity are regions of instability. A word of caution must be given at this point. We have been assuming that $g_2(q)$ is a function of the induction B_0. However, it is not B_0 that one controls experimentally, but an external magnetic field H_0. This point must certainly be kept in mind in thinking about what instabilities are realizable. For the $q = 0$ instabilities, both the discontinuous jump in the magnetization of a long thin rod and the domain state of a sample with finite demagnetizing factor occur slightly before[20] the point where $g_2(q = 0, B_0) = 1$. When these instabilities occur, whole regions of values of B_0 are not realized (e.g., for a long thin rod the magnetization jumps from some value $-M_1$ to a value M_1 at an applied field H; thus values of B between $H - 4\pi M_1$ and $H + 4\pi M_1$ are not realized within the sample). A peak of $g_2(q, B_0)$ at a finite value of q in a region of B_0 which is unrealized because of a $q = 0$ instability will not in general lead to a MDW state.

Clearly, Eq. (6. 2) is sufficiently complicated that a tremendous variety of situations can arise by properly choosing $a_1, a_2, f_1, f_2, \delta_1, \delta_2, r_{c1}$, and r_{c2}. We present some numerical results for one particular model in which the MDW state certainly occurs. Let the Fermi surface consist of two identical cigar-shaped ellipsoids whose major axes are oriented along the x and y directions, respectively. If the dc magnetic field is tilted very slightly off the z axis, the two extremal cross sections of the Fermi surface will differ in area by a very small amount. For a 1% difference, the beats resulting from the two slightly different de Haas–van Alphen frequencies will lead to almost completely distructive interference over hundred cycles of the main de Haas–van Alphen period. Consider $g_2(q, B_0)$ for a value of B_0 in such a region. The contributions to $g_2(q=0, B_0)$ from each of the orbits are exactly out of phase, giving a very small result. In Fig. 1 we plot $g_2(q_x, q_y=0, B_0)$ as a function of q_x. At $q_x=0$, the two contributions are out of phase, leading to the small value of g_2 mentioned above. However, as q_x increases, each of the orbits displays geometric resonances in their contributions to $g_2(q_x, B_0)$. Because the ellipsoid whose long axis is oriented along the y direction has a larger orbital diameter in the x direction, its contribution to $g_2(q_x)$ decreases very rapidly compared to that for the other orbit. The resulting maximum in $g_2(q_x, q_y=0, B_0)$ occurs at finite q_x and, if the amplitudes a_1 and a_2 are sufficiently large, will lead to a MDW state. Notice that there are no maxima of $g_2(q=0, B_0)$ for any nearby values of B_0, because it takes a hundred cycles for the two orbital contributions to constructively interfere. In Fig. 2 we plot contours of constant $g_2(q_x, q_y=0, B_0)$ in the q_x, B_0 plane. The values of the parameters appearing in Eq. (6. 2) which have been chosen in plotting these graphs are $\delta_1=0$, $\delta_2=\pi$, $\eta=1.0$ $\gamma=r_{c2}/r_{c1}=5$, $a_1=1.2$, and $a_2=1.1$. When using this model to calculate the coefficient b appearing in Eq. (4. 7), b is always positive when $g_2>1$.

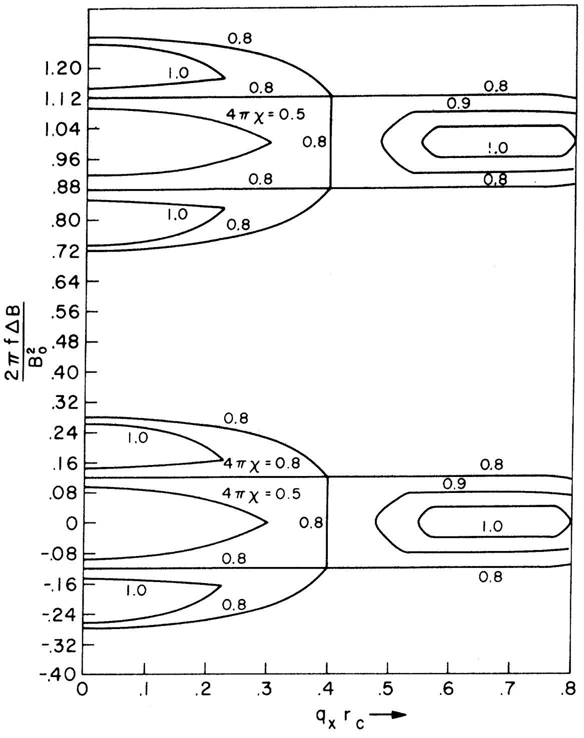

FIG. 2. Contours of constant $g_2(q_xq_y=0, B_0)$ in the q_x, B_0 plane for the model described in Fig. 1. The only maxima of $g_2(q, B_0)$ in this region of field occur at finite values of q.

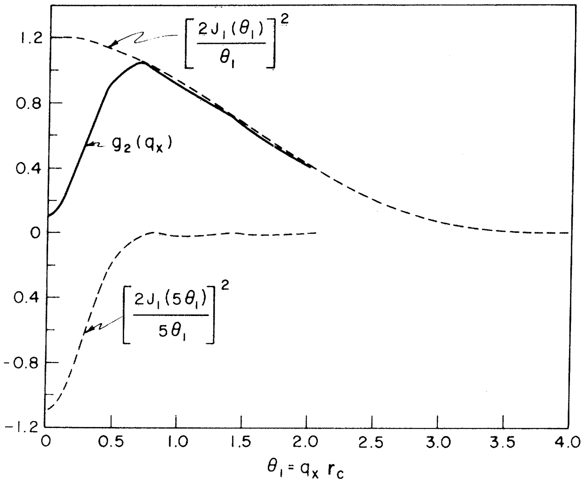

FIG. 1. Plot of $g_2(q_x, q_y, =0, B_0)$ versus q_x for a model consisting of two cigar-shaped ellipsoids of approximately equal area. The contributions of the two ellipsoids to g_2 at $q=0$ are out of phase, giving a very small value for $g_2(q=0, B_0)$. Because the orbital radii in the x direction differ, the cancellation does not hold at finite q, and a maximum of $g_2(q_x, B_0)$ occurs at finite q.

Clearly, we have investigated a very special model with particularly simple properties. For a real metal with a sufficiently complicated Fermi surface, many interesting instabilities caused by diamagnetic interactions among conduction electrons may occur.

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[19] This form for the thermodynamics potential was suggested by Azbel' in Ref. 3 without proof.

[20] Dr. E. I. Blount and Dr. J. Condon pointed out (in private discussion) that the domain-type transition actually occurs slightly before the point $4\pi\chi(q=0,\ B_0)=1$ is reached. Hence, in order to be absolutely sure that the system is stable against domain formation $4\pi\chi(q=0)$ has to be considerably less than unity.

[21] We have omitted a cross term in the derivative of A. This kind of term can always be removed by effecting a transformation of coordinate systems.

[22] When magnetostructure effects are neglected, the free energy is the same as the thermodynamic potential.

[23] Since $g_2(q)$ has a maximum at $q=\kappa$, $-\partial^2 g_2/\partial\kappa_i^2>0$ for $i=1,\ 2$.

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