

## Spin Susceptibility of an Electron Gas

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The generalized random phase approximation is used to investigate the effects of electron-electron interaction on the spin susceptibility of an electron gas. Within this approximation, the induced spin density is determined by the solution of an integral equation that describes exchange scattering between virtually excited particles. Solutions to this equation are obtained in simple cases. They indicate that the exchange scattering enhances the susceptibility over that predicted by the Ruderman-Kittel formula by factors which, for electron densities comparable to those found in good metals, are in the range 1-2. These results can also be derived by summing certain classes of diagrams in many-body perturbation theory. The structure of these graphs shows that the random phase approximation takes account of the simplest sort of self-energy effect and the simplest type of scattering of virtually excited particles.

### I. INTRODUCTION

LOCALIZED magnetic fields in metals, such as those due to paramagnetic impurities or nuclear moments, induce spin polarization in the conduction electrons in their vicinity. A theory of this effect, based upon the independent electron model, was developed by Ruderman and Kittel<sup>1</sup> and yields a simple formula for the amplitude and spatial variation of the spin density. It is well known, however, that in real metals electron-electron interactions are *not* weak. Thus a complete theory of the spin polarization must include the effects of Coulomb interactions between the electrons. As a first step in this direction we study in this paper the response of a degenerate interacting electron gas to an applied magnetic field. This system is, of course, a rather crude approximation to an actual metal, but does contain, in full, the many-body effects whose nature we would like to investigate. Thus it may serve as a useful model for understanding their nature in real crystals.

Our analysis of the many-body problem is based upon the random phase approximation (RPA)<sup>2</sup> in a form that includes exchange interactions between the electrons.<sup>3</sup> This approximation leads to an integral equation (in momentum space) whose solution determines the spin density. The relation of this equation to the Ruderman-Kittel result is quite straightforward. The latter is calculated by second-order perturbation theory that contains, as an intermediate state, a configuration in which one electron is excited outside the Fermi sea and there is an empty level (which we will call a hole) below the Fermi surface. These virtual particles may, however, scatter against one another. The Schrödinger equation that (with due allowance for the exclusion principle) describes this process is,

in momentum space, the integral equation characteristic of the RPA.

This integral equation is generally quite difficult to solve, but in the long-wavelength limit or for a delta-function interparticle potential (which is not too bad an approximation to the screened Coulomb interaction), solutions are obtained readily. The spin density calculated from them is enhanced over that predicted by the Ruderman-Kittel formula, and also has a slightly broader distribution in space. Since the solutions in the two limiting cases have exactly the same form it is not unreasonable to expect that an exact solution of the integral equation would lead to similar conclusions.

The RPA contains, of course, only a part of the electron-electron interaction. In view of this fact, it is of considerable interest to inquire which terms (in a perturbation theory sense) lead to the integral equation obtained from it. To answer this question it is necessary to restudy the problem with many-body perturbation theory of the Goldstone<sup>4</sup> type. In the final section of the paper we indicate briefly how such an analysis may be carried out, and display those terms in the perturbation expansion that give rise to the integral equation. These terms arise from a certain type of graph whose structure indicates that the RPA has the twofold effect of including direct Coulomb scatterings between virtual particles created by the external field, and taking account of the simplest self-energy corrections to the propagators of these particles.

### II

The system with which we shall deal in the following pages consists of a degenerate gas of electrons (of density  $n$ ) that interact with one another via the Coulomb field. The electron field operator for this system will be denoted by  $\psi(\mathbf{r})$  and has the usual expansion

$$\psi(\mathbf{r}) = \sum_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma} |\sigma\rangle e^{i\mathbf{k} \cdot \mathbf{r}} \quad (1)$$

in terms of creation operators  $c_{\mathbf{k}, \sigma}$  for plane wave

<sup>1</sup> M. A. Ruderman and C. Kittel, *Phys. Rev.* **96**, 99 (1954). See also K. Yoshida, *Phys. Rev.* **106**, 893 (1957).

<sup>2</sup> D. Pines, in *Solid-State Physics*, edited by F. Seitz and D. Turnbull (Academic Press Inc., New York, 1955), Vol. 1, p. 367. K. Sawada, K. A. Brueckner, N. Fukuda, and R. Brout, *Phys. Rev.* **108**, 507 (1957).

<sup>3</sup> P. W. Anderson, *Phys. Rev.* **112**, 1900 (1958).

<sup>4</sup> J. Goldstone, *Proc. Roy. Soc. (London)* **A240**, 539 (1957).

states of momentum  $\mathbf{k}$  and spin  $\sigma$ . The Hamiltonian  $H$  consists of two parts: the kinetic energy<sup>5</sup>

$$H_0 = \int \bar{\psi}(\mathbf{r}) \left( -\frac{\nabla^2}{2m} \right) \psi(\mathbf{r}) d^3r = \sum_{\mathbf{k}, \sigma} \left[ \bar{c}_{\mathbf{k}, \sigma} c_{\mathbf{k}, \sigma} \frac{k^2}{2m} \right], \quad (2)$$

and the electron-electron interaction

$$\begin{aligned} V &= \frac{1}{2} \int \bar{\psi}(\mathbf{r}) \bar{\psi}(\mathbf{r}') v(\mathbf{r}-\mathbf{r}') \psi(\mathbf{r}') \psi(\mathbf{r}) d^3r d^3r' \\ &= \frac{1}{2} \sum_{\mathbf{q}} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} [v(\mathbf{q}) \bar{c}_{\mathbf{k}+\mathbf{q}, \sigma} \bar{c}_{\mathbf{k}'-\mathbf{q}, \sigma'} c_{\mathbf{k}', \sigma'} c_{\mathbf{k}, \sigma}] \end{aligned} \quad (3)$$

[here  $v(\mathbf{q})$  is the Fourier transform of the interparticle potential,  $v(\mathbf{r})$ ]. To calculate the spin susceptibility we now imagine that a weak magnetic field  $\mathbf{B}(\mathbf{r})$ —which for simplicity we take in the  $z$  direction—is applied to the system defined by Eqs. (1)–(3). Its coupling to the electron spins is described by the interaction Hamiltonian

$$\begin{aligned} H_1 &= (\mu g) \int \bar{\psi}(\mathbf{r}) \sigma_z B(\mathbf{r}) \psi(\mathbf{r}) d^3r \\ &= (\mu g) \sum_{\mathbf{k}, \mathbf{q}} (\bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow} - \bar{c}_{\mathbf{k}+\mathbf{q}, \downarrow} c_{\mathbf{k}, \downarrow}) B(\mathbf{q}), \end{aligned} \quad (4)$$

where  $B(\mathbf{q})$  is the Fourier transform of  $B(\mathbf{r})$ . From this equation it is clear that the spin density (at wave vector  $\mathbf{q}$ ) is determined by the operators  $\bar{c}_{\mathbf{k}+\mathbf{q}, \sigma} c_{\mathbf{k}, \sigma}$ . To study their behavior we consider the equation of motion which is obtained from the commutator

$$[\bar{c}_{\mathbf{k}+\mathbf{q}, \sigma} c_{\mathbf{k}, \sigma}, H + H_1].$$

Evaluation of this commutator is a straightforward but tedious matter. The result is a very complicated expression involving a sum of products of either two or four annihilation and creation operators. Of the fourfold products we retain only those terms in which one pair has a nonvanishing expectation value in the unperturbed ground state. Thus, for instance, in a sum such as

$$\sum_{\mathbf{k}'\mathbf{p}} [v(\mathbf{p}) \bar{c}_{\mathbf{k}+\mathbf{q}} \bar{c}_{\mathbf{k}'-\mathbf{p}} c_{\mathbf{k}', \sigma} c_{\mathbf{k}-\mathbf{p}}], \quad (5)$$

we keep terms in which  $\mathbf{k}' = \mathbf{k} + \mathbf{q}$ ,  $\mathbf{k} - \mathbf{p} = \mathbf{k} + \mathbf{q}$  and  $\mathbf{k} - \mathbf{p} = \mathbf{k}' - \mathbf{p}$ . The corresponding operator products  $\bar{c}_{\mathbf{k}+\mathbf{q}} c_{\mathbf{k}+\mathbf{q}}$  and  $\bar{c}_{\mathbf{k}-\mathbf{p}} c_{\mathbf{k}-\mathbf{p}}$  are then replaced by their expectation values, the zero-order occupation numbers  $n_{\mathbf{k}+\mathbf{q}}$  and  $n_{\mathbf{k}-\mathbf{p}}$ . This is the basic approximation of the RPA which greatly simplifies the equations of motion.

<sup>5</sup> We set  $\hbar=1$  and denote the conjugate of an operator or function  $\psi$  by  $\bar{\psi}$ .

After using it the commutator takes the form

$$\begin{aligned} &[\bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow}, H + H_1] \\ &= \left[ \frac{k^2}{2m} - \frac{(\mathbf{k}+\mathbf{q})^2}{2m} \right] \bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow} \\ &\quad - \sum_{\mathbf{k}'} \{ [v(\mathbf{k}-\mathbf{k}') - v(\mathbf{k}+\mathbf{q}-\mathbf{k}')] n_{\mathbf{k}', \uparrow} \} \bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow} \\ &\quad + \sum_{\mathbf{k}\sigma} \{ v(\mathbf{q}) \bar{c}_{\mathbf{k}'+\mathbf{q}, \sigma} c_{\mathbf{k}', \sigma} \} [n_{\mathbf{k}+\mathbf{q}, \uparrow} - n_{\mathbf{k}, \uparrow}] \\ &\quad - \sum_{\mathbf{k}'} \{ v(\mathbf{k}-\mathbf{k}') c_{\mathbf{k}'+\mathbf{q}, \uparrow} c_{\mathbf{k}', \uparrow} \} [n_{\mathbf{k}+\mathbf{q}, \uparrow} - n_{\mathbf{k}, \uparrow}] \\ &\quad - (\mu g) B(\mathbf{q}) [n_{\mathbf{k}+\mathbf{q}, \uparrow} - n_{\mathbf{k}, \uparrow}]. \end{aligned} \quad (6)$$

The first term on the right-hand side of Eq. (6) is the commutator of  $\bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow}$  with the kinetic energy; the second gives the exchange self-energy of the states involved and corrects the individual particle energy from  $k^2/2m$  to

$$\epsilon(\mathbf{k}) = \frac{k^2}{2m} - \int_{k < k_F} v(\mathbf{k}-\mathbf{k}') \frac{d^3k'}{(2\pi)^3}; \quad (7)$$

the third is a plasma term that describes coupling to charge density fluctuations; and the fourth an exchange term that gives rise to scattering between the two virtual particles in states  $\mathbf{k}+\mathbf{q}$  and  $\mathbf{k}$ . Finally, the inhomogeneous term  $\mu g B(\mathbf{q}) (n_{\mathbf{k}+\mathbf{q}, \uparrow} - n_{\mathbf{k}, \uparrow})$  arises from the coupling to the external magnetic field. To simplify the succeeding analysis we now define a quantity

$$\theta_{\mathbf{k}, \mathbf{q}} = [\bar{c}_{\mathbf{k}+\mathbf{q}, \uparrow} c_{\mathbf{k}, \uparrow} - c_{\mathbf{k}+\mathbf{q}, \downarrow} c_{\mathbf{k}, \downarrow}]. \quad (8)$$

This operator does not generate charge density fluctuations. Thus, all plasma terms cancel from its equation of motion [as one may readily verify by subtracting from Eq. (6) the corresponding expression with spins reversed], and one obtains the relatively simple formula

$$\begin{aligned} i\dot{\theta}_{\mathbf{k}, \mathbf{q}} &= [\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{q})] \theta_{\mathbf{k}, \mathbf{q}} \\ &\quad - \sum_{\mathbf{k}'} \{ v(\mathbf{k}-\mathbf{k}') \theta_{\mathbf{k}', \mathbf{q}} \} (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}) \\ &\quad - \mu g B(\mathbf{q}) (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}). \end{aligned} \quad (9)$$

We now take the expectation value of this equation with respect to the wave function of the perturbed system. The result is the formula

$$\begin{aligned} i \frac{\partial}{\partial t} \langle \theta_{\mathbf{k}, \mathbf{q}} \rangle &= [\epsilon(\mathbf{k}) - \epsilon(\mathbf{k}+\mathbf{q})] \langle \theta_{\mathbf{k}, \mathbf{q}} \rangle \\ &\quad - \sum_{\mathbf{k}'} [v(\mathbf{k}-\mathbf{k}') \langle \theta_{\mathbf{k}', \mathbf{q}} \rangle] (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}) \\ &\quad - \mu g B(\mathbf{q}) (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}). \end{aligned} \quad (10)$$

It is clear from this equation that  $\langle \theta_{\mathbf{k}, \mathbf{q}} \rangle$  is proportional to  $(n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}})$ . Thus, we define a quantity  $\varphi(\mathbf{k}, \mathbf{q})$  through the relation

$$\langle \theta_{\mathbf{k}, \mathbf{q}} \rangle = (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}) \varphi(\mathbf{k}, \mathbf{q}). \quad (11)$$

Under steady-state conditions  $\varphi(\mathbf{k}, \mathbf{q})$  is determined by

the integral equation

$$[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k} + \mathbf{q})]\varphi(\mathbf{k}, \mathbf{q}) - \sum_{\mathbf{k}'} v(\mathbf{k} - \mathbf{k}') (n_{\mathbf{k}'+\mathbf{q}} - n_{\mathbf{k}'}) \varphi(\mathbf{k}', \mathbf{q}) = \mu g B(\mathbf{q}). \quad (12)$$

The solution of Eq. (12) determines the spin density through the relation

$$\langle \sigma_z(\mathbf{q}) \rangle = \sum_{\mathbf{k}} [\varphi(\mathbf{k}, \mathbf{q}) (n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}})]. \quad (13)$$

Equation (12) is a sort of Schrödinger equation describing scattering of particles excited into states  $\mathbf{k}$  and  $\mathbf{k} + \mathbf{q}$  by the external field. As was mentioned earlier, this equation is generally rather difficult to solve. Some feeling for the nature of its solution may be obtained, however, by making the assumption  $v(\mathbf{k} - \mathbf{k}') = \text{constant} = \bar{v}$ . If  $v(\mathbf{k} - \mathbf{k}')$  were the Fourier transform of the bare Coulomb potential this approximation would be very bad. Hubbard<sup>6</sup> has pointed out, though, that the exchange interaction should be screened. Under these circumstances the assumption  $v = \bar{v}$  greatly improves, and one may hope it will give some insight into the solution of the correct problem. After this approximation is made, Eq. (12) is readily soluble. One finds the induced spin density

$$\langle \sigma_z(\mathbf{q}) \rangle = \frac{\mu g B(\mathbf{q}) F(\mathbf{q})}{[1 - \bar{v} F(\mathbf{q})]}, \quad (14)$$

where

$$F(\mathbf{q}) = - \sum_{\mathbf{k}} \left[ \frac{n_{\mathbf{k}+\mathbf{q}} - n_{\mathbf{k}}}{\epsilon(\mathbf{k} + \mathbf{q}) - \epsilon(\mathbf{k})} \right] \quad (15)$$

is the counterpart of the Ruderman-Kittel susceptibility function, and reduces to their formula if one sets  $\epsilon(\mathbf{k}) = k^2/2m$ . From Eqs. (14) and (15) we see that, within the RPA, the Coulomb interaction has a twofold effect on the spin susceptibility. It renormalizes the particle energies [to the extent of replacing  $k^2/2m$  by  $\epsilon(\mathbf{k})$ ], and causes exchange scattering between virtual particles created by the external field. These scatterings give rise to the denominator  $[1 - \bar{v} F(\mathbf{q})]$  in Eq. (14), which has the effect of enhancing the spin density [note that  $F(\mathbf{q}) \geq 0$ ] over that predicted by the Ruderman-Kittel formula. Moreover, since  $F(\mathbf{q})$  is a monotonically decreasing function, this correction is greatest for small  $q$ . Hence the spin density (in  $\mathbf{q}$  space) is also slightly sharpened by the exchange interaction, which means that it is broader in real space.

The previous results have been obtained by replacing  $v(\mathbf{k} - \mathbf{k}')$  by  $\bar{v}$ . It is also of interest to investigate Eq. (12) in the limit  $q/k_F \ll 1$  (here  $k_F$  is the Fermi momentum). The factor  $(n_{\mathbf{k}'+\mathbf{q}} - n_{\mathbf{k}'})$  in this equation then limits the  $\mathbf{k}'$  integration to the vicinity of the Fermi surface. Furthermore, from Eq. (13), we see that to compute the spin density we only need know  $\varphi(\mathbf{k}, \mathbf{q})$  for  $k \sim k_F$ . Therefore, in solving Eq. (12), we may assume that both  $\mathbf{k}$  and  $\mathbf{k}'$  lie on the surface of the Fermi sphere and write  $\mathbf{k} = k_F \boldsymbol{\Omega}$  and  $\mathbf{k}' = k_F \boldsymbol{\Omega}'$ , where  $\boldsymbol{\Omega}$  and  $\boldsymbol{\Omega}'$  are unit

vectors. Lastly, we set

$$\varphi(\mathbf{k}, \mathbf{q}) = \frac{\psi(\mathbf{k}, \mathbf{q})}{[\epsilon(\mathbf{k}) - \epsilon(\mathbf{k} + \mathbf{q})]}. \quad (16)$$

In the limit  $q/k_F \ll 1$ , Eq. (12) then becomes

$$\psi(k_F \boldsymbol{\Omega}, \mathbf{q}) + \sum_{\mathbf{k}'} \frac{v(k_F \boldsymbol{\Omega} - k_F \boldsymbol{\Omega}') \varphi(k_F \boldsymbol{\Omega}', \mathbf{q}) (n_{\mathbf{k}'+\mathbf{q}} - n_{\mathbf{k}'})}{(\nabla_{\mathbf{k}'} \epsilon) \cdot \mathbf{q}} = \mu g B(\mathbf{q}). \quad (17)$$

The integral over the magnitude of  $\mathbf{k}'$  may now be evaluated, and the equation takes the form

$$\psi(k_F \boldsymbol{\Omega}, \mathbf{q}) - \int \frac{d\Omega'}{(2\pi)^3} \left( \frac{k_F^2}{v_F} \right) v[k_F(\boldsymbol{\Omega} - \boldsymbol{\Omega}')] \psi(k_F \boldsymbol{\Omega}', \mathbf{q}) = \mu g B(\mathbf{q}), \quad (18)$$

where

$$v_F = (\partial \epsilon / \partial k) |_{k=k_F}.$$

This equation has a solution

$$\psi(k_F \boldsymbol{\Omega}, \mathbf{q}) = \frac{\mu g B(\mathbf{q})}{1 - \int \frac{d\Omega'}{(2\pi)^3} \frac{v[k_F(\boldsymbol{\Omega} - \boldsymbol{\Omega}')] k_F^2}{v_F}}, \quad (19)$$

since  $\int [d\Omega' / (2\pi)^3] v[k_F(\boldsymbol{\Omega} - \boldsymbol{\Omega}')] k_F^2$  is independent of  $\boldsymbol{\Omega}$ . The corresponding spin density is obtained from Eq. (13) and turns out to be

$$\langle \sigma_z(\mathbf{q}) \rangle = \frac{\mu g B(\mathbf{q}) \frac{4\pi k_F^2}{(2\pi)^3 v_F}}{\left\{ 1 - \frac{k_F^2}{v_F} \int \frac{d\Omega'}{(2\pi)^3} v[k_F(\boldsymbol{\Omega} - \boldsymbol{\Omega}')] \right\}}. \quad (20)$$

With the aid of Eq. (15) this expression may be rewritten in the form

$$\langle \sigma_z(\mathbf{q}) \rangle = \frac{\mu g B(\mathbf{q}) F(0)}{1 - F(0) \int \frac{d\Omega'}{4\pi} v[k_F(\boldsymbol{\Omega} - \boldsymbol{\Omega}')]}, \quad (21)$$

which is then similar to that of Eq. (14).

From Eqs. (14) and (21) one sees that exchange scattering has an important effect on the spin susceptibility when  $\bar{v} F(\mathbf{q})$  or (in the limit  $q \rightarrow 0$ )

$$F(0) \int (d\Omega' / 4\pi) v(k_F \boldsymbol{\Omega}')$$

are of order unity. There is, in fact, a divergence of  $\langle \sigma_z(\mathbf{q}) \rangle$  when either of these quantities is equal to unity. It is clear from Eq. (12) that this infinity corresponds to the existence of a finite spin density in the absence of any magnetic field—that is, to ferromagnetism of the electron gas. In particular, one may show that the denominator of Eq. (21) (which gives the spin density in the  $q=0$  limit) vanishes at that electron

<sup>6</sup> J. Hubbard, Proc. Roy. Soc. (London) A243, 336 (1958).

density which corresponds to Bloch's<sup>7</sup> criterion for differential ferromagnetism of the electron gas.<sup>8</sup> If  $v(\mathbf{k})$  is the bare Coulomb interaction this criterion is satisfied when the density parameter  $r_s$  is about six—with a screened interaction the divergence occurs at an even lower electron density. We conclude, therefore, that in an electron gas of density comparable to that found in good metals, the enhancement of the Ruderman-Kittel susceptibility by exchange scattering is not particularly large. Typically, one may expect enhancement factors in the range 1.25–2.0.

Finally, it should be observed that our entire analysis is based upon perturbation expansion about an *unpolarized* ground state. It must, therefore, fail when the exchange interaction is sufficiently strong (or the gas sufficiently dilute) that the electron system is ferromagnetic. For the case of the delta-function interaction ferromagnetism sets in when the denominator of Eq. (14) vanishes for  $q=0$ —that is, when  $\bar{v}F(0)=1$ . This equation also has infinities, corresponding to standing spin waves, when its denominator goes to zero for finite  $q$ . Since  $F(q)$  is a monotonically decreasing function, however, these roots only occur at electron densities so low that the gas becomes ferromagnetic—that is, in a range in which Eq. (14) has no physical meaning. Overhauser<sup>9</sup> has suggested, on the basis of an analysis somewhat similar to ours, that such spin waves actually exist in metals. The preceding remarks imply, however, that before the exchange interaction is sufficiently strong to generate them, the electron gas becomes ferromagnetic, under which circumstances both his and our analyses fail.

### III

Having discussed the spin susceptibility from the point of view of the RPA, we now wish briefly to consider the same problem with the aid of many-body perturbation theory. Since the techniques of this method, as well as many of the formulas we shall need, have been given elsewhere, we will only indicate the essential points in the development. Our point of

departure is the fact that the field  $B(\mathbf{r})$  that causes the spin polarization is weak. We may, therefore, use first-order perturbation theory to calculate its effect on the electron system. Assuming that this system is initially in its ground state  $\psi_0$  one finds by a straightforward computation that the expectation value of the spin density is given by the formula

$$\langle \sigma_z(\mathbf{r}) \rangle = \left( \frac{1}{i} \right) \int_0^\infty e^{-\eta t} \langle \psi_0, [\sigma_z(\mathbf{r}, t), H_1] \psi_0 \rangle dt, \quad (22)$$

where  $\sigma_z(\mathbf{r}, t) = e^{iH_0 t} \sigma_z(\mathbf{r}) e^{-iH_0 t}$  is the Heisenberg operator for the spin density, and  $\eta$  a small, positive convergence factor. Equation (22) has the form of a vacuum expectation value and may be evaluated with techniques that have been developed for treating such quantities. A straightforward calculation, which exactly parallels the discussion given by Schweber, Bethe, and de Hoffman,<sup>10</sup> leads to the formula

$$\langle \sigma_z(\mathbf{r}) \rangle = 2 \operatorname{Im} \left\{ \int_0^\infty e^{-\eta t} \langle \varphi_0, T[S \sigma_z^{\text{int}}(\mathbf{r}, t) H_1] \varphi_0 \rangle dt \right\}. \quad (23)$$

Here  $\sigma_z^{\text{int}}(\mathbf{r}, t) = e^{iH_0 t} \sigma_z(\mathbf{r}) e^{-iH_0 t}$  is the spin-density operator in the interaction representation, “ $T$ ” is Wick's<sup>11</sup> time-ordering operator,  $\varphi_0$  is the ground-state eigenfunction of  $H_0$ , and the  $S$  matrix is to be evaluated with the expansion

$$S = \sum_{n=0}^{\infty} \left( \frac{1}{i} \right)^n \frac{1}{n!} \int_{-\infty}^{\infty} dt_1 \cdots \times \int_{-\infty}^{\infty} dt_n T[V(t_1) \cdots V(t_n)], \quad (24)$$

where  $V(t) = e^{iH_0 t} V e^{-iH_0 t}$ .

As in the RPA, it is more convenient to deal with the Fourier transform of the spin density,  $\langle \sigma_z(\mathbf{q}) \rangle = \int \langle \sigma_z(\mathbf{r}) \rangle e^{-i\mathbf{q} \cdot \mathbf{r}} d^3r$ , rather than with  $\langle \sigma_z(\mathbf{r}) \rangle$  itself. By combining Eq. (4) with Eq. (23) and making use of translational invariance and the reality of  $B$ , one may obtain the result

$$\langle \sigma_z(\mathbf{q}) \rangle = 2\mu g B(\mathbf{q}) \operatorname{Im} \left\{ \int_0^\infty e^{-\eta t} \langle \varphi_0, T[S \sigma_z^{\text{int}}(\mathbf{q}, t) \sigma_z(-\mathbf{q}, 0)] \varphi_0 \rangle dt \right\}. \quad (25)$$

This formula, which provides the starting point for the perturbation calculation, is in precisely the form to which Wick's theorem applies and thus leads directly to a diagrammatic analysis of the spin density.

To develop Eq. (25) in powers of  $e^2$  we replace  $S$  by its expansion [Eq. (24)]. Wick's theorem then permits

one to write each term in the series as a set of diagrams of the Goldstone type. Most of the rules required to evaluate these diagrams are given in the literature and will not be repeated here. A formulation due to Du Bois<sup>12</sup> is particularly convenient for our purposes and will be used throughout this section. The operators  $\sigma_z(\mathbf{q}, 0)$  and  $\sigma_z(\mathbf{q}, t)$  do not appear in his work, however,

<sup>7</sup> F. Bloch, *Z. Physik* **57**, 545 (1929). See also F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940), p. 601.

<sup>8</sup> I am grateful to P. W. Anderson for pointing out to me the relationship between Eq. (23) and Bloch's work.

<sup>9</sup> A. W. Overhauser, *Phys. Rev. Letters* **3**, 414 (1959).

<sup>10</sup> S. S. Schweber, H. A. Bethe, and F. de Hoffman, *Mesons and Fields* (Row, Peterson and Company, Evanston, Illinois, 1955), Vol. 1, p. 384.

<sup>11</sup> G. C. Wick, *Phys. Rev.* **80**, 268 (1950).

<sup>12</sup> D. F. Du Bois, *Ann. Phys.* **7**, 174 (1959).

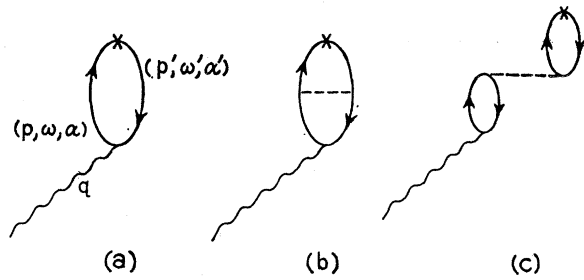


FIG. 1. Diagrams illustrating the effect of spin operators in Eq. (25).

so we must consider how they are to be incorporated into the graphical analysis. Their effect can probably be best understood by examination of simple examples. In Fig. 1(a), we show the diagram that arises from Eq. (25) when  $S$  is set equal to unity. The incoming wavy line in the graph represents the interaction of the electron system with the external field [operator  $\sigma_z(-\mathbf{q}, 0)$  of Eq. (25)], whereas the cross corresponds to the spin-measuring operator  $\sigma(\mathbf{q}, t)$ . It is clear that these operators bring momentum  $\pm\mathbf{q}$  into the diagram—thus one has momentum conservation at each of the vertices of Fig. 1(a). On the other hand, the energy conservation rule, which applies at the vertices corresponding to Coulomb scattering, is modified or absent. For Coulomb vertices this conservation condition arises from the infinite time integral, that appears in Eq. (24). No time integral at all is associated with the vertex due to the perturbing field—thus there is no corresponding frequency condition. At the spin-measuring vertex the time integration goes from zero to infinity. Thus in Fig. 1(a), instead of setting  $\omega = \omega'$  at the upper vertex we introduce a factor  $i/(\omega - \omega' + i\eta)$  and integrate over both  $\omega$  and  $\omega'$ . In static problems, however, only the delta-function part of this expression contributes.

The preceding remarks take care of the momentum and frequency conditions at vertices arising from the  $\sigma$  operators in Eq. (25). We must finally examine their spin dependence. For this purpose label the particle lines of a graph according to their spin states  $\alpha, \alpha'$ , etc. It is then clear that the spin operators in Eq. (25) give the matrix element  $\langle \alpha | \sigma_z | \alpha' \rangle$ , between incoming and outgoing lines, at the vertex. Thus, in Fig. 1(a), the spin sum is

$$\sum_{\alpha\alpha'} \langle \alpha | \sigma_z | \alpha' \rangle \langle \alpha' | \sigma_z | \alpha \rangle = \frac{1}{2}. \quad (28)$$

In considering more complicated diagrams it is important to realize that a particle's spin is unchanged in scattering. Thus, in Fig. 1(b), the spins of electron and hole are the same before and after the scattering, and the spin sum again has the value  $\frac{1}{2}$ . On the other hand, in cases such as that shown in Fig. 1(c) in which the two spin operators are on *different* particle lines,

the spin sum is of the form

$$\sum_{\alpha\alpha'} \langle \alpha | \sigma_z | \alpha \rangle \langle \alpha' | \sigma_z | \alpha' \rangle,$$

and vanishes. The principles embodied in these observations are quite general and greatly simplify the succeeding analysis. Henceforth we may ignore spin and consider only those diagrams in which the two spin operators appear on the *same* particle line.

We are now in a position to discuss the diagrams that contribute to the RPA. These are graphs containing the simplest sort of self-energy correction and electron-hole scattering. A typical such graph is illustrated in Fig. 2 and involves exchange self-energy corrections to the propagators and direct Coulomb interactions between the virtual electron-hole pair. The effect of including the exchange self-energy in all possible ways (that is, to all orders) in such graphs is quite simple. It merely replaces the energy  $k^2/2m$  in the propagators by the expression given in Eq. (7). Assuming that the summation over all possible exchange self-energy insertions has been performed, we are then left with the set of graphs shown in Fig. 3 [which are to be evaluated with propagators renormalized to the extent of replacing  $k^2/2m$  by  $\epsilon(k)$ ] to sum. The first diagram gives a contribution to  $\langle \sigma_z(\mathbf{q}) \rangle$  of the form

$$2\mu g B(\mathbf{q}) \operatorname{Im} \int \frac{iS(\mathbf{k}\omega)S(\mathbf{k}+\mathbf{q}, \omega')}{(\omega - \omega' + i\eta)} \frac{d^3k}{(2\pi)^3} \frac{d\omega}{(2\pi)} \frac{d\omega'}{(2\pi)}, \quad (29)$$

where

$$S(\mathbf{k}, \omega) = -i \left\{ \frac{\theta(k - k_F)}{[\omega - \epsilon(k) + i\eta]} + \frac{\theta(k_F - k)}{[\omega - \epsilon(k) - i\eta]} \right\}, \quad (30)$$

and  $\theta(x)$  is the step function defined by

$$\begin{aligned} \theta(x) &= 1 & x \geq 0, \\ \theta(x) &= 0 & x < 0. \end{aligned} \quad (31)$$

One may readily show that only the  $\delta(\omega' - \omega)$  term contributes to Eq. (29). Thus we obtain

$$\mu g B(\mathbf{q}) \operatorname{Im} \int S(\mathbf{k}, \omega) S(\mathbf{k} + \mathbf{q}, \omega) \frac{d^3k d\omega}{(2\pi)^4}, \quad (32)$$

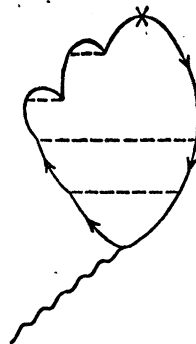


FIG. 2. A typical diagram that contributes to the RPA.

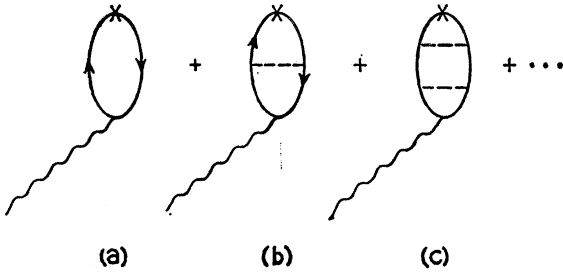


FIG. 3. Diagrams that are summed to give the RPA integral equation.

which can be evaluated by contour integration to give

$$\mu g B(\mathbf{q}) \int \frac{d^3 k}{(2\pi)^3} \frac{(n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}})}{[\epsilon(\mathbf{k}+\mathbf{q}) - \epsilon(\mathbf{k})]} \quad (33)$$

The integral in this expression is just the function  $F(\mathbf{q})$  defined in the previous section, and Eq. (33) is, once again, the Ruderman-Kittel result for the susceptibility. From the structure of the graph that leads to Eq. (33) one might also suspect that  $F(\mathbf{q})$  is the pair propagator. Comparison with Du Bois' work shows that this surmise is, indeed, correct.

We now go on to consider diagram 3(b), in which there is a single exchange scattering between the electron and hole. Using Du Bois' rules one finds, after some minor manipulations, that this graph contributes an amount

$$\mu g B(\mathbf{q}) \int \frac{d^3 k d^3 k'}{(2\pi)^6} \frac{d\omega d\omega'}{(2\pi)^2} [S(\mathbf{k}, \omega) S(\mathbf{k}+\mathbf{q}, \omega) \times v(\mathbf{k}-\mathbf{k}') S(\mathbf{k}', \omega') S(\mathbf{k}'+\mathbf{q}, \omega')] \quad (34)$$

to  $\langle \sigma_z(\mathbf{q}) \rangle$ . To simplify succeeding expressions we introduce the function

$$R(\mathbf{p}, \mathbf{q}) = \left( \frac{1}{i} \right) \int_{-\infty}^{\infty} \frac{d\omega}{(2\pi)} S(\mathbf{p}, \omega) S(\mathbf{p}+\mathbf{q}, \omega) = \left[ \frac{n_{\mathbf{p}} - n_{\mathbf{p}+\mathbf{q}}}{\epsilon(\mathbf{p}+\mathbf{q}) - \epsilon(\mathbf{p})} \right] \quad (35)$$

With this abbreviation the sum of the two lowest order diagrams in Fig. 3 is

$$\mu g B(\mathbf{q}) \left\{ \int \frac{d^3 k}{(2\pi)^3} R(\mathbf{k}, \mathbf{q}) + \int \int \frac{d^3 k}{(2\pi)^3} \frac{d^3 k'}{(2\pi)^3} R(\mathbf{k}, \mathbf{q}) v(\mathbf{k}-\mathbf{k}') R(\mathbf{k}', \mathbf{q}) \right\} \quad (36)$$

From the structure of this expression one guesses—and

may verify by direct computation—that the contribution of the entire set of diagrams shown in Fig. 3 is obtained from the solution of an integral equation. This equation is

$$T(\mathbf{k}, \mathbf{q}) = \mu g B(\mathbf{q}) R(\mathbf{k}, \mathbf{q}) + R(\mathbf{k}, \mathbf{q}) \int v(\mathbf{k}-\mathbf{k}') T(\mathbf{k}', \mathbf{q}) \frac{d^3 k'}{(2\pi)^3}; \quad (37)$$

from its solution one obtains the induced spin density (due to graphs in Fig. 3) through the relation

$$\langle \sigma_z(\mathbf{q}) \rangle = \int T(\mathbf{k}, \mathbf{q}) \frac{d^3 k}{(2\pi)^3} \quad (38)$$

If we make the identification  $T(\mathbf{k}, \mathbf{q}) = (n_{\mathbf{k}} - n_{\mathbf{k}+\mathbf{q}}) \varphi(\mathbf{k}, \mathbf{q})$  we see that Eq. (37) reduces to Eq. (12), and that Eq. (38) is precisely equivalent to the expression we obtained earlier [Eq. (13)] for the induced spin density. Thus, the set of diagrams shown in Fig. 3 gives the same spin susceptibility as the RPA. This approximation may, therefore, be characterized by saying that it takes into account (to all orders) the simplest possible propagator renormalizations and the simplest type of scattering between the virtual electron and hole created by the external field.

## CONCLUSION

The calculations outlined above indicate that, within the RPA at least, Coulomb interactions enhance the spin polarizability of an electron gas. For the completely free gas, at densities comparable to those found in good metals, the change is probably less than a factor two. However, one can well imagine that the effect of the lattice, which causes electrons to move in Bloch waves rather than plane waves, might considerably increase this figure. This is a point which certainly deserves further investigation.

We have shown that the RPA is equivalent to the summation of certain selected terms in perturbation theory. It thus neglects a great part of the Coulomb interaction and one can hardly expect its formulas to be numerically accurate at metallic densities. On the other hand, the general form of the results is physically very reasonable and doubtless indicates the sort of effect to be expected from an accurate treatment of the electron-electron interaction. Since such a treatment is presently rather far from realization, it has seemed worthwhile to investigate, in some detail, the rather simple RPA.

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