

Exchange Energy of an Electron Gas in a Strong Magnetic Field*

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The magnetic field variation of the exchange energy of a free-electron gas is calculated by deriving the form of the "Fermi hole" around each electron. The wave functions which are used exactly diagonalize the kinetic energy. The resulting charge distribution is integrated to find the exchange energy. The exchange energy has the same periodicity in the reciprocal magnetic field which is displayed by the kinetic energy. Hence, it is concluded that the de Haas-van Alphen effect is unchanged by the field variation of the exchange energy except for a possible shift in the phase of the oscillations.

RECENT investigations by Gell-Mann and Brueckner,¹ Sawada,² and Sawada *et al.*³ have revived interest in the calculation of the ground-state energy of a dense free-electron gas. The ground-state energy per particle in the presence of a uniform background of positive charge is

$$E = \left[\frac{2.21}{r_s^2} - \frac{0.916}{r_s} + E_C \right] \text{ ry}, \quad (1)$$

in which the terms on the right are the mean kinetic energy, the exchange energy, and the correlation energy in that order. The quantity, r_s , is the radius of the Wigner-Seitz sphere, measured in units of the Bohr radius, and the energy is measured in Rydbergs. In the original work, Wigner and Seitz calculated the exchange energy,⁴ while the correlation energy was estimated by Wigner.⁵ The recent studies¹⁻³ give an explicit quantum mechanical derivation of the correlation energy.

The magnetic properties of a free-electron gas have been examined by Wentzel⁶ using the Sawada formalism.² For weak magnetic fields Wentzel found the diamagnetic susceptibility to be unaffected by the Coulomb interactions; that is, the result of Landau and Peierls⁷ was verified. However, the perturbation treatment used by Wentzel⁶ is not applicable to the case of strong magnetic fields, which is also physically interesting. Experimental studies of high-field quantum effects, such as the de Haas-van Alphen effect, have supplied valuable information relating to the electronic structure of metals.

To date, calculation of the de Haas-van Alphen effect has been limited to consideration of the magnetic field dependence of the kinetic energy. In this work the effect of the magnetic field on the exchange energy term is in-

vestigated. The field variation of the correlation energy, though probably important, is not considered here.

The wave functions which diagonalize the kinetic energy term in the Hamiltonian are

$$\Psi_{nkq} = (L_x L_z)^{-\frac{1}{2}} [\exp i(kx + qz)] \phi_n(y + \lambda^2 q), \quad (2)$$

in which the static magnetic field, H , is along the x direction and in which ϕ_n is the harmonic oscillator wave function in state n , $\lambda^2 = \hbar(m\omega_c)^{-1}$, and $\omega_c = eH/(mc)^{-1}$. The normalization of Ψ is in a box of rectangular cross section, $L_x L_z$, and the eigenstates are designated by n , and the wave numbers k and q . The energy eigenvalues associated with the wave functions are

$$\epsilon_{nk} = (2m)^{-1} \hbar^2 k^2 + \hbar \omega_c (n + \frac{1}{2}). \quad (3)$$

The mean kinetic energy per particle is given by

$$E_{KE} = \left\{ \sum f_0(\epsilon_{nk}) \right\}^{-1} \sum \epsilon_{nk} f_0(\epsilon_{nk}), \quad (4)$$

in which f_0 is the Fermi-Dirac distribution function and the summation is over the quantum numbers, n , k , q . At 0°K, Eq. (4) yields for the ground-state energy

$$E_{KE} = \frac{2.21}{r_s^2} (1 + g) \text{ ry}, \quad (5)$$

where

$$g = \frac{2}{3} - \frac{10}{9} \frac{\hbar \omega_c}{\eta} \sum_{n=0}^{n_F} (n_F - n)^{\frac{3}{2}} / \sum_{n=0}^{n_F} (n_F - n)^{\frac{1}{2}}, \quad (6)$$

$\eta =$ Fermi energy, and $n_F = (\eta/\hbar\omega_c) - \frac{1}{2}$. The upper limit in the summation over n is taken to be the largest integer $\leq n_F$. The magnetic field dependence of E_{KE} is contained in g and is shown in Fig. 1. The periodicity in $\eta/\hbar\omega_c$ observed in this plot is characteristic of the de Haas-van Alphen effect.

This work treats the exchange energy in the presence of strong magnetic fields by calculating the form of the "Fermi hole" around each electron in the gas using the wave functions which exactly diagonalize the kinetic energy, i.e., Eq. (2). Treating the Coulomb energy as a perturbation, one obtains as the first order correction to the energy

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¹ M. Gell-Mann and K. Brueckner, *Phys. Rev.* **106**, 364 (1957).

² K. Sawada, *Phys. Rev.* **106**, 372 (1957).

³ Sawada, Brueckner, Fukuda, and Brout, *Phys. Rev.* **108**, 507 (1957).

⁴ See, for example, N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, London, 1936), p. 139.

⁵ E. P. Wigner, *Phys. Rev.* **46**, 1002 (1934).

⁶ G. Wentzel, *Phys. Rev.* **108**, 1593 (1957).

⁷ N. F. Mott and H. Jones, reference 4, p. 201.

$$E_1 = \frac{1}{4} \{ \sum f_0(\epsilon_{nk}) \}^{-2} \sum f_0(\epsilon_{nk}) f_0(\epsilon_{n'k'}) \times \int d\mathbf{x}_1 \int d\mathbf{x}_2 e^2 |\mathbf{x}_1 - \mathbf{x}_2|^{-1} \times | \Psi_{nkq}(\mathbf{x}_1) \Psi_{n'k'q'}(\mathbf{x}_2) - \Psi_{nkq}(\mathbf{x}_2) \Psi_{n'k'q'}(\mathbf{x}_1) |^2. \quad (7)$$

This expression contains both an exchange term and a direct Coulomb interaction, the latter term being cancelled by the interaction with the uniform positive charge density. The relative probability per unit volume, $P(r)$, that another electron with parallel spin will be found a distance r from a given electron is⁸

$$P(r) = \frac{1}{2} \{ \sum f_0(\epsilon_{nk}) \}^{-2} \sum f_0(\epsilon_{nk}) f_0(\epsilon_{n'k'}) \times | \Psi_{nkq}(\mathbf{x}_1) \Psi_{n'k'q'}(\mathbf{x}_2) - \Psi_{nkq}(\mathbf{x}_2) \Psi_{n'k'q'}(\mathbf{x}_1) |^2, \quad (8)$$

where $r = |\mathbf{x}_1 - \mathbf{x}_2|$. The evaluation of Eq. (8) using plane waves (i.e., $H=0$) for the eigenfunctions gives

$$P(r) = 1 - 9(k_F r)^{-6} (\sin k_F r - k_F r \cos k_F r)^2, \quad (9)$$

in which k_F is the value of the wave number at the Fermi surface. By subtracting the interaction with the uniform positive charge background, the exchange energy per particle is found to be

$$E_{ex} = 2\pi e^2 \int_0^\pi \sin\theta d\theta \int_0^\infty r dr [P(r) - 1]. \quad (10)$$

The substitution of Eq. (9) into Eq. (10) yields the exchange energy term of Eq. (1).

The evaluation of Eq. (8) for an electron in a magnetic field can be carried out using the Landau wave functions of Eq. (2). The result is

$$P(x, \rho) = 1 - \left\{ \sum_{n=0}^{n_F} \sqrt{2\lambda}^{-1} x (n_F - n)^{\frac{1}{2}} \right\}^{-2} \times \left\{ \sum_{n=0}^{n_F} \sin[\sqrt{2\lambda}^{-1} x (n_F - n)^{\frac{1}{2}}] \right\} \times \exp[-\rho^2/4\lambda^2] L_n(\rho^2/2\lambda^2)^2, \quad (11)$$

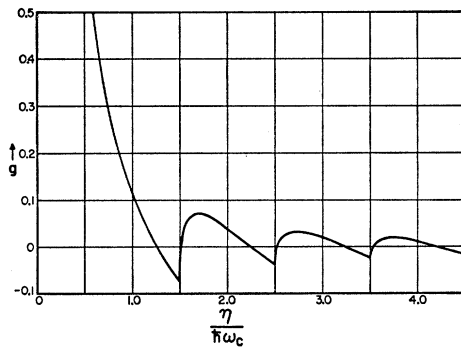


FIG. 1. Magnetic field dependence of the mean kinetic energy of a free-electron gas. $1+g$ is proportional to the mean kinetic energy per particle and $(\eta/\hbar\omega_c)$ is the Fermi energy relative to the magnetic energy.

⁸ E. Wigner and F. Seitz, Phys. Rev. 43, 804 (1933).

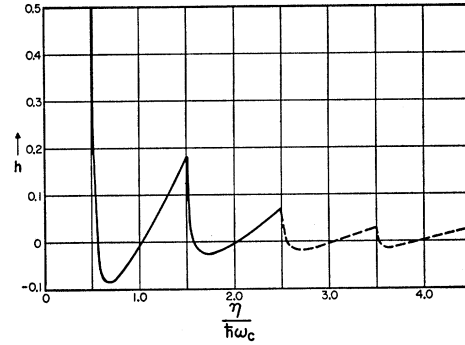


FIG. 2. Magnetic field dependence of the exchange energy. $1+h$ is proportional to the exchange energy per particle and $(\eta/\hbar\omega_c)$ is the Fermi energy relative to the magnetic energy. The dashed curve for $(\eta/\hbar\omega_c) > 2.5$ has been inferred from the integrals calculated for $(\eta/\hbar\omega_c) < 2.5$.

in which the cylindrical coordinates, ρ and x , are used because of the symmetry of the problem, and $L_n(x)$ is the Laguerre polynomial of order n defined by⁹

$$\sum_{n=0}^{\infty} L_n(x) z^n = (1-z)^{-1} \exp\left(\frac{xz}{1-z}\right). \quad (12)$$

In the limit of zero magnetic field, Eq. (11) can be shown to reduce to Eq. (9) if the summations are replaced by integrations and the asymptotic expansion for large n is used for the Laguerre polynomial,

$$\exp(-x^2/2) L_n(x^2) \approx J_0[2x(n+\frac{1}{2})^{\frac{1}{2}}], \quad (13)$$

in which J_0 is the zero-order Bessel function.

The exchange energy per electron is obtained by substituting Eq. (11) into the integral of (10), yielding

$$E_{ex} = -\frac{0.916}{r_s} (1+h) \text{ ry}, \quad (14)$$

where

$$h = -1 + \left(\frac{2}{9}\right) \left(\frac{\eta}{\hbar\omega_c}\right) \left\{ \sum_{n=0}^{n_F} (n_F - n)^{\frac{1}{2}} \right\}^{-2} \sum_{i,j=0}^{n_F} \mathfrak{S}_{ij}, \quad (15)$$

and

$$\mathfrak{S}_{ij} = 2 \int_0^\infty d\nu \nu^{-2} \sin[2\nu(n_F - i)^{\frac{1}{2}}] \sin[2\nu(n_F - j)^{\frac{1}{2}}] \times \int_0^\infty \mu d\mu (\nu^2 + \mu^2)^{-\frac{1}{2}} \exp(-\mu^2) L_i(\mu^2) L_j(\mu^2). \quad (16)$$

Inserting the generating function for Laguerre polynomials (12), one obtains

⁹ A. Erdélyi et al., Higher Transcendental Functions (McGraw-Hill Book Company, Inc., New York, 1953), Vol. 1, Chap. 6.

$$\mathfrak{S}_{ij} = \frac{1}{\sqrt{\pi}} \sum_{k,l,n=0}^{\infty} \frac{(-1)^{i+j-n} \Gamma(n+l+1) \Gamma(\frac{1}{2}+n)}{\Gamma(l+1) \Gamma(i-l-k+1) \Gamma(j-l+k-n+1) \Gamma(n-i+l+1) \Gamma(n+l-j+1)} \\ \times \int_0^{\infty} d\nu \nu^{-2} \sin[2\nu(n_F-i)^{\frac{1}{2}}] \sin[2\nu(n_F-j)^{\frac{1}{2}}] \Psi(\frac{1}{2}+n, \frac{1}{2}; \nu^2), \quad (17)$$

where

$$\Psi(\frac{1}{2}+n, \frac{1}{2}; \nu^2) = \frac{1}{\Gamma(\frac{1}{2}+n)} \int_0^{\infty} \frac{t^{n-\frac{1}{2}} \exp(-\nu^2 t) dt}{(1+t)^{n+1}}, \quad (18)$$

and the factorials have been written as gamma functions.

The field variation of E_{ex} in the limit of high fields is presented in Fig. 2 by plotting h vs $\eta/\hbar\omega_c$. In the interval, $0 < (\eta/\hbar\omega_c) \leq 0.5$, h has a logarithmic singularity. The use of a screened Coulomb potential would obviate this singularity.†

The results of Fig. 2 can be understood qualitatively as follows. The condition,

$$n_F = (\eta/\hbar\omega_c) - \frac{1}{2} = 0, 1, 2, \dots, \quad (19)$$

corresponds to a given harmonic oscillator state's being exactly filled. When the condition (19) is satisfied, the helical orbits of the electrons fill coordinate space with a maximum overlap of the electronic wave functions; hence a maximum in the exchange energy is produced. As the magnetic field, H , decreases just below the value needed to satisfy condition (19) (i.e., n_F increases), there is a rapid decrease in E_{ex} . When electrons start to fill a new oscillator state, they position themselves so as to minimize E_{ex} . Since the overlap of the wave functions increases with increasing population of the unfilled oscillator state, E_{ex} increases until the state is filled.

† *Note added in proof.*—The singularity in h at large fields is a result of allowing the number of electrons to vary so that all the states labeled by q are filled. The result obtained here is thus an upper limit on the exchange energy for an electron gas containing a fixed number of electrons. For fixed concentration the exchange energy should vanish for infinite fields because in this limit the electrons are so localized that no overlap exists.

For $H=0$, E_{KE} and E_{ex} are opposite in sign and their relative magnitude depends on the electron concentration [see Eq. (1)]. For example, for the alkali metals, $E_{\text{ex}}/E_{\text{KE}} = -0.415r_s \simeq -1.5$. Almost the entire correlation between electrons of parallel spin is contained in E_{ex} , while the electrons with antiparallel spin contribute to E_C ($[E_C/E_{\text{KE}}] = -0.398r_s^2/(r_s+7.8) \simeq -0.5$ in the alkali metals).

Although E_{KE} and E_{ex} exhibit the same periodicity as a function of H , the two terms are of opposite sign and have a different dependence on electron concentration, as is seen in the following equation:

$$E_{\text{KE}} + E_{\text{ex}} = \left\{ \frac{2.21}{r_s^2} - \frac{0.916}{r_s} + \frac{2.21}{r_s^2} [g - 0.415r_s h] \right\} \text{ ry.} \quad (20)$$

Since g and h are generally of opposite sign, the effect of E_{ex} is to increase the magnitude of the field dependence of the total energy, with the contributions from E_{KE} and E_{ex} being approximately equal.

In experimental studies of the de Haas-van Alphen effect, the periodicity in H^{-1} and the phase of the oscillations of the susceptibility, χ , are observed. The inclusion of E_{ex} in a calculation of χ leaves the period of the oscillations unchanged, though their phase may be altered. Previous work⁴ has shown that for $H=0$, E_{KE} , E_{ex} , and E_C are of comparable magnitude. The present study has, furthermore, yielded a comparable field dependence of E_{KE} and E_{ex} . The details of the de Haas-van Alphen effect may be affected by E_{ex} and probably also by E_C .