

# Contribution of the second Landau level to the exchange energy of the three-dimensional electron gas in a high magnetic field

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We derive a closed analytical expression for the exchange energy of the three-dimensional interacting electron gas in strong magnetic fields, which goes beyond the quantum limit ( $L=0$ ) by explicitly including the effect of the second,  $L=1$ , Landau level and arbitrary spin polarization. The inclusion of the  $L=1$  level brings the fields to which the formula applies closer to the laboratory range, as compared to previous expressions, valid only for  $L=0$  and complete spin polarization. We identify and explain two distinct regimes separated by a critical density  $n_c$ . Below  $n_c$ , the per particle exchange energy is lowered by the contribution of  $L=1$ , whereas above  $n_c$  it is increased. As special cases of our general equation we recover various known more limited results for higher fields, and we identify and correct a few inconsistencies in some of these earlier expressions.

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## I. INTRODUCTION

The calculation of the exchange energy of an interacting Fermi gas in high magnetic fields is a fundamental problem of many-body physics, with applications in fields as diverse as semiconductor physics,<sup>1-3</sup> astrophysics,<sup>1,4,5</sup> atomic and molecular physics,<sup>1,4,5</sup> and density-functional theory.<sup>6-9</sup>

In a seminal 1971 paper, Danz and Glasser<sup>10</sup> (hereafter DG) calculated the exchange energy,  $e_x$ , of a three-dimensional electron gas in high magnetic fields by means of Green's-function techniques. The key results are analytical expressions for the dependence of  $e_x$  on density  $n$  and magnetic field  $B$ , valid if the electrons are fully spin polarized and occupy only the spin-down sublevel of the lowest Landau level. In an equally important 1974 paper, Banerjee, Constantinescu, and Rehak<sup>11</sup> (hereafter BCR) also calculated this exchange energy and obtained a result that looks very similar to that of DG. The calculations of DG and BCR provided the background for a large body of later work on the exchange and correlation energies of the electron gas in high magnetic fields<sup>1,12-18</sup> and are also frequently quoted as input for the local-density approximation to current-density-functional theory in strong magnetic fields.<sup>18-22</sup>

A major limitation of these early calculations is their restriction to complete spin polarization and the lowest Landau level, which in three dimensions requires either magnetic fields that are beyond what is currently achievable in the laboratory or restriction to low-density low-effective-mass systems. Here we extend the DG many-body calculations to the case of arbitrary spin polarization, and we include the contribution of the second,  $L=1$ , Landau level. As a consequence, the range of magnetic fields to which the resulting expression applies is extended toward weaker fields, as compared to earlier expressions.

Our formula reveals a rather complex behavior of the exchange energy once higher Landau levels are included: As a function of the density  $n$ ,  $e_x$  first drops with a discontinuous derivative at density  $n_d$  corresponding to the onset of occupation of  $L=1$  and then passes through two regimes sepa-

rated by a critical density  $n_c$ . Below  $n_c$ , the per particle exchange energy is lowered (in modulus) by occupation of the  $L=1$  level, whereas above  $n_c$  it is increased (in modulus). The crossover between both regimes corresponds to a local minimum of  $e_x(n)$  at  $n_c$ . The physics of the drop and of both regimes can be understood in terms of the Landau-level structure. For currently achievable fields,  $n_c$  falls into the metallic density regime, and thus it should be observable.

Next, we consider various special cases of our general expression in order to make contact with more restricted results previously available in the literature, in particular those of DG and BCR. Scrutiny of these earlier expressions reveals a number of small inconsistencies and mistakes, which we correct on the basis of our more general expression.

## II. EXCHANGE ENERGY INCLUDING THE SECOND LANDAU LEVEL

The extension of the DG calculation to include higher Landau levels had, up to now, not been achieved in closed form. DG, and many other workers,<sup>1,11-18</sup> went beyond the quantum limit by rewriting the exchange integrals via expansion in infinite series, which cannot be resummed; or calculate them numerically. Neither approach yields analytical expressions that can be used, e.g., in the construction of density functionals for current-density-functional theory.<sup>6,7</sup> Motivated by the need for analytical expressions for lower fields (including  $L=1$ ) and by the observation of small inconsistencies in available results for  $L=0$  (see below), we have recalculated the exchange energy along the same lines as in the DG calculation for  $L=0$  but kept all contributions from the  $L=1$  level. The result turns out to permit a closed analytical expression which, although lengthy, can be expressed in terms of the same special functions and physical variables as the original DG formula for  $L=0$ . To be concise, we here just present the final result. More details on its derivation

can be found in Appendix A.

Three types of terms contribute: one,  $e_x^{(0)}$ , arises exclusively from  $L=0$ , another,  $e_x^{(1)}$ , arises from  $L=1$ , and a third,  $e_x^{(0,1)}$ , arises from interlevel exchange involving contributions

from  $L=0$  and  $L=1$ . As a function of the occupation numbers  $n_L^\sigma$  of the spin-up and spin-down sublevels of the  $L=0$  and  $L=1$  Landau levels, the final result for the per volume exchange energy can be written,

$$e_x(n_0^\uparrow, n_0^\downarrow, n_1^\uparrow, n_1^\downarrow, B) = \frac{e^2}{8\pi^3} \left( \frac{m\omega_c}{\hbar} \right)^2 \sum_\sigma [e_x^{(0)}(n_0^\sigma, B) + e_x^{(0,1)}(n_0^\sigma, n_1^\sigma, B) + e_x^{(1)}(n_1^\sigma, B)], \quad (1)$$

where

$$e_x^{(0)}(n_0^\sigma, B) = C + \ln \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_0^{\sigma 2} \right) - \exp \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_0^{\sigma 2} \right) Ei \left( - \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_0^{\sigma 2} \right) - \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_0^{\sigma 2} \right)^{1/4} G_{23}^{22} \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_0^{\sigma 2} \middle| \begin{matrix} 3/4, 5/4 \\ 3/4, 3/4, 1/4 \end{matrix} \right), \quad (2)$$

$$\begin{aligned} e_x^{(0,1)}(n_0^\sigma, n_1^\sigma, B) &= 4 \ln \left( \frac{n_0^\sigma + n_1^\sigma}{n_0^\sigma - n_1^\sigma} \right) + 2 \exp \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma - n_1^\sigma)^2 \right] Ei \left[ - \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma - n_1^\sigma)^2 \right] - 2 \exp \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma + n_1^\sigma)^2 \right] \\ &\times Ei \left[ - \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma + n_1^\sigma)^2 \right] + \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma - n_1^\sigma)^2 \right]^{1/4} G_{23}^{22} \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma - n_1^\sigma)^2 \middle| \begin{matrix} 3/4, 5/4 \\ 3/4, 3/4, 1/4 \end{matrix} \right] \\ &- \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma + n_1^\sigma)^2 \right]^{1/4} G_{23}^{22} \left[ \frac{2\pi^4 \hbar^3}{m^3 \omega_c^3} (n_0^\sigma + n_1^\sigma)^2 \middle| \begin{matrix} 3/4, 5/4 \\ 3/4, 3/4, 1/4 \end{matrix} \right], \end{aligned} \quad (3)$$

and

$$\begin{aligned} e_x^{(1)}(n_1^\sigma, B) &= C + \ln \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right) - \exp \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right) Ei \left( - \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right) - \frac{3}{4} \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right)^{1/4} G_{23}^{22} \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \middle| \begin{matrix} 3/4, 5/4 \\ 3/4, 3/4, 1/4 \end{matrix} \right) \\ &+ \frac{1}{2} \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right) \exp \left( \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right) Ei \left( - \frac{8\pi^4 \hbar^3}{m^3 \omega_c^3} n_1^{\sigma 2} \right). \end{aligned} \quad (4)$$

Here  $\omega_c(B) = eB/mc$  is the cyclotron frequency,  $C = 0.57722$  is the Euler constant,  $G_{23}^{22}$  is the Meijer  $G$  function,<sup>23</sup> and  $Ei$  is the exponential integral. In principle, this expression holds for arbitrary values of the  $g$  factor, as long as  $L \leq 1$ . However we note that if the free-electron value  $g=2$  is employed, an accidental degeneracy between the spin-up subband of  $L=1$  level and the spin-down subband of  $L=2$  occurs. Restriction to  $L \leq 1$  is thus only rigorously possible if either  $g < 2$  (a common situation in semiconductors) or if the  $L=1$  level is fully polarized so that its spin-up subband is empty.

The condition  $L \leq 1$  implies a restriction on the allowable values of density and magnetic field. In terms of the magnetic length  $l(B) = \sqrt{\hbar c / (eB)}$  and the density parameter  $r_s(n) a_0 = [3 / (4\pi n)]^{1/3}$ , where  $a_0 = \hbar^2 / (me^2)$  is the Bohr radius, this restriction is conveniently written as

$$\frac{l}{r_s a_0} < \left[ \frac{4}{3\pi} (1 + \sqrt{2}) \right]^{1/3}, \quad (5)$$

for  $g=2$  and

$$\frac{l}{r_s a_0} < \left[ \frac{4}{3\pi} (2 + \sqrt{2}) \right]^{1/3}, \quad (6)$$

for  $g=0$ . These conditions are derived in Appendix B.

Regarding the spin dependence, we note that spin-up and spin-down contributions do not mix, i.e., their contribution to  $e_x$  can be evaluated separately. Equations (1)–(4) permit one to do this for arbitrary values of the occupation numbers  $n_L^\sigma$  and thus also for arbitrary spin polarizations  $m \propto (n_\uparrow - n_\downarrow)$ , where  $n_\sigma = \sum_L^{\text{occ}} n_L^\sigma$ .

As illustration of Eq. (1), Fig. 1 displays the exchange energy for a combination of densities and magnetic fields, for which both  $L=0$  and  $L=1$  levels contribute, and compares it with the (erroneous) use of the  $L=0$  expression alone in the same regime.

Figure 1 reveals interesting behavior of  $e_x$  that appears only once  $L > 0$  is allowed for: Upon adding more particles (increasing the density), the per particle exchange energy suddenly drops (in modulus) once the  $L=1$  level starts to be occupied at density  $n_d$  and then passes through two regimes. Initially, it continues to decrease, while for larger densities it increases (in modulus) up to values larger than those obtained by allocating all particles in  $L=0$ . The first regime is entered with a discontinuous derivative in the  $e_x(n)$  curve, indicating a zero-temperature phase transition. The second regime is entered via a gradual crossover. Both regimes are separated by a critical density  $n_c$ , at which  $e_x(n)$  goes through a local minimum.

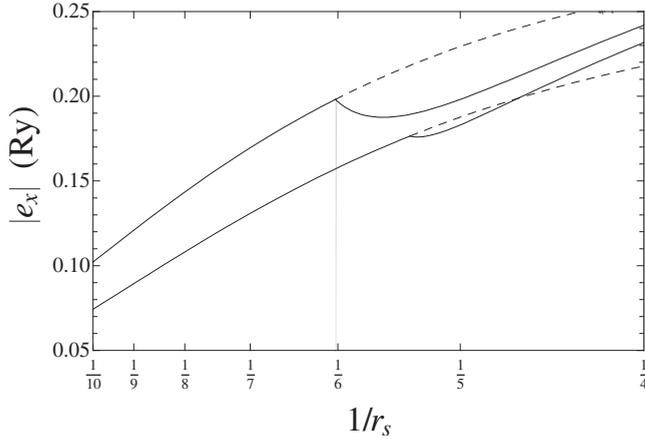


FIG. 1. Full curves: Exchange energy per particle obtained from Eq. (1) by dividing it by the density, as a function of  $r_s^{-1} \propto n^{1/3}$ . Dashed curves: (erroneous) continuation of the  $L=0$  expression into the  $L=1$  regime. Upper set of two curves:  $g=2$  and  $B=1.4448 \times 10^4$  T. Lower set of two curves:  $g=0$  and  $B=1.1474 \times 10^4$  T.

This intricate behavior finds its explanation in the Landau-level structure: Due to the differences in the spatial part of the Landau-level wave functions, the intralevel exchange integrals are larger than the interlevel integrals. As long as only  $L=0$  contributes, the exchange energy naturally increases with the number of particles. Once particles are allocated also in the  $L=1$  level, the reduced spatial overlap of their orbitals with those of the particles in  $L=0$  leads to a reduction in the per particle exchange energy. As the number of particles in  $L=1$  increases, their intralevel exchange energy also increases and overcompensates the initial drop (as seen in the crossing of the full and the dashed curve).

For  $g=2$ , the initial drop is much more pronounced than for  $g < 2$  because for this value occupation of the spin-down subband of the  $L=1$  level occurs simultaneously with that of the energetically degenerate spin-up subband of the  $L=0$  level so that the exchange energy of some of the additional particles is not only reduced by small spatial overlap but strictly zero due to zero-spin overlap with the spin-down particles already occupying  $L=0$ . The resulting larger drop may be so large that for fields and densities compatible with  $L \leq 1$ ,  $e_x(n)$  does not recover the hypothetical value obtained by filling only the  $L=0$  level (as illustrated in the upper set of two curves in Fig. 1).

This complex behavior of  $e_x(n)$  implies that magnetic-field Thomas-Fermi-Dirac theory,<sup>1,14,15</sup> current-density-functional theory,<sup>6,7</sup> and magnetic-field-density-functional theory<sup>8,9</sup> should have a much richer solution space than have ordinary Thomas-Fermi-Dirac and spin-density-functional theories, where  $e_x(n)$  is strictly monotonous. The density  $n_d$  where the discontinuous drop occurs and the critical density  $n_c$  where  $e_x(n)$  goes through its minimum depend on the magnetic field. For sufficiently large fields both fall in the metallic density range (i.e., both regimes, as well as the crossover between them, should be observable in the laboratory).

### III. HIGHER FIELDS AND LIMITING CASES

In the quantum limit,  $B$  is so high that only the  $L=0$  level is occupied. In this limit, the exchange energy is given by

keeping only  $e_x^{(0)}$  in Eq. (1). If the free-electron value  $g=2$  is employed, an accidental degeneracy between the spin-up subband of  $L=0$  level and the spin-down subband of  $L=1$  occurs. Restriction to  $L=0$  is thus only rigorously possible if either  $g < 2$  or if the system is fully polarized so that the spin-up subband of  $L=0$  level is empty too. Moreover, the conditions guaranteeing  $L=0$  are stricter than those limiting occupation to  $L \leq 1$ , given above, and read

$$\frac{l}{r_s a_0} < \left( \frac{2\sqrt{2}}{3\pi} \right)^{1/3}, \quad (7)$$

for  $g=2$ ,

$$\frac{l}{r_s a_0} < \left( \frac{4\sqrt{2}}{3\pi} \right)^{1/3}, \quad (8)$$

for  $g=0$ , and

$$\frac{l}{r_s a_0} < \left[ \frac{2}{3\pi} (\sqrt{2-|g|} + \sqrt{2}) \right]^{1/3}, \quad (9)$$

for generic  $g \in (-2, 2)$ . These conditions are derived in Appendix B. As long as these conditions are satisfied, Eq. (1) with the contribution from just  $e_x^{(0)}$  can be used for arbitrary occupation of the up and down subbands, i.e., for arbitrary spin polarization.

The further restriction to full spin polarization, i.e., an empty spin-up subband, then leads to

$$e_x(n, B) = \frac{e^2}{8\pi^3} \left( \frac{m\omega_c}{\hbar} \right)^2 \left[ C + \ln(p) - e^p Ei(-p) - p^{1/4} G_{23}^{22} \left( p \left| \begin{matrix} 3/4, 5/4 \\ 3/4, 3/4, 1/4 \end{matrix} \right. \right) \right], \quad (10)$$

which was the result obtained by DG.<sup>10</sup> Here the particle density  $n$  is equal to the occupation  $n_{L=0}^{\sigma=1}$ . We defined, following DG,  $p(n, B) := 8\pi^4 \hbar^3 n^2 / (m^3 \omega_c^3)$ . As long as no higher levels are occupied and  $g=2$ , we also have  $p(n, B) = 4\epsilon_F / \hbar \omega_c$ , where  $\epsilon_F$  is the Fermi energy. (This equality breaks down if other spin states or Landau levels are involved, or  $g \neq 2$ .)

If  $\epsilon_F / \hbar \omega_c \ll 1$ , then only the bottom of the lowest subband is occupied and the preceding equation reduces to

$$e_x(n, B) = \frac{\pi e^2 \hbar}{m \omega_c} n^2 [\ln(p) - 3 + C]. \quad (11)$$

In units in which  $\hbar=c=1$ , Eq. (11) can be written as

$$e_x(n, B) = \frac{2\pi e^2}{eB} n^2 \left\{ \ln \left[ \frac{n}{(eB)^{3/2}} \right] + 2.117\,79 \right\}, \quad (12)$$

which was first obtained by DG (Ref. 10) and can be directly compared with the corresponding Eq. (47) of BCR,<sup>11</sup>

$$e_x(n, B)^{\text{BCR}} = \frac{2\pi e^2}{eB} n^2 \left\{ \ln \left[ \frac{n}{(eB)^{3/2}} \right] + 2.329\,18 \right\}, \quad (13)$$

featuring a different numerical value inside the brackets. This difference was also noticed in Refs. 13 and 14.

For ultrastrong magnetic fields (quantified in Fig. 2) or for extremely low densities, that value (be it 2.117 79 or

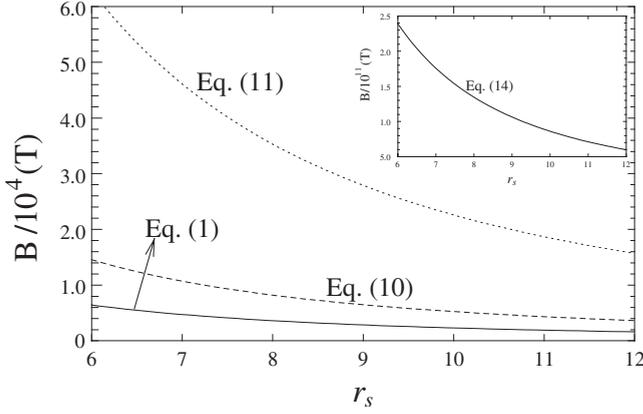


FIG. 2. Applicability of the four expressions discussed here. The curves represent the lowest magnetic fields, for which the indicated expression is valid for the free-electron value of  $m$  and  $g=2$ .

2.329 18) becomes negligible relative to the logarithmic term, and the DG and BCR expressions become identical both reducing to

$$\frac{e_x(r_s, B)}{Ry} = -\frac{27}{4\pi a_0^3 r_s^6} \left(\frac{\hbar\omega_c}{Ry}\right)^{-1} \ln\left(0.141 r_s^2 \frac{\hbar\omega_c}{Ry}\right), \quad (14)$$

where  $e_x/Ry$  and  $\hbar\omega_c/Ry$  denote exchange and cyclotron energies measured in Rydberg [ $1Ry=e^2/2a_0=13.6$  eV]. In DG this limit appears as their Eq. (1.1),

$$\frac{e_x(r_s, B)^{DG}}{Ry} = -\frac{27}{16\pi a_0^3 r_s^6} \left(\frac{\hbar\omega_c}{Ry}\right)^{-1} \ln\left(0.282 r_s^2 \frac{\hbar\omega_c}{Ry}\right), \quad (15)$$

which differs in two ways from Eq. (14): the numerical factor inside the logarithm is  $0.282=2\times 0.141$  and the prefactor is  $27/16$  instead of  $27/4$ .

Our general expression (1) contains all these limits as special cases, and we can therefore verify which of the conflicting expressions is correct. In the high-field limit of the quantum limit, we find that the DG Eq. (12) is correct, while the BCR Eq. (13) is not. In the ultrastrong field limit, we find that Eq. (14) is correct, while the DG Eq. (15) is not. In this latter case, we suspect that DG inadvertently used Hartree units instead of Rydberg units ( $1H=e^2/a_0=2Ry$  is the atomic unit of energy) but denoted them as Rydberg, as this would explain both the factor of two inside and the factor of  $1/4$  outside the logarithm.<sup>24</sup>

Figure 2 illustrates the magnetic-field and density regimes, for which each of the above equations is valid. The curves represent the *lowest* magnetic fields, for which the indicated expression is valid for the free-electron value of  $m$  and  $g=2$ . For all  $B(r_s)$  above the full curve,  $L\leq 1$  and Eq. (1) with arbitrary values of  $n_0^\downarrow$ ,  $n_0^\uparrow$ , and  $n_1^\downarrow$  may be applied. For  $g=2$ ,  $n_1^\uparrow$  must be zero to avoid degeneracy with the  $L=2$  Landau level, not included in our formula. For  $g<2$ ,  $n_1^\uparrow$  is also arbitrary.

For values of  $B(r_s)$  above the dashed curve, Eq. (10) with arbitrary values of  $n=n_0^\downarrow$  may be applied. For  $g=2$ ,  $n_0^\uparrow$  must be zero to avoid degeneracy with the  $L=1$  Landau level, not

included in the DG formula. For  $g<2$ ,  $n_0^\uparrow$  is also arbitrary. The relevant expression in this case is our Eq. (1) but with only the  $e_x^{(0)}$  term kept.

The restrictions  $L=0$  and  $L\leq 1$  are precisely defined and easily applied. The restriction  $p\ll 1$ , which leads from Eq. (10) to Eq. (11), and the condition  $|\ln[n/(eB)^{3/2}]|\gg 2.11779$ , which leads from Eq. (11) to Eq. (14), are less precisely defined, and we simply adopt as validity criterium that  $p\leq 0.05$  and that 2.11779 is less than 5% of the logarithmic term. From these criteria, we find that for  $B(r_s)$  above the dotted curve the high-field limit [Eq. (11)] becomes valid. The inset shows the values of  $B(r_s)$ , above which the ultra-high-field limit [Eq. (14)] is valid.

To generate Figs. 1 and 2, we used the free-electron value of the electron mass  $m$ , requiring very high magnetic fields to satisfy conditions (5)–(9). Such high fields are not without physical relevance. Continuous fields  $\sim 40$  T and pulsed fields  $\sim 10^4$  T can be produced in the laboratory, white dwarfs have surface fields of order  $\sim 10^4$  T, and neutron stars can have fields in excess of  $10^8$ – $10^9$  T. For effective masses smaller than the free-electron mass, the required fields are considerably lower. The use of effective masses  $m^*=\gamma m$  rescales all  $B$  values by  $B\rightarrow\gamma^2 B$  so that a reduction of  $m$  by a factor of ten allows a reduction of  $B$  by a factor of 100. Small effective masses and low densities thus bring these fields into the laboratory range.

#### IV. CONCLUSIONS

Our key result is Eq. (1), for the exchange energy of the three-dimensional Fermi gas in magnetic fields, for which both the lowest and the second-lowest Landau level contribute and the fermions may have arbitrary spin polarization. This equation predicts the existence of two physically distinct regimes, one (entered with a discontinuous derivative) in which the occupation of the  $L=1$  level lowers the per particle exchange energy and one (entered through a gradual crossover) in which it increases it. For high, but achievable, fields both the discontinuous drop and the gradual crossover between the two regimes occur in the metallic density range. Thus both regimes should be experimentally observable. We predict that similar separation in two regimes occurs every time a new Landau level is included in the calculation.

The availability of an analytical expression for the exchange energy of the electron gas in high magnetic fields facilitates the construction of density functionals for magnetic-field Thomas-Fermi-Dirac theory,<sup>1,14,15</sup> current-density-functional theory,<sup>6,7</sup> and magnetic-field density-functional theory.<sup>8,9</sup> However the intricate structure of  $e_x(n, B)$  implies that their local approximations must display a much more complex behavior than those of the ordinary Thomas-Fermi-Dirac and spin-density-functional theory.

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**APPENDIX A: DETAILS ON THE DERIVATION OF EQS. (1)–(4)**

From Eq. (2.1) of DG and following their procedure until their Eq. (2.5), we find the per volume exchange energy,

$$e_x = -\frac{e^2}{4\pi^3} \left(\frac{m\omega_c}{\hbar}\right)^2 \sum_{\sigma} \int_{-\infty}^{\infty} dr_z \int_0^{\infty} d\bar{r} \frac{\bar{r} e^{-\frac{m\omega_c}{2\hbar}\bar{r}^2}}{(\bar{r}^2 + r_z^2)^{1/2} r_z^2} \times \left\{ \sum_{L=0}^{\infty} \Theta(C_L^{\sigma}) \sin(r_z D_L^{\sigma}) L_L \left(\frac{m\omega_c}{2\hbar} \bar{r}^2\right) \right\}^2, \quad (\text{A1})$$

where  $\Theta(x)$  is the step function,  $L_L(x)$  are Laguerre polynomials, and

$$C_L^{\sigma} = \mu - \left(L + \frac{1}{2}\right) \hbar \omega_c - g \mu_0 B \sigma, \quad (\text{A2})$$

$$D_L^{\sigma} = \sqrt{\frac{2m}{\hbar^2} \left[ \mu - \left(L + \frac{1}{2}\right) \hbar \omega_c - g \mu_0 B \sigma \right]}, \quad (\text{A3})$$

where  $\mu_0 = e\hbar/2mc$  is the Bohr magneton.

Keeping the contributions from the  $L=0$  and  $L=1$  levels and performing the change of variable,

$$\bar{r}^2 = \frac{2\hbar}{m\omega_c} \left( r_z t + \frac{\hbar}{2m\omega_c} t^2 \right), \quad (\text{A4})$$

we obtain

$$e_x = -\frac{e^2}{2\pi^3} \frac{m\omega_c}{\hbar} \sum_{\sigma} \int_0^{\infty} dt e^{-\hbar t^2/2m\omega_c} \int_0^{\infty} dr_z \frac{e^{-r_z t}}{r_z^2} \left\{ \Theta(C_0^{\sigma}) \sin^2(D_0^{\sigma} r_z) + \Theta(C_1^{\sigma}) \sin^2(D_1^{\sigma} r_z) \left(1 - tr_z - \frac{\hbar t^2}{2m\omega_c}\right) + 2\Theta(C_0^{\sigma})\Theta(C_1^{\sigma}) \sin(D_0^{\sigma} r_z) \sin(D_1^{\sigma} r_z) \left(1 - tr_z - \frac{\hbar t^2}{2m\omega_c}\right) \right\}. \quad (\text{A5})$$

Using Laplace transforms to perform the  $r_z$  integral,<sup>25</sup> we find

$$e_x = -\frac{e^2}{2\pi^3} \frac{m\omega_c}{\hbar} \sum_{\sigma} \int_0^{\infty} dt e^{-\hbar t^2/2m\omega_c} \left\{ \Theta(C_0^{\sigma}) \left[ D_0^{\sigma} \tan^{-1} \left( \frac{2D_0^{\sigma}}{t} \right) - \frac{1}{4} t \ln \left( 1 + \frac{4D_0^{\sigma 2}}{t^2} \right) \right] + \Theta(C_0^{\sigma})\Theta(C_1^{\sigma}) \left[ \left( t - \frac{\hbar}{4m\omega_c} t^3 \right) \ln \left( \frac{t^2 + (D_0^{\sigma} - D_1^{\sigma})^2}{t^2 + (D_0^{\sigma} + D_1^{\sigma})^2} \right) + \left( \frac{\hbar}{2m\omega_c} t^2 - 1 \right) (D_0^{\sigma} - D_1^{\sigma}) \tan^{-1} \left( \frac{D_0^{\sigma} - D_1^{\sigma}}{t} \right) + \left( 1 - \frac{\hbar}{2m\omega_c} t^2 \right) (D_0^{\sigma} + D_1^{\sigma}) \tan^{-1} \left( \frac{D_0^{\sigma} + D_1^{\sigma}}{t} \right) \right] + \Theta(C_1^{\sigma}) \left[ D_1^{\sigma} \left( 1 - \frac{\hbar}{2m\omega_c} t^2 \right) \tan^{-1} \left( \frac{2D_1^{\sigma}}{t} \right) + \left( -\frac{3t}{4} + \frac{\hbar}{2m\omega_c} t^3 - \frac{\hbar^2}{16m^2\omega_c^2} t^5 \right) \ln \left( 1 + \frac{4D_1^{\sigma 2}}{t^2} \right) + 2D_1^{\sigma 2} \frac{t}{t^2 + 4D_1^{\sigma 2}} \right] \right\}. \quad (\text{A6})$$

The integral over the first term, involving only contributions from  $L=0$ , can be calculated following the procedure of Appendix A of the DG paper.<sup>10</sup> The other integrals are calculated by integration by parts and Laplace transforms. In particular, the integrals involving  $\tan^{-1}(x)$  can be calculated by using the result of the first integral.

$C_L^{\sigma}$  and  $D_L^{\sigma}$  can be written in terms of the occupation number  $n_L^{\sigma}$  as  $C_L^{\sigma} = (2\pi^4 \hbar^2 l^4 / m) n_L^{\sigma 2}$  and  $D_L^{\sigma} = 2\pi^2 l^2 n_L^{\sigma}$ . The step functions turn out to be unnecessary because the term arising from  $L=1$  and the mixed term containing contributions from  $L=0$  and  $L=1$  are automatically zero when  $n_1^{\sigma} = 0$ . We thus find the exchange energy as given by Eqs. (1)–(4). More details of the calculation are available through Ref. 26.

An extension of these analytical calculations to higher  $L$  values seems extraordinarily cumbersome. To include, e.g.,  $L=2$ , one must keep one more term in the sum of Eq. (A1), which gives rise to not just one more intralevel integral in Eq. (A5) but also to many new interlevel integrals. In the general case, for arbitrary  $L$ , there is no guarantee that the

resulting integrals can all be solved by the Laplace transforms and be reduced to some known special function. The three-dimensional case is, in this regard, more complicated than the two-dimensional one<sup>27</sup> due to the additional  $k_z$  dependence of the single-particle energies and the resulting Landau-level dispersion. Numerical work on the general case is under way.

**APPENDIX B: DETAILS ON THE DERIVATION OF EQS. (5)–(9)**

The conditions specifying the fields and densities, for which restriction to  $L=0$  or  $L \leq 1$  is valid, depend on the Landau-level degeneracy. The single-particle dispersion in the spin  $\sigma$  sublevel of Landau level  $L$  is

$$\epsilon(k_z, L, \sigma) = \frac{\hbar^2}{2m} k_z^2 + \left(L + \frac{1}{2}\right) \hbar \omega_c + g \mu_0 B \sigma. \quad (\text{B1})$$

In each subband, the Fermi momentum is related to the partial density by  $k_{FL}^{\sigma} = 2\pi^2 l^2 n_L^{\sigma}$ . The degeneracy of these levels

depends on the value of  $g$ . For the free-electron value  $g=2$ , the spin-up subband of level  $L$  and the spin-down subband of level  $L+1$  are degenerate. For  $g=0$ , on the other hand, the spin-up and spin-down sublevels of Landau level  $L$  are degenerate. We first deal with  $g=2$ .

The restriction to  $L=0$  implies

$$\epsilon(k_z=0, L=1, \downarrow) = \epsilon(k_z=0, L=0, \uparrow), \quad (\text{B2})$$

$$> \epsilon_F = \epsilon(k_{F0}^\downarrow, L=0, \downarrow). \quad (\text{B3})$$

From Eq. (B1) and using the fact that for  $L=0$  and  $g=2$ ,  $n_0^\downarrow=n$ , we immediately find

$$n^2 < \frac{1}{2\pi^4 l^6}, \quad (\text{B4})$$

which is equivalent to Eq. (7) of the main text. Similarly, the restriction to  $L \leq 1$  implies

$$\epsilon(k_z=0, L=2, \downarrow) = \epsilon(k_z=0, L=1, \uparrow), \quad (\text{B5})$$

$$> \epsilon_F = \epsilon(k_{F1}^\downarrow, 1, \downarrow) = \epsilon(k_{F0}^\uparrow, 0, \uparrow) = \epsilon(k_{F0}^\downarrow, 0, \downarrow). \quad (\text{B6})$$

The total density is  $n=n_0^\downarrow+n_0^\uparrow+n_1^\downarrow$ . Solving this set of equations for  $n$  yields

$$n < \frac{2 + \sqrt{2}}{\sqrt{2}\pi^2 l^3}, \quad (\text{B7})$$

which is equivalent to Eq. (5) of the main text.

The corresponding conditions for  $g=0$  follow in the same way. The case  $g=0$  is occasionally used as a methodological device in theoretical work because it allows us to cleanly separate the effects of spin magnetism from those of orbital magnetism. Experimentally,  $g=0$  occurs, e.g., in systems studied in the context of  $g$ -factor engineering of devices.<sup>28</sup>

When  $|g| < 2$  and  $g \neq 0$ , no such degeneracy occurs. The restriction to  $L=0$  then implies  $n=n_0^\uparrow+n_0^\downarrow$  and

$$n < \frac{\sqrt{2-|g|} + \sqrt{2}}{2\pi^2 l^3}, \quad (\text{B8})$$

which is equivalent to Eq. (9).

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<sup>24</sup>After completion of this work we became aware of footnote 22 of A. R. P. Rau, R. O. Mueller, and L. Spruch, Phys. Rev. A **11**, 1865 (1975); which confirms our suspicion regarding Eq. (15). Some other equations of Ref. 10 are also in need of minor corrections: in their Eq. (2.3), the exponent of the last exponential should be  $-\hbar n \omega_c s$  instead of  $-\hbar n \omega_c s/2$ , and in their Eq. (2.6)  $(\bar{r}^2 + r_c^2)^{1/2}$  should be  $(\bar{r}^2 + r_c^2)^{-1/2}$ . These problems seem to be mere misprints, however, since their correction leads to Eq. (11) [equivalent to Eq. (2.9) of DG] as published in DG and reproduced by us. The wrong factors in Eq. (15) [equivalent to Eq. (1.1) of DG], on the other hand, are completely independent of these additional corrections, as is the difference between the DG and BCR expressions.

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