

Magnetic Susceptibility of an Electron Gas at High Density

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The magnetic susceptibility of an electron gas at high density is determined using the exact theory of Gell-Mann and Brueckner.

THE magnetic susceptibility of the electron gas has been given by Pines¹ on the basis of the approximate theory of Bohm and Pines. In this note we shall determine the susceptibility using the exact high-density theory of Gell-Mann and Brueckner (to be referred to in the following as I). This theory has been previously applied to the determination of the correlation energy,² specific heat,³ and collective properties of the electron gas.

The susceptibility of the electron gas is determined by the change in energy of the system as its spins are polarized. We denote the number of electrons with spin up and down by N_+ and N_- , and introduce a parameter p defining the polarization by the equations

$$N_+ = \frac{1}{2}N(1+p), \quad N_- = \frac{1}{2}N(1-p), \quad (1)$$

where N is the total number of electrons. The Fermi momentum in the polarized system, measured in units of the Fermi momentum in the unpolarized system, then is

$$p_+ = (1+p)^{\frac{1}{3}}, \quad p_- = (1-p)^{\frac{1}{3}}. \quad (2)$$

The change in kinetic and exchange energy per particle, measured in Rydbergs, to lowest order in p , is

$$E_F(p) + E_{\text{ex}}(p) - E_F(0) - E_{\text{ex}}(0) = \frac{1}{4}p^2(\alpha_F + \alpha_{\text{ex}}), \quad (3)$$

where

$$\begin{aligned} \alpha_F &= (20/9)E_F = 4.91/r_s^2, \\ \alpha_{\text{ex}} &= (8/9)E_{\text{ex}} = -0.814/r_s. \end{aligned} \quad (4)$$

To determine the change in the correlation energy upon spin polarization, we first note that the exchange correlation energy per particle² (neglecting terms of order r_s and higher),

$$E_{\text{ex}}(\text{correlation}) = 0.046 \text{ Rydberg},$$

does not depend on the electron density and hence is unaltered by spin polarization, at least to this order. Consequently the entire correlation contributed to the susceptibility comes from the nonexchange terms. This contribution cannot be evaluated from the second-order nonexchange energy alone, since this diverges for small

momentum transfers. To avoid this difficulty, we must as in I include all orders of perturbation theory in the class of "ring diagrams" or, equivalently, the terms which remain after the random phase approximation has been applied. This approximation, as shown in I, is exact in the high-density limit.

To determine the nonexchange contribution, we rewrite Eq. (19) of I for the correlation energy per particle in Rydbergs as

$$\begin{aligned} \epsilon'(p) &= -\frac{3}{4\pi^5} \int_0^\infty \frac{dq}{q} \int_{-\infty}^\infty du \sum_{n=2}^\infty \frac{(-1)^n}{n} \\ &\quad \times \left[\frac{Q_q^+(u) + Q_q^-(u)}{2} \right]^n \left(\frac{\alpha r_s}{\pi q^2} \right)^{n-2}, \end{aligned} \quad (5)$$

where

$$\begin{aligned} Q_q^\pm(u) &= \int_{|p+\mathbf{q}| > p_\pm, p < p_\pm} d^3p \int_{-\infty}^\infty e^{i\mathbf{t}u\mathbf{q}} \\ &\quad \times \exp\{-|\mathbf{t}|[\frac{1}{2}q^2 + \mathbf{q} \cdot \mathbf{p}]\} dt. \end{aligned} \quad (6)$$

As in I we evaluate the integral over q by taking the small q limit in all terms in the sum except the second-order term which must be treated more carefully. This allows us to rewrite Eq. (5) as

$$\begin{aligned} \epsilon'(p) &= -\frac{3}{4\pi^5} \int_0^1 \frac{dq}{q} \int_{-\infty}^\infty du \sum_{n=2}^\infty \frac{(-1)^n}{n} \\ &\quad \times \left[\frac{Q_0^+(u) + Q_0^-(u)}{2} \right]^n \left(\frac{\alpha r_s}{\pi q^2} \right)^{n-2} + \delta(p), \end{aligned} \quad (7)$$

where

$$\begin{aligned} \delta(p) &= \frac{3}{8\pi^5} \int_0^1 \frac{dq}{q} \int_{-\infty}^\infty du \left[\frac{Q_0^+(u) + Q_0^-(u)}{2} \right]^2 \\ &\quad - \frac{3}{32\pi^6} \int \frac{d^3q}{q^3} \int_{-\infty}^\infty du \left[\frac{Q_q^+(u) + Q_q^-(u)}{2} \right]^2. \end{aligned} \quad (8)$$

To evaluate the first term in Eq. (7), we expand $\frac{1}{2}[Q_0^+(u) + Q_0^-(u)]$ in powers of the polarization parameter p , which gives

$$\frac{1}{2}[Q_0^+(u) + Q_0^-(u)] = 4\pi[R(u) + p^2g(u)], \quad (9)$$

where

$$\begin{aligned} R(u) &= 1 - u \tan^{-1}(1/u), \\ g(u) &= -(1/9)(1+u^2)^{-2}. \end{aligned} \quad (10)$$

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¹ D. Pines, Phys. Rev. **95**, 1090 (1954); in *Solid State Physics*, edited by F. Seitz and D. Turnbull (Academic Press, Inc., New York, 1955), Vol. 1, p. 368.

² M. Gell-Mann and K. A. Brueckner, Phys. Rev. **106**, 364 (1957); K. Sawada, Phys. Rev. **106**, 372 (1957); Sawada, Brueckner, Fukuda, and Brout, Phys. Rev. **108**, 507 (1957).

³ M. Gell-Mann, Phys. Rev. **106**, 369 (1957).

Inserting this result into Eq. (7) and carrying out the sum over n and integral over q , we find in the limit of small r_s

$$\begin{aligned} \epsilon'(\phi) - \epsilon'(0) &= -\frac{6\phi^2}{\pi^3} \int_{-\infty}^{\infty} du R(u)g(u) \ln \frac{4\alpha r_s R(u)}{\pi} + \delta(\phi) - \delta(0) \\ &= -\frac{\phi^2}{6\pi^2} \left\{ \ln \frac{4\alpha r_s}{\pi} + \langle \ln R \rangle_{Av} \right\} + \delta(\phi) - \delta(0), \end{aligned} \quad (11)$$

where

$$\langle \ln R \rangle_{Av} = \frac{\int_{-\infty}^{\infty} du R(u)g(u) \ln R(u)}{\int_{-\infty}^{\infty} du R(u)g(u)}. \quad (12)$$

The evaluation of the correction $\delta(\phi) - \delta(0)$ is straightforward but lengthy; the details are given in the Appendix. The result is

$$\delta(\phi) - \delta(0) = (\phi^2/3\pi^2) \{ \ln 2 + \frac{1}{2} \}. \quad (13)$$

Collecting these results, we find for the correlation contribution to the spin polarization energy

$$\epsilon'(\phi) - \epsilon'(0) = \frac{1}{4}\phi^2\alpha_c,$$

where

$$\alpha_c = \frac{2}{3\pi^2} \left[1 - \ln \frac{\alpha r_s}{\pi} - \langle \ln R \rangle_{Av} \right]. \quad (14)$$

Numerical integration gives for $\langle \ln R \rangle_{Av}$ the value of -0.534 . Inserting this value together with the other numerical factors into Eq. (14) gives for the final result

$$\alpha_c = 0.225 - 0.0676 \ln r_s, \quad (15)$$

which is exact to terms of order r_s .

The appearance of the logarithmic term in Eq. (15) shows that the long-range screening effects associated with the collective properties of the electron gas are altered by spin polarization, a not unexpected result. The previous estimate by Pines¹ gave $\alpha_c = 0.162 - 0.043r_s^{-\frac{1}{2}} - 0.0032r_s$; the discrepancy between his and our results appears to be the consequence of the approximate nature of his theory and also of his assumption that the change in screening can be neglected.

APPENDIX. EVALUATION OF $\delta(\phi)$

We rewrite $\delta(\phi)$ as defined in Eq. (8) as

$$\delta(\phi) = \frac{1}{4} [f(+,+) + f(-,-) + 2f(+,-)], \quad (A1)$$

where

$$\begin{aligned} f(x,y) &= -\frac{3}{2\pi^4} \lim_{\beta \rightarrow 0} \left\{ \int_{\beta}^{\infty} \frac{dq}{q^2} \int_{\substack{p_1 < x \\ |p_1+q| > x}} d^3p_1 \int_{\substack{p_2 < y \\ |p_2+q| > y}} d^3p_2 \right. \\ &\quad \times \frac{1}{q^2 + \mathbf{q} \cdot (\mathbf{p}_1 + \mathbf{p}_2)} \int_{\beta}^1 \frac{dq}{q} \lim_{\alpha \rightarrow 0} \frac{1}{q} \int_{\substack{p_1 < x \\ |p_1+q| > x}} d^3p_1 \\ &\quad \left. \times \int_{\substack{p_2 < y \\ |p_2+q| > y}} d^3p_2 \frac{1}{q^2 + \mathbf{q} \cdot (\mathbf{p}_1 + \mathbf{p}_2)} \right\}. \end{aligned} \quad (A2)$$

To carry out the integration of this expression, we first expand in powers of $(p_+ - 1)$ and $(p_- - 1)$. The result is

$$\begin{aligned} \delta(\phi) - \delta(0) &= \left\{ [(\phi_+ - 1) + (\phi_- - 1)] \frac{\partial f(x,1)}{\partial x} \right. \\ &\quad + \frac{1}{2} [(\phi_+ - 1)^2 + (\phi_- - 1)^2] \frac{\partial^2 f(x,1)}{\partial x^2} \\ &\quad + \frac{1}{4} [(\phi_+ - 1)^2 + (\phi_- - 1)^2 + 2(\phi_+ - 1)(\phi_- - 1)] \\ &\quad \left. \times \frac{\partial^2 f(x,y)}{\partial x \partial y} \right\}_{x=y=1}. \end{aligned} \quad (A3)$$

Now using the expansions of p_+ and p_- in powers of ϕ , we find

$$\delta(\phi) - \delta(0) = \frac{1}{8}\phi^2 \left\{ -2 \frac{\partial f(x,1)}{\partial x} + \frac{\partial^2 f(x,1)}{\partial x^2} \right\}_{x=1}. \quad (A4)$$

This can be brought into a form more easily integrated if we use the fact that $f(x,x)$ is proportional to x^3 , which leads to the identity

$$\left\{ -2 \frac{\partial f(x,1)}{\partial x} + \frac{\partial^2 f(x,1)}{\partial x^2} + \frac{\partial^2 f(x,y)}{\partial x \partial y} \right\}_{x=y=1} = 0. \quad (A5)$$

Using this result and Eq. (A4), we have

$$\delta(\phi) - \delta(0) = -\frac{1}{8}\phi^2 \left[\frac{\partial^2}{\partial x \partial y} f(x,y) \right]_{x=y=1}. \quad (A6)$$

In this form the integral is now easily evaluated; the result is given in Eq. (13).