#### **ACKNOWLEDGMENTS**

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# APPENDIX: CALCULATION OF CRITICAL TEMPERATURE OF McMILLAN MODEL

The method utilizes the fact that  $\Delta_s^{ph}$  goes to zero when T goes to  $T_c$ .

First, new variables x, y, and  $\gamma$  are defined by

$$\Delta_S = \chi \ \Delta_S^{ph}, \quad \Delta_N = y \ \Delta_N^{ph}, \quad \Delta_N^{ph} = \gamma \ \Delta_S^{ph}.$$
 (A1)

The new variables are introduced into Eqs. (1) and (2) of Ref. 1 and the equations are calculated in the limit  $\Delta_S^{ph} \rightarrow 0$ , giving

$$x\left(1 + \frac{i\Gamma_{S}}{E}\right) - y\frac{i\Gamma_{S}}{E} = 1,$$

$$x\frac{i\Gamma_{N}}{E} - y\left(1 + \frac{i\Gamma_{N}}{E}\right) = -\gamma$$
(A2)

and

$$\gamma = \lambda_N \int_0^{\omega_c^N} \operatorname{Re}\left(\frac{y}{E}\right) \tanh\frac{E}{2T} dE$$
,

Equations (A2) can be solved for x and y and the results put into Eqs. (A3). When eliminating  $\gamma$  from Eqs. (A3), after substitution of x and y, we get

$$F = \frac{\lambda_N \lambda_S \Gamma_N \Gamma_S I_1 I_3}{1 - \lambda_N I_2 / (\Gamma_S + \Gamma_N) - \lambda_N \Gamma_S I_1} + \frac{\lambda_S I_4}{\Gamma_S + \Gamma_N} + \lambda_S \Gamma_N I_3 - 1 = 0, \quad (A4)$$

where

$$I_1 = \int_0^{\omega_c^N} D(E) dE, \quad I_2 = \int_0^{\omega_c^N} E^2 D(E) dE,$$

$$I_3 = \int_0^{\omega_c^S} D(E) dE$$
,  $I_4 = \int_0^{\omega_c^S} E^2 D(E) dE$ ,

and

$$D(E) = \frac{\Gamma_N + \Gamma_S}{E^2 + (\Gamma_N + \Gamma_S)^2} \frac{1}{E} \tanh \frac{E}{2T}.$$

The temperature for which F=0 is the critical temperature of the McMillan model. This equation has more than one root, but the one of physical interest lies in the temperature interval between 1.2 and 3.8  $^{\circ}$ K.

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### Exchange Energy of an Electron Gas in a Magnetic Field

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The exchange energy of an electron gas is calculated in the zero-temperature limit. In high magnetic fields, it is shown that the exchange energy dominates the independent-particle energy, but in low and intermediate fields becomes much less important. Modifications due to band structure and application to the de Haas-van Alphen effect are discussed briefly.

#### I. INTRODUCTION

The free energy of a dense electron gas, which forms a basis for studying the thermodynamic properties of metals, is assumed to have a con-

vergent expression in powers of the parameter describing the electron-electron Coulomb interaction. (This parameter is customarily related to the mean interelectron spacing  $r_s$ .) The leading

 $<sup>1 = \</sup>lambda_S \int_0^{\omega_c^S} \operatorname{Re}\left(\frac{x}{E}\right) \tanh\frac{E}{2T} dE.$  (A3)

<sup>\*</sup>Research supported in part by the National Research Council of Canada.

<sup>&</sup>lt;sup>1</sup>J. Vrba and S. B. Woods, Phys. Rev. B <u>3</u>, 2243 (1971).

<sup>&</sup>lt;sup>2</sup>J. Vrba and S. B. Woods, in *Proceedings of the Twelfth International Conference on Low-Temperature Physics*, edited by E. Kanda (Academic Press of Japan, Tokyo, 1971).

<sup>&</sup>lt;sup>3</sup>W. L. McMillan, Phys. Rev. <u>175</u>, 537 (1968).

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<sup>&</sup>lt;sup>6</sup>S. M. Freake and C. J. Adkins, Phys. Letters <u>29A</u>, 382 (1969).

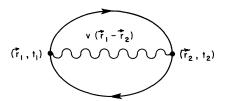


FIG. 1. Feynman diagram representing the secondorder exchange energy.

term in this expansion is simply the free particle or Fermi term and has been exhaustively studied in the absence and in the presence of a uniform magnetic field. <sup>1</sup> The second term consists of two parts: the mean-field electron-electron interaction, which is canceled exactly by the Coulomb interaction with a uniform charged background, and the exchange term which corresponds to the usual bubble diagram in Fig. 1. The remaining terms are lumped together and called the correlation energy.

The exchange energy in a uniform magnetic field has been examined previously by Dresselhaus<sup>2</sup> and Ichimura and Tanaka. 3 Dresselhaus calculated the exchange energy numerically in the high-magnetic-field regime (Fermi energy ~ Zeeman energy) by deriving the form of the exchange hole about each electron and then integrating the resulting charge distribution to obtain the exchange energy. In doing this, however, he effectively allowed the electron density to be field dependent to maintain a fixed occupation of the highest occupied Landau level. This introduces a spurious divergence for large fields and provides only an upper limit to the exchange energy. Dresselhaus concluded from his calculation that including the field dependence of the exchange energy should not affect the de Haas-van Alphen (dHvA) oscillations as calculated on the basis of the Fermi term alone, other than enhancing the amplitudes in the high-field regime.

Ichimura and Tanaka treated the diagram in Fig. 1 on the basis of Matsubara's propagator formalism and extracted the dominant oscillatory behavior at intermediate-field strengths. However, they did not include electron spin in their consideration and their numerical calculation of the field dependence of the amplitude was insufficiently convergent, which introduced spurious oscillatory behavior into their results. Their results, however, are accurate for sufficiently low magnetic fields where spin effects are not crucial and their numerical integrations converge well.

In this paper we reevaluate the behavior of the exchange energy in the high- and intermediate-field regimes by including spin properly and taking due account of the Landau level occupation. In

Sec. II we examine the strong-field limit  $\hbar\omega_c > \zeta$ , where  $\omega_c = e\hbar H/2mc$  is the cyclotron frequency and  $\zeta$  is the chemical potential. We find, per unit volume,

$$E_{\rm ex} = -\frac{27}{16\pi} \frac{\Re}{a_0^3} r_s^{-6} h^{-1} \ln(0.282 h r_s^2)$$
 (1.1)

for  $\hbar\omega_c\gg\xi$ , where  $\Re=1$  Ry,  $a_0=$  Bohr radius, and  $h=\hbar\omega_c/\Re$ . We also have

$$\zeta = \rho^2 \frac{(2\pi\hbar)^4}{(2m)^3 \omega_c^2} = \frac{9}{8} \pi^2 \Re h^{-2} r_s^{-6}, \qquad (1.2)$$

where  $\rho$  is the density. We note that the exchange energy does not diverge as  $H \rightarrow \infty$ , as in Dresselhaus's calculation. Furthermore, it is no longer correct to eliminate  $e^2$  in terms of  $r_s$  as is done in the zero-field case, since the relation between density and chemical potential is field dependent.

Section III contains a calculation of the dominant oscillatory contribution to the exchange energy in the intermediate-field regime  $(\zeta \gg \hbar \omega_c > kT)$ . It is found that this contribution to the dHvA term is weighted by the factor  $r_s^{-1}$   $(\hbar \omega_c/\xi)^{3/2}$ , whereas the neglected terms are weighted by  $r_s^{-1}$   $(\hbar \omega_c/\xi)^n$ , where  $n > \frac{3}{2}$ . This was not made explicit in Ref. 3. We find, in agreement with Ichimura and Tanaka, that at intermediate magnetic fields, the exchange and free-particle energies are not generally in phase. In addition we find that the exchange and Fermi terms depend differently on effective mass and g factor, which may have consequences for the thermodynamics of semimetals and degenerate semiconductors in high fields. The Appendices are concerned with some mathematical points.

## II. EXCHANGE ENERGY AT HIGH-FIELD STRENGTHS

By evaluating the diagram in Fig. 1, using the Martin-Schwinger propagator formalism as adapted by Horing, 4 we have, at zero temperature,

$$E_{\text{ex}} = \frac{1}{2} \operatorname{Tr} \left\{ \int d\overset{\leftarrow}{\mathbf{r}}_{1} \int d\overset{\leftarrow}{\mathbf{r}}_{2} v \left(\overset{\leftarrow}{\mathbf{r}}_{1} - \overset{\leftarrow}{\mathbf{r}}_{2}\right) \right.$$

$$\times \left[ \overline{G}_{<} (1, 2, \sigma_{3}) \overline{G}_{<} (2, 1, \sigma_{3}) \right]_{t_{1} = t_{2}} \right\}, \quad (2.1)$$

where

$$\begin{split} \overline{G}_{\varsigma}(1,2,\sigma_{3})_{t_{1}=t_{2}} &= C(\mathbf{r}_{1},\mathbf{r}_{2}) \int \frac{d\overline{p}}{(2\pi)^{3}} e^{i\overline{p}\cdot\overline{r}} \int d\omega i f_{0}(\omega) \\ &\times \int_{\delta-i\infty}^{\delta+i\infty} \frac{ds}{2\pi i} \exp \left[ s \left( \hbar \omega - \frac{\hbar^{2} p_{x}^{2}}{2m} - \mu_{0} H \sigma_{3} \right) \right] \\ &\times \operatorname{sech}(\frac{1}{2} \hbar \omega_{c} s) \exp \left[ - \left( \frac{\hbar \overline{p}^{2}}{m \omega_{s}} \tanh(\frac{1}{2} \hbar \omega_{c} s) \right) \right]. \quad (2.2) \end{split}$$

The trace in (1.1) is over spin  $\sigma_3 = \pm 1$ ;  $\rho_z$  and  $\overline{\rho}$  are the components of  $\overline{p}$  along and normal to the magnetic field,  $\overrightarrow{r} = \overrightarrow{r}_1 - \overrightarrow{r}_2$ ,  $\beta = 1/kT$ ;  $C(\overrightarrow{r}_1, \overrightarrow{r}_2)$  is a unitary phase factor,  $\mu_0 = ge\hbar/2m_0c$ ; and  $f_0(\omega)$  is the Fermi-Dirac distribution function. We consider an effective mass m which may differ from the free-electron mass  $m_0$ .

By using the expansion

$$\mathrm{sech}(\tfrac{1}{2}\hbar\omega_c s)\exp\left[-\left(\frac{\hbar\,\overline{p}^2}{m\,\omega_c}\,\tanh(\tfrac{1}{2}\hbar\omega_c s)\right)\right]$$

$$=2\sum_{n=0}^{\infty}(-1)^{n}e^{-\hbar\bar{p}^{2}/m\omega_{c}}L_{n}\left(\frac{2\,\bar{h}\,\bar{p}^{2}}{m\,\omega_{c}}\right)e^{-\hbar\omega_{c}s/2}e^{-\hbar n\omega_{c}s/2}$$
(2.3)

in terms of Laguerre polynomials  $L_n(x)$ , the s and  $\omega$  integrations in (2.2) are trivial and we find, introducing cylindrical coordinates,

$$\begin{split} & \overline{G}_{\zeta}(\overrightarrow{\mathbf{r}}_{1}, \overrightarrow{\mathbf{r}}_{2}, \sigma_{3})_{t_{1}=t_{2}} \\ &= 2iC(\overrightarrow{\mathbf{r}}_{1}, \overrightarrow{\mathbf{r}}_{2}) \sum_{n=0}^{\infty} (-1)^{n} \int_{-\infty}^{\infty} \frac{dp_{z}}{(2\pi)} \int_{0}^{\infty} \frac{\overline{p}d\overline{p}}{2\pi} \int_{-\pi}^{\pi} \frac{d\theta}{2\pi} \\ & \times e^{i\overline{p}r\sin\theta} e^{ip_{z}r_{z}} e^{-\hbar\overline{p}^{2}/m\omega_{c}} L_{n} \left(\frac{2\overline{h}\overline{p}^{2}}{m\omega_{c}}\right) \\ & \times f_{0} \left(\frac{\hbar^{2}p_{z}^{2}}{2\omega_{c}} + (n + \frac{1}{2}) \hbar\omega_{c} + \frac{1}{2}\sigma_{3} \hbar\omega_{c}\right) . \end{split}$$

The  $\theta$  integration gives  $J_0(\overline{p}\,\overline{r}),$  the  $p_z$  integration yields

$$\begin{split} &(\pi r_z)^{-1} \eta_+ (\zeta - (n + \frac{1}{2}) \hbar \omega_c - \frac{1}{2} \sigma_3 \hbar \omega_c) \\ &\times \text{sin} r_z \Big\{ (2m/\hbar^2) \big[ \zeta - (n + \frac{1}{2}) \hbar \omega_c - \frac{1}{2} \sigma_3 \hbar \omega_c \big] \big\}^{1/2} \,, \end{split}$$

where

$$\eta_{+}(x) = 0$$
 if  $x < 0$ ,  $\eta_{+}(x) = 1$  if  $x > 0$ .

while the  $\bar{p}$  integral is tabulated. Thus, after making the coordinate transformation  $\vec{r} = \vec{r}_1 - \vec{r}_2$ ,  $\vec{R} = \frac{1}{2}(\vec{r}_1 + \vec{r}_2)$ , we obtain (per unit volume)

$$E_{ex} = -4\pi e^{2} \sum_{\sigma_{3}} \int_{-\infty}^{\infty} dr_{z} \int_{0}^{\infty} \overline{r} \, d\overline{r} \, (r_{z}^{2} + \overline{r}^{2})^{-1/2}$$

$$\times \left\{ \sum_{n=0}^{\infty} \eta_{+} \left( \xi - (n + \frac{1}{2}) \overline{h} \omega_{c} - \frac{1}{2} \sigma_{3} \overline{h} \omega_{c} \right) \frac{m \omega_{c}}{4 \pi^{2} \overline{h} r_{z}} \right\}$$

$$\times \sin \left[ r_{z} \left( \frac{2m}{h^{2}} \left[ \xi - (n + \frac{1}{2} + \sigma_{3}) \overline{h} \omega_{c} \right] \right)^{1/2} \right]$$

$$\times e^{-m \omega_{c}} \overline{r}^{2/4h} L_{n} \left( \frac{m \omega_{c} \overline{r}^{2}}{2 \overline{h}} \right) \right\}^{2} . \quad (2.5)$$

In the strong-field limit  $(\hbar \omega_c > \zeta)$ , (2.5) becomes

$$E_{ex} = -\frac{4e^2}{(2\pi)^3} \left(\frac{m\omega_c}{\hbar}\right)^2 \int_0^\infty dr_z r_z^{-2} \sin^2\left[\left(\frac{2m\xi}{\hbar^2}\right)^{1/2} r_z\right] \times \int_0^\infty d\overline{r} \, \overline{r} \, (\overline{r}^2 + r_z^2)^{1/2} e^{-(m\omega_c/2\hbar)\overline{r}^2} \,. \tag{2.6}$$

After making the change of variable  $\bar{r}^2 = (2\hbar/m\omega_c) \times (r_z t + \hbar t^2/2m\omega_c)$ , and obtaining the  $r_z$  integral from a table of Laplace transforms, <sup>6</sup> we find

$$E_{ex} = -(e^{2}/4\pi^{3})(m\omega_{c}/\bar{n})^{2} \left[ p \int_{0}^{\infty} dx \, x \ln(x^{2}) e^{-\rho x^{2}} \right]$$
$$-p \int_{0}^{\infty} dx \, x \ln(x^{2}+1) e^{-\rho x^{2}}$$
$$+2p \int_{0}^{\infty} dx \, e^{-\rho x^{2}} \tan^{-1}(1/x) \right], \quad (2.7)$$

where  $p = (4\xi/\hbar\omega_c)$ . In Appendix A it is shown that this may be written, where C is Euler's constant 0.5772...,

$$E_{ex} = (e^2/8\pi^3)(m\omega_c/\hbar)^2 \left[\ln p + C - e^p \text{Ei}(-p) - p^{1/4}G_{23}^{22} \left(p \mid_{3/4,3/4,1/4}^{3/4,5/4}\right)\right].$$
 (2.8)

From this we find the behavior for  $p \ll 1$ :

$$E_{\rm ex}(p) \simeq (e^2/8\pi^3)(m\omega_c/\hbar)^2 p[\ln p - (3-C)].$$
 (2.9)

In conjunction with (2.9) we note that at fixed electron concentration  $(\xi = 2\pi^4 \, \hbar^4 \, \rho^2/m^3 \omega_c^2)$  the exchange energy vanishes as the magnetic field becomes infinite, and exceeds the free-particle energy per unit volume

$$E_F = \frac{1}{3} \frac{m^{3/2} \zeta^{3/2} \omega_c}{2^{1/2} \pi^2 \hbar^2} = \frac{9}{32} \pi \left(\frac{\Re}{a_0^3}\right) h^{-2} r_s^{-9}$$
 (2. 10)

in this limit; whereas if one considers a band model in high magnetic field [all electrons in the lowest Landau state with spins antiparallel to the magnetic field or  $\frac{1}{2}(1+\nu)\hbar\omega_c > \zeta$  where  $\nu = gm/2m_0$ ], one finds that the exchange energy is given by (2.8) and (2.9), with

$$p = \frac{4\left[\zeta - \frac{1}{2}(1 - \nu)\hbar\omega_c\right]}{\hbar\omega},$$

and is less than the free-particle energy in the limit  $p \ll 1$ ,

$$\begin{split} E_F &= \frac{2(2m)^{1/2}}{(2\pi)^2} \;\; \frac{m\,\omega_c}{\hbar^2} \; \left\{ \left[ \xi - \frac{1}{2}(1-\nu)\,\hbar\omega_c \right]^{1/2}\, \tfrac{1}{2}\, (1-\nu)\,\hbar\omega_c \\ &\quad + \tfrac{1}{3} \left[ \xi - \tfrac{1}{2}(1-\nu)\,\hbar\omega_c \right]^{3/2} \right\}, \end{split}$$

with 
$$\zeta - \frac{1}{2}(1 - \nu)\bar{h}\omega_c = 2\pi^4 \,\bar{h}^4 \,\rho^2/m^3 \,\omega_c^2$$
.

# III. EXCHANGE ENERGY AT INTERMEDIATE-FIELD STRENGTH

Here essentially we follow the work of Ichimura and Tanaka but with spin effects included in the propagator. The integral over  $\vec{p}$  in (2.2) is performed by transforming to cylindrical coordinates as before and we find (including the effect of a non-free-electron g factor)

$$E_{ex} = -e^{2} \left(\frac{m^{3/2}\omega_{c}}{2^{5/2}\pi^{3/2}\hbar^{2}}\right)^{2} \int \frac{d\mathbf{r}}{r} \int_{0}^{\infty} d\omega \frac{df_{0}(\omega)}{d\omega} \int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} \frac{e^{s\hbar\omega}}{s^{3/2}\sinh(\frac{1}{2}\hbar\omega_{c}s)} \cosh\left(\frac{gm}{m_{0}} \left(\frac{1}{2}\hbar\omega_{c}\right)(s+s')\right) e^{-mr_{z}^{2}/2s\hbar^{2}}$$

$$\times \exp\left(-\frac{m\omega_{c}\overline{r}^{2}}{4\hbar\tanh(\frac{1}{2}\hbar\omega_{c}s)}\right) \int_{0}^{\infty} d\omega' \frac{df_{0}(\omega')}{d\omega'} \int_{c-i\infty}^{c+i\infty} \frac{ds'}{2\pi i} \frac{e^{s'\hbar\omega}}{(s')^{3/2}\sinh(\frac{1}{2}\hbar\omega_{s}')} e^{-mr_{z}^{2}/2s'\hbar^{2}} \exp\left(-\frac{m\omega_{c}\overline{r}^{2}}{4\hbar\tanh(\frac{1}{2}\hbar\omega_{c}s')}\right). \tag{3.1}$$

The singularities of the s and s' integrals in (3.1) are of two types: (a) isolated essential singularities along the imaginary axis at s, s'=  $2\pi ni/\hbar\omega_c$ ,  $n=\pm 1,\pm 2,\ldots$ , and (b) a branch cut along the negative real axis with branch points at 0 and  $-\infty$ . These singularities give rise to characteristic behavior in the exchange energy. At intermediate magnetic fields ( $\hbar\omega_c < \zeta$ ) the leading dHvA contribution to the exchange energy comes from terms due to the isolated singularity contributions to the two s integrals in (3.1). We evaluate these terms by retaining the leading term of the Laurent expansion of the hyperbolic functions appearing in the integrand. By a simple change of variables the contour integral corresponding to each of the isolated singularities can be transformed to one of the form

$$\int \frac{dx}{2\pi i} e^{x\xi} x^{-1} e^{-m\bar{r}^2/2\hbar^2 x} = J_0 \left[ 2 \left( \frac{m\bar{r}^2 \zeta}{2\hbar^2} \right)^{1/2} \right] ,$$

where the contour encircles x=0. The branch line contribution to the s integrals is evaluated by expanding the integrand in powers of  $\omega_c$ ; the leading term of this series expansion gives rise to an integral of the form

$$\int_{c-i\infty}^{c+i\infty} \frac{ds}{2\pi i} e^{s\xi} s^{-5/2} e^{-mr^2/2\hbar^2 s}$$

$$=J_{3/2}\left[2\left(\frac{\xi m r^2}{2\hbar^2}\right)^{1/2}\right]\left(\frac{2\hbar^2 \xi}{m r^2}\right)^{3/4}.$$

The leading dHvA contribution to the exchange energy is given in terms of the branch cut of one and dHvA contributions of the other s integrals. Therefore we have

$$E_{\text{ex}} = -e^{2} \frac{m^{3}}{\hbar^{6}8\pi^{3}} \left(\frac{2\hbar^{2}\zeta}{m}\right)^{3/4} \sum_{\substack{n=1\\\sigma=\pm 1}}^{\infty} (-1)^{n} \frac{2\pi^{2}n\sigma/\hbar\omega_{c}\beta}{\sinh(2\pi^{2}n\sigma/\hbar\omega_{c}\beta)} \frac{e^{2\pi i n\sigma\xi/\hbar\omega_{c}}}{2\pi i n\sigma/\hbar\omega_{c}}$$

$$\times \left\{ \left[\cos\left(\frac{gm}{m_{0}}\right)\pi n\right] + 1\right\} \int d\mathbf{r} \, \mathbf{r}^{-5/2} J_{0} \left[2\left(\frac{m\overline{r}^{2}\zeta}{2\hbar^{2}}\right)^{1/2}\right] \exp\left(\frac{i m r_{z}^{2}\omega_{c}}{4\hbar\pi n}\right) J_{3/2} \left[2\left(\frac{\zeta m r^{2}}{2\hbar^{2}}\right)^{1/2}\right]. \tag{3.2}$$

By separating the r integral in spherical polar coordinates we have

$$E_{\text{ex}} = B \sum_{n=1}^{\infty} \frac{(-1)^n}{n^{3/2}} \frac{2\pi^2 n/\hbar \omega_c \beta}{\sinh(2\pi^2 n/\hbar \omega_c \beta)} \left[ 1 + \cos\left(\frac{gm}{m_0} \pi n\right) \right] \overline{Q}(p) , \qquad (3.3)$$

where

$$\rho B = \frac{m^2 e^2 (\hbar \omega_c)^{3/2} \zeta^{1/2}}{2^4 \pi^{9/2} \hbar^4} = r_s^{-1} \left[ \frac{9(\frac{1}{4}\pi)^{1/3}}{2^5 \pi^{5/2}} \right] \left( \frac{\hbar \omega_c}{\zeta} \right)^{3/2}, \tag{3.4}$$

$$\overline{Q}(p) = \cos\left(\frac{2\pi n\zeta}{\hbar\omega_c} - \frac{\pi}{4}\right)S(p) + \sin\left(\frac{2\pi n\zeta}{\hbar\omega_c} - \frac{\pi}{4}\right)C(p),$$

$$\frac{C(p)}{S(p)} = \int_0^\infty dx \, x^{-1/2} J_{3/2}(x) \int_{-1}^1 dz \, J_0 \left[ x (1 - z^2)^{1/2} \right] \begin{cases} \cos(p x^2 z^2) \\ \sin(p x^2 z^2) \end{cases}, \tag{3.5}$$

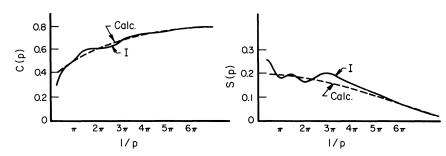


FIG. 2. Amplitude factors given by Eq. (3.5). The solid curves denoted I are the results of Ichimura and Tanaka. The dashed curve shows the present results.

and  $p = \hbar \omega_c / 8\pi \zeta n$ . Equations (3.3)-(3.5) correspond to Eqs. (3.8)-(3.10) in Ref. 3. It is shown in Appendix B that C(p) and S(p) may be expressed as

$$C(p) = (2/\pi)^{1/2} - (2\pi)^{-1}p^{-1/2}[C_0(p) + S_0(p)],$$
(3.6a)

$$S(p) = -(2\pi)^{-1} p^{-1/2} \left[ C_0(p) - S_0(p) \right], \tag{3.6b}$$

where

$$\frac{C_0(p)}{S_0(p)} = -\int_0^\infty dt \, t^2 (1+t^2)^{-1/2} \ln \left( \frac{(1+t^2)^{1/2}-1}{(1+t^2)^{1/2}+1} \right) \begin{cases} \cos(t^2/4p) \\ \sin(t^2/4p) \end{cases}$$
 (3.7)

For small p we find

$$C(p) \cong (2/\pi)^{1/2}, \quad S(p) \cong -p(2/\pi)^{1/2} \ln(\frac{1}{4}p).$$
 (3.8)

Ichimura and Tanaka calculated the complicated double integrals in Eq. (3.5) numerically. The fact that we have reduced them to rapidly convergent single integrals allows us to obtain a more accurate picture of the behavior of these functions. In particular, we find that the irregular oscillations found by these authors are absent and we obtain the simple behavior shown in Fig. 2.

We find from Eqs. (3.3) that the exchange energy is not in phase with the free-particle energy and that the free-particle and exchange energy depend differently on the effective mass and g factor.

$$E_{F}/E_{F}^{0} = (m_{0}/m)\cos(gm\pi/m_{0}),$$

$$E_{ex}/E_{ex}^{0} = \frac{1}{2}[1 + \cos(gm\pi/m_{0})].$$
(3.9)

In the case of simple metals, the exchange energy is small compared to the free-particle energy at intermediate-field strength, and these facts are of little consequence for thermodynamic properties such as the magnetic susceptibility where

$$\frac{\chi_{\rm ex}\,({\rm dHvA})}{\chi_F\,({\rm dHvA})} \sim \left(\frac{\zeta}{\hbar\omega_c}\right) \gamma_s.$$

It is interesting to note that Berlincourt and Steele<sup>7</sup> point out that the field dependence of the amplitude of the obserfed dHvA magnetic susceptibility in zinc is one power lower in magnetic field strength than

the free-particle susceptibility. For semimetals and degenerate semiconductors where the quantum limit is easily reached, however, it appears that the field dependence of the exchange energy must be taken into account in comparing theory and experiment.

### ACKNOWLEDGMENT

We wish to thank Dr. N. Winter for programming the numerical integration.

### APPENDIX A

The first two integrals in (1.7) may be obtained from a table of Laplace transforms. Consider

$$F(a) = \int_0^\infty e^{-a^2x^2} \tan^{-1}(1/x) dx$$
.

By a simple change of variable we have

$$F(a) = a^{-1} \int_0^\infty e^{-t^2} \tan^{-1} \left(\frac{a}{t}\right) dt$$
$$= \left(\frac{\pi^{1/2}}{2a}\right) \int_0^\infty \frac{\partial}{\partial t} \left(\operatorname{erf} t\right) \tan^{-1} \left(\frac{a}{t}\right) dt$$
$$= \left(\frac{1}{2}\pi^{1/2}\right) \int_0^\infty \frac{\operatorname{erf} t}{a^2 + t^2} dt ,$$

where we have integrated by parts. Now by noting that

$$\operatorname{erf} t = (2/\pi^{1/2}) t^{-1/2} e^{-t^2/2} M_{-1/4,1/4}(t^2)$$

and letting  $x = t^2$  we obtain

$$F(a) = \frac{1}{2} \int_0^\infty \frac{t^{-3/4} e^{-t/2} M_{-1/4,1/4}(t)}{a^2 + t}$$
$$= \frac{1}{4} a^{-3/2} G_{23}^{22} \left(a^2 \left| \frac{3/4}{3/4} \right|_{1/4}^{5/4} \right) ,$$

which is a known Stieltjes transform. 8

#### APPENDIX B

Let

$$I_1 = 2 \int_0^1 dz \ J_0[x (1-z)^{1/2}] \begin{cases} \cos(px^2z^2) \\ \sin(px^2z^2) \end{cases}$$

We note the Fourier cosine transform pairs

$$\eta_{+}(1-z)J_{0}[x(1-z^{2})^{1/2}] \cdot \sim (x^{2}+y^{2})^{-1/2}\sin(x^{2}+y^{2})^{1/2}$$

$$\frac{\cos(px^2z^2)}{\sin(px^2z^2)} \left\langle - - \frac{1}{4x} \left( \frac{2\pi}{p} \right)^{1/2} \left[ \cos\left( \frac{y^2}{4px^2} \right) \pm \sin\left( \frac{y^2}{4px^2} \right) \right] \right].$$

So, by Parseval's theorem, we have

$$I_1 = \frac{1}{x} \left(\frac{2}{\pi p}\right)^{1/2} \int_0^\infty (1+y^2)^{-1/2} \sin[x(1+y^2)^{1/2}]$$

$$\times \left[\cos\left(\frac{y^2}{4p}\right) \pm \sin\left(\frac{y^2}{4p}\right)\right] dy$$
 .

Next, note that

$$\begin{split} I_2 &= \int_0^\infty dx \, x^{-3/2} J_{3/2}(x) \sin(ax) \\ &= (\frac{1}{2}\pi a)^{1/2} \int_0^\infty dx \, x^{-1} J_{3/2}(x) J_{1/2}(ax), \end{split}$$

where

$$a = (1 + y^2)^{1/2}$$

which is a Weber-Schaftheitlin integral and has the value

$$\begin{split} I_2 &= \frac{1}{3} a^{-1} (2/\pi)^{1/2} \,_2 F_1(\frac{1}{2}, \, 1; \, \frac{5}{2}; \, 1/a^2) \\ &= \frac{1}{4} \left( \frac{2}{\pi} \right)^{1/2} (1 - a^2) \, \left[ \ln \left( \frac{a+1}{a-1} \right) \, + \frac{2a}{1-a^2} \right], \quad a > 1 \ . \end{split}$$

Thus we obtain

$$\frac{C(p)}{S(p)} = \left(\frac{1}{2\pi}\right) p^{-1/2} \int_0^\infty dy \, y^2 (1+y^2)^{-1/2} \\
\times \left[ 2y^{-2} (1+y^2)^{1/2} + \ln\left(\frac{(1+y^2)^{1/2} - 1}{(1+y^2)^{1/2} + 1}\right) \right] \\
\times \left[ \cos\left(\frac{y^2}{4p}\right) \pm \sin\left(\frac{4^2}{4p}\right) \right],$$

which is equivalent to (3.6) and (3.7).

Series and Products (Academic, New York, 1965), Eq. 7.421.

<sup>6</sup>A. Erdélyi *et al.*, *Tables of Integral Transforms* (McGraw-Hill, New York, 1954), Vol. I, p. 160, Eq. 83. <sup>7</sup>T. G. Berlincourt and M. C. Steele, Phys. Rev. <u>94</u>, 1421 (1954).

<sup>8</sup>Reference 6, Vol. II, p. 231.

PHYSICAL REVIEW B

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## Magnetization of Dirty Superconductors near the Upper Critical Field\*

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The magnetic behavior of a type-II superconductor with very short electron mean free path (dirty limit) near its upper critical field  $B_{c2}(T)$  is investigated. A calculation of the magnetization up to the second order in the difference between  $B_{c2}(T)$  and the external magnetic field is presented which is valid for all temperatures. A triangular and a square lattice of flux lines are considered. A numerical calculation suggests that the triangular lattice remains stable despite the fact that the difference in the thermodynamical potentials between the two lattices decreases due to these second-order terms.

## I. INTRODUCTION

The magnetic behavior of type-II superconductors was first explained theoretically by Abrikosov.<sup>1</sup>

On the basis of the Ginzburg-Landau theory, <sup>2</sup> Abrikosov showed that a type-II superconductor exhibits a mixed state between the two critical magnetic fields  $B_{\rm cl}(T)$  and  $B_{\rm cl}(T)$  in which the mag-

<sup>&</sup>lt;sup>1</sup>A. H. Wilson, *The Theory of Metals*, 2nd ed. (Cambridge U. P., Cambridge, England, 1954).

<sup>&</sup>lt;sup>2</sup>G. Dresselhaus, Phys. Rev. 114, 736 (1959).

<sup>&</sup>lt;sup>3</sup>H. Ichimura and S. Tanaka, Progr. Theoret. Phys. (Kyoto) 25, 315 (1961).

<sup>&</sup>lt;sup>4</sup>N. J. Horing, Ann. Phys. (N. Y.) 31, 1 (1965).

<sup>&</sup>lt;sup>5</sup>I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals*,