

## Electron-electron interaction in simple metals

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We calculate  $V_{ee}$ , the effective screened interaction between two electrons in a simple metal. The result is derived by a self-consistent perturbation theory based on Hartree-Fock theory. Exchange and correlation are treated in local approximation. We consider the lattice to be a smooth but elastically deformable, charged medium in which the electrons move. Our results is a generalization of the Fröhlich interaction to include exchange and correlation. The effective interaction is spin dependent and may be written  $V_{ee}(q, \omega) = V_0(q, \omega) - J(q, \omega) \vec{\sigma}_1 \cdot \vec{\sigma}_2$ . Explicit expressions for  $V_0$  and  $J$  are given in terms of the lattice stiffness and the same local exchange and correlation potentials of the electron gas which are needed to calculate the dielectric function and the spin susceptibility.

### I. INTRODUCTION

This paper presents a calculation of the effective screened interaction between two electrons in a simple metal. Exchange and correlation are taken into account in a local approximation, and the lattice is treated as a smooth but elastically deformable medium in which the electrons move. Our results are derived by a self-consistent perturbation theory based on Hartree-Fock theory. This approach yields coupled algebraic equations for the coupled electron-ion system. The expression for the electron-electron interaction is given in terms of the same local exchange and correlation potentials which are needed to calculate the dielectric function  $\epsilon$ , and the spin susceptibility,  $\chi$ . We also calculate these quantities as well as the electron-test-charge interaction in order to define our notation and to show that the standard expressions are obtained.

Our results will be of interest to those concerned with electron-electron scattering and transport theory, superconductivity, charge and spin density waves, and other properties of the coupled electron-lattice system. Previous work in this area has been limited. Kukkonen and Wilkins<sup>1</sup> have shown the importance of exchange on the electron-electron interaction, but they approximated the lattice by a *rigid* uniform background. They found the electron-electron interaction to be strongly repulsive and they used their result in a calculation of transport properties. Fröhlich<sup>2</sup> first showed how lattice screening leads to an attractive electron-electron interaction. This work provided insight into the problem of superconductivity, but the

Fröhlich interaction does not include the effects of exchange and correlation. The present theory includes both exchange and correlation and the effect of lattice screening.

In Sec. II, we present the results of the Hartree-Fock theory of the electronic response, assuming a rigid uniform background of positive charge and treating exchange in a local approximation. We generalize the theory to include correlation in Sec. III, and we treat the spin response to an external magnetic field in Sec. IV. We note that the effect of correlation is to enhance the dielectric response but reduce the spin response. The electron-electron interaction depends on both of these responses. Screening by the lattice is included in Sec. V, where we obtain our final results. A brief discussion of the implications of our results is given in Sec. VI. The Hartree-Fock approach is outlined in Appendix.

### II. EXCHANGE EFFECTS

In this section we use the results of standard Hartree-Fock and linear response theories<sup>3</sup> to calculate in a simple way the effective many-body interaction  $V_{ee}(q)$  between two electrons in a metal. We introduce our notation by rederiving the known effective interactions between two test charges,  $V_{tt}(q)$ , and between an electron and a test charge,  $V_{et}(q)$ . We then introduce the simple extension required to obtain  $V_{ee}$ . Since this section is based on Hartree-Fock theory, our results include only exchange effects. In Sec. III we generalize the Hartree-Fock ap-

proach to include Coulomb correlations explicitly.

We first consider the standard problem of an electron gas perturbed by a weak external potential such as that due to a test-charge density with Fourier components  $\rho_{\text{ext}}(q, \omega)$ . The Fourier components of the potential are obtained from Poisson's equation, as

$$V_{\text{ext}}(q, \omega) = v(q) \rho_{\text{ext}}(q, \omega), \quad (1)$$

where  $v(q) = 4\pi e^2/q^2$ . For convenience we will not remind the reader of the wave vector and frequency dependence of most quantities at each step, e.g., Eq. (1) will become  $V_{\text{ext}} = v\rho_{\text{ext}}$ . We take the lattice charge density as uniform and rigid. Our discussion of this problem parallels that of Hedin and Lundqvist.<sup>4</sup>

The external perturbation induces a density response  $\Delta n$  in the electron gas. The total potential seen by another test charge is simply the electrostatic potential

$$V_{\text{tt}} = v(\rho_{\text{ext}} + \Delta n). \quad (2)$$

The dielectric function  $\epsilon(q, \omega)$  is defined by

$$V_{\text{tt}} = \frac{V_{\text{ext}}}{\epsilon}. \quad (3)$$

The problem is to calculate the density response  $\Delta n$ . This is done self-consistently in Hartree-Fock theory. An electron in the Fermi sea feels a self-consistent potential  $V_{\text{et}}$ , which is the sum of the local electrostatic potential ( $V_{\text{ext}}$  plus Hartree term) and a nonlocal exchange potential  $V_{\text{x}}$  (Fock term) caused by  $\Delta n$ . Since the nonlocal problem is difficult, we make the usual approximation that  $V_{\text{x}}$  is a local potential,

$$V_{\text{x}} = -vG_{\text{x}}\Delta n. \quad (4)$$

This expression may be viewed as the definition of  $G_{\text{x}}$  which we will discuss later. With this approximation we obtain the fundamental equation

$$V_{\text{et}} = V_{\text{tt}} + V_{\text{x}} = v[\rho_{\text{ext}}(q) + (1 - G_{\text{x}})\Delta n]. \quad (5)$$

First-order perturbation theory shows that the induced density is linearly related to  $V_{\text{et}}$  by

$$\Delta n = -\Pi^0 V_{\text{et}}. \quad (6)$$

$\Pi^0$  is the free-electron response function,

$$\Pi^0 = \frac{q_{\text{TF}}^2}{4\pi e^2} \left[ \frac{1}{2} + \frac{k_{\text{F}}}{2q} \left[ 1 - \left( \frac{q}{2k_{\text{F}}} \right)^2 \right] \ln \left| \frac{1 + \frac{q}{2k_{\text{F}}}}{1 - \frac{q}{2k_{\text{F}}}} \right| \right],$$

where  $q_{\text{TF}}^2$  is the Thomas-Fermi screening wave vector and  $k_{\text{F}}$  is the Fermi wave vector ( $q_{\text{TF}}^2 = 4me^2k_{\text{F}}/\pi\hbar^2$ ). The self-consistent electron-test-charge potential is found by eliminating  $\Delta n$  from

Eqs. (5) and (6) to be

$$V_{\text{et}} = \frac{V_{\text{tt}}}{1 - G_{\text{x}}Q} = \frac{V_{\text{ext}}}{1 + (1 - G_{\text{x}})Q}. \quad (7)$$

The test-charge-test-charge interaction is given by Eq. (3) and thus the dielectric function is, from Eq. (7),

$$\epsilon = 1 + Q/(1 - G_{\text{x}}Q), \quad (8)$$

where  $Q \equiv v\Pi^0$ . These results have forms identical to previous work,<sup>5</sup> but our  $G_{\text{x}}$  includes only the effect of exchange. Correlation will be included in Sec. II A.

### A. Electron-electron interaction

Our goal is to use the same Hartree-Fock theory to calculate the effective interaction between two electrons. The first problem in the formal theory is to determine what the perturbation is. For an external test charge the answer is clear, but when the perturbing particle is an electron, identical to those in the Fermi sea, the problem is more difficult. We postpone the discussion of the rigorous Hartree-Fock solution to Appendix A, and instead we present a physical argument that reproduces the Hartree-Fock result (using a local approximation for the exchange potential).

The electron-electron interaction is obtained as follows. Consider two "particular" electrons in the Fermi sea with momenta and spin,  $k_1\sigma_1$  and  $k_2\sigma_2$ , and with densities  $\rho_{\sigma_1}$  and  $\rho_{\sigma_2}$ . We consider one to be the perturbing particle, say  $\rho_1$  and the other to feel the perturbation. Although we focus on two "particular" electrons, we must remember that these two electrons are indistinguishable from others in the Fermi sea and are indistinguishable from each other if they have parallel spins. This indistinguishability is the crucial difference between a perturbation due to an external test charge  $\rho_{\text{ext}}$  and that due to an electron,  $\rho_1$ . The main contribution of this paper is the simple recognition that when considering the electron-electron interaction one must take into account that the perturbing electron has an exchange interaction with *all* other electrons of parallel spin. This interaction is absent for a test-charge perturbation.

The perturbation due to  $\rho_1$  induces a density response in the electron gas that includes contributions from electrons with both spins,  $\Delta n_{\uparrow}$  and  $\Delta n_{\downarrow}$ . The second particular electron then interacts with  $\rho_1$  and with  $\Delta n_{\uparrow}$  and  $\Delta n_{\downarrow}$ . The first step then is to calculate the density response.

If the perturbing electron has spin up, a down spin electron in the Fermi sea will feel the net electrostatic

potential.

$$V_{\text{electrostatic}} = v(\rho_1 + \Delta n_1 + \Delta n_1), \quad (9)$$

and it will also feel an exchange potential due to the induced density of the same spin  $\Delta n_1$ . In the local approximation the exchange potential is given by

$$V_x^{\text{ex}} = -2vG_x\Delta n_1. \quad (10)$$

The inclusion of the factor of 2 retains the usual definition of  $G_x$ ,  $V_x = -vG_x\Delta n$  [Eq. (4)] for an unpolarized system where  $\Delta n = \Delta n_1 + \Delta n_1 = 2\Delta n_1$ .

A spin-up electron in the Fermi sea will also feel the electrostatic potential and it will feel an exchange potential due to  $\Delta n_1$ . *The difference between an electron with spin up and one with spin down is that the spin-up electron will have an additional exchange interaction directly with the perturbing electron  $\rho_1$ .* In the local approximation, the direct exchange potential is

$$\bar{V}_{11}^{\text{dir ex}} = -2vG_x\rho_1. \quad (11)$$

This simple observation is the new ingredient required to form the electron-electron interaction.

We can now write the coupled equations that determine the density response of the electron gas perturbed by an electron with spin up as

$$V_{11} = v[\rho_1 + \Delta n_1 + (1 - 2G_x)\Delta n_1] \quad (12)$$

and

$$\bar{V}_{11} = v[(1 - 2G_x)\rho_1 + (1 - 2G_x)\Delta n_1 + \Delta n_1]. \quad (13)$$

The equation for parallel spins has the form

$$\bar{V}_{11} = V_{11} + \bar{V}_{11}^{\text{dir ex}}, \quad (14)$$

which includes a term  $V_{11}$ , like Eq. (12), and a term due to the direct exchange of the two electrons under consideration. If the direct exchange term were absent, these equations would reduce to those for a test-charge perturbation. The density responses are related to the effective potentials by

$$\Delta n_1 = -\Pi^0 \bar{V}_{11}/2,$$

and

$$\Delta n_1 = -\Pi^0 V_{11}/2. \quad (15)$$

Substituting these into Eqs. (12) and (13) one obtains

$$V_{11} = \left( \frac{1}{1 - G_x Q} \right)^2 \frac{v\rho_1}{\epsilon}, \quad (16)$$

and

$$\bar{V}_{11} = V_{11} - \frac{2G_x v\rho_1}{1 - G_x Q}, \quad (17)$$

which yield the density responses via Eq. (15). We check the consistency of our results by using  $\Delta n_1$  and

$\Delta n_1$  to calculate the electrostatic potential due to a perturbing electron. A test charge would feel only this potential. We find that this potential  $V_{te}$  is exactly the same as the self-consistent potential  $V_{et}$  an electron feels due to a perturbing test charge.

The last point to consider is the relation of these potentials,  $V_{11}$  and  $\bar{V}_{11}$ , to those one should use to calculate scattering amplitudes. Consider simple two-electron scattering via a potential  $U(r)$  which is spin independent. The scattering event is  $k_1\sigma_1$ ;  $k_2\sigma_2 \rightarrow k_1 + q, \sigma_1$ ;  $k_2 - q, \sigma_2$ . For electrons with antiparallel spins, the scattering amplitude in the Born approximation is

$$M_{11} \propto U(q). \quad (18)$$

If the electrons have parallel spins however, the scattering amplitude must be antisymmetric under interchange of the two particles and is given by

$$M_{11} \propto U(q) - U(k_2 - k_1 - q), \quad (19)$$

where the first term is the direct term and the second is the exchange term. Because  $\bar{V}_{11}$  is not antisymmetric under interchange of the two electrons, it is not a proper scattering amplitude. The reason is that  $\bar{V}_{11}$ , Eq. (17), is based on the approximate expression Eq. (11), for direct exchange. We remedy the situation by subtracting the direct exchange term from  $\bar{V}_{11}$ , Eq. (14), to obtain  $V_{11}$ . The result is,

$$V_{11} = \bar{V}_{11} - \frac{2G_x^2 Q v\rho_1}{1 - G_x Q}. \quad (20)$$

We then stipulate that the scattering amplitude  $M_{11}$  for a parallel-spin event is

$$M_{11} \propto V_{11}(q) - V_{11}(k_2 - k_1 - q), \quad (21)$$

which incorporates the direct exchange in a manifestly antisymmetric way. Of course, the antiparallel-spin scattering amplitude is simply

$$M_{11} \propto V_{11}. \quad (22)$$

These results can be justified by formal many-body theory.<sup>6</sup>

The result for  $V_{11}$  was previously obtained by Kukkonen and Wilkins<sup>1</sup> based on a Feynman diagram analysis of the Bethe-Salpeter equations. Their diagrammatic analysis for  $V_{11}$  included all the diagrams that sum to our present expression Eq. (20). However, they did not realize that those diagrams that yield the second term in Eq. (20) could be summed explicitly and they neglected this term.

The fact that  $V_{11} \neq \bar{V}_{11}$  shows that the potentials themselves are spin dependent. We exhibit the spin dependence explicitly by writing

$$V_{\vec{\sigma}_1, \vec{\sigma}_2} = V_0 - J \vec{\sigma}_1 \cdot \vec{\sigma}_2, \quad (23)$$

where  $\vec{\sigma}$  is the Pauli spin operator and

$$V_0 = \frac{1}{2}(V_{\uparrow\uparrow} + V_{\downarrow\downarrow}) = V_{\uparrow\uparrow} - \frac{G_x^2 Q v \rho_{\uparrow}}{1 - G_x Q}, \quad (24)$$

$$J = -\frac{1}{2}(V_{\uparrow\downarrow} - V_{\downarrow\uparrow}) = \frac{G_x^2 Q v \rho_{\uparrow}}{1 - G_x Q}. \quad (25)$$

These results are the complete solution within the Hartree-Fock theory of the electron-electron interaction when a local approximation to the exchange interaction is used. The only unknown is the *same* exchange interaction  $G_x$ , needed to form  $V_u$  and  $V_{et}$ . We now turn our attention to a generalization of the Hartree-Fock theory to include Coulomb correlations among electrons.

### III. EXCHANGE AND CORRELATION EFFECTS

A local correlation potential is included by the following analogy with the local approximation of the exchange potential in Hartree-Fock theory. The self-consistent Hartree-Fock charge density around an electron with wave vector  $k$  and a given spin consists of a uniform density of antiparallel spin electrons, but electrons with parallel spins are kept away by the Pauli principle. This exchange charge density is nonlocal and leads to a nonlocal exchange potential. The local approximation to exchange is obtained by averaging the nonlocal exchange potential. The resulting exchange charge density represents a local, spherically symmetric exchange hole or absence of parallel-spin electrons around the electron under consideration. The exchange hole is a kinematic effect of the Pauli principle that results from the antisymmetry of the wave functions.

Correlation effects are defined as those effects due to the mutual Coulomb repulsion of electrons that are not included in Hartree-Fock theory. The most important effect of correlation on the charge density surrounding an electron with a given spin is the Coulomb repulsion of electrons with opposite spins. This causes a correlation hole in the density of these electrons. Coulomb correlations also modify the exchange hole, but this effect is presumed to be smaller because parallel spins are already kept away from each other by the Pauli principle. These effects of correlation are included by replacing the local exchange potential in Hartree-Fock theory by a local exchange and correlation potential.

To illustrate this we calculate the response of electrons in the Fermi sea to a perturbation by a test charge,  $\rho_{ext}$ . An electron with spin up feels the potential

$$V_{e\uparrow} = v[\rho_{ext} + (1 - 2G_x)\Delta n_{\uparrow} + (1 - 2G_C)\Delta n_{\downarrow}], \quad (26)$$

where the local exchange and correlation potential

between electrons with parallel spins is

$$V_{xc}^{\uparrow\uparrow} = -2vG_x\Delta n_{\uparrow}, \quad (27)$$

and  $G_x = G_x + \delta G$ ;  $G_x$  is the exchange contribution defined in Eq. (4) and  $\delta G$  is the correlation correction for parallel spins. The local correlation potential between electrons with antiparallel spins is

$$V_C^{\uparrow\downarrow} = -2vG_C\Delta n_{\downarrow}. \quad (28)$$

Equation (26) is the generalization of the Hartree-Fock result [Eq. (5)] to include correlation explicitly. The density responses are related to the effective potentials by the usual relation, Eq. (15). Because the perturbation is a test charge,  $V_{e\uparrow} = V_{e\downarrow}$ . Using this, the solution is immediately obtained as

$$V_{et} = \frac{V_{ext}}{1 + [1 - (G_x + G_C)]Q}, \quad (29)$$

which has precisely the form obtained in Hartree-Fock theory Eq. (7), but  $G_x$  has been replaced by  $G_x + G_C$ . The test charge-test charge interaction  $V_u$  is also obtained by the same substitution. As we will see this is no longer true however for the electron-electron interactions or for the spin susceptibility, where the effects of correlation enter in a different way. The effect of correlation on  $V_u$  and  $V_{et}$  has been obtained previously.<sup>4</sup>

The calculation of electron-electron interactions is similar to the Hartree-Fock theory. The potentials felt by electrons in the Fermi sea due to the perturbing electron  $\rho_{\uparrow}$  are

$$\tilde{V}_{\uparrow\uparrow} = v[(1 - 2G_x)\rho_{\uparrow} + (1 - 2G_x)\Delta n_{\uparrow} + (1 - 2G_C)\Delta n_{\downarrow}] \quad (30)$$

and

$$\tilde{V}_{\uparrow\downarrow} = v[(1 - 2G_C)\rho_{\uparrow} + (1 - 2G_C)\Delta n_{\uparrow} + (1 - 2G_x)\Delta n_{\downarrow}]. \quad (31)$$

These equations differ in form from the Hartree-Fock equations, Eqs. (12) and (13), by the inclusion of antiparallel spin correlations  $G_C$ , with the induced density and directly with the perturbing electron. The inclusion of the latter is the reason for the tilde over  $V_{\uparrow\uparrow}$ . Using Eq. (15) to relate the density responses to the potentials and after some algebra, one finds

$$\tilde{V}_{\uparrow\uparrow} = \left( \frac{1}{1 - G_+ Q} \right)^2 \frac{v\rho_{\uparrow}}{\epsilon} + \frac{G_- v\rho_{\uparrow}}{1 - G_- Q} - \frac{G_+ v\rho_{\uparrow}}{1 - G_+ Q}, \quad (32)$$

and

$$\tilde{V}_{\uparrow\downarrow} = \tilde{V}_{\uparrow\uparrow} - \frac{2G_- v\rho_{\uparrow}}{1 - G_- Q}, \quad (33)$$

where  $G_+ = G_x + G_C$  and  $G_- = G_x - G_C$ , and  $\epsilon$  is given by Eq. (8) with  $G_x$  replaced by  $G_+$ . Again we check our results by using the derived  $\Delta n_{\uparrow}$  and  $\Delta n_{\downarrow}$

to calculate the electrostatic potential due to a perturbing electron, and we find the same result

$$V_{\text{electrostatic}} \equiv V_{te} = V_{et},$$

given in Eq. (29).

The effective potentials  $V_{\uparrow\uparrow}$  and  $V_{\downarrow\downarrow}$  needed to calculate scattering amplitudes are obtained from the average potentials by subtracting the term  $-2vG_X\rho_{\uparrow}$  from  $\bar{V}_{\uparrow\uparrow}$  and  $-2vG_C\rho_{\downarrow}$  from  $\bar{V}_{\downarrow\downarrow}$ . This removes the local approximation to direct exchange and correlation between the two electrons with parallel spins. Direct exchange may be then taken into account by using the antisymmetric form, Eq. (21). The above prescription also removes the local approximation to direct correlation between electrons with antiparallel spins. Direct correlation may be then included by calculating the scattering amplitude beyond the first Born approximation. This yields the modification of the wave functions due to the scattering. Because there is no particular simplification, we do not give these interactions, but rather their sum and difference which yield the explicit spin dependent form shown in Eq. (23). The spin-independent term is

$$V_0 = \frac{1}{2}(V_{\uparrow\uparrow} + V_{\downarrow\downarrow}) = \frac{[1 + (1 - G_+)G_+Q]v\rho_{\uparrow}}{1 + (1 - G_+)Q} \quad (34)$$

and the spin-dependent term is given by

$$J = -\frac{1}{2}(V_{\uparrow\uparrow} - V_{\downarrow\downarrow}) = \frac{G_-^2 Q v \rho_{\downarrow}}{1 - G_- Q} \quad (35)$$

We note that  $V_0$  depends only on  $G_+$  while  $J$  depends only on  $G_-$ , which shows that correlation affects a charge response differently from a magnetic or spin response. The magnetic response is discussed in Sec. IV.

#### IV. SPIN SUSCEPTIBILITY

We calculate the spin susceptibility  $\chi$ , in order to assure the reader that our approach yields the standard result and to show clearly that the effect of correlations among electrons with parallel spins (primarily due to exchange) is to enhance  $\chi$ , while antiparallel spin correlations (due to the Coulomb interaction) reduce the susceptibility. We consider a magnetic perturbation,  $H^{\text{int}} = \mu_B H \sigma_z \cos \vec{q} \cdot \vec{r}$ , where  $\mu_B$  is the Bohr magneton,  $H$  is the field amplitude, and  $\sigma_z$  is the spin operator. An electron with its spin parallel (antiparallel) to the  $z$  axis has its energy raised (lowered) by the field. Consequently electrons will tend to flip their spins to align themselves opposite to the field and lower their energy. This tendency is opposed by the increase in kinetic energy caused by increasing  $n_{\uparrow}$  at the expense of  $n_{\downarrow}$ . The susceptibility calculated in Hartree-Fock theory is larger than that calculated in Hartree theory because this increase

in kinetic energy is partially offset by an increase in the size of the exchange energy which has the opposite sign.

The qualitative effects of exchange and correlation may be understood from the following simple argument. The external field tends to flip spins and polarize the electrons. Therefore the effect of exchange and correlation on the susceptibility is determined by the effect of this polarization on the exchange and correlation energies. Both these energies are negative. Roughly speaking the exchange energy is proportional to the number of possible pairs of parallel spin electrons,

$$E_x \propto - \left[ \frac{N_{\uparrow}(N_{\uparrow}-1)}{2} + \frac{N_{\downarrow}(N_{\downarrow}-1)}{2} \right] \quad (36)$$

The correlation energy, however, derives mostly from antiparallel spins and therefore is roughly proportional to the number of possible pairs of antiparallel spins,

$$E_c \propto -N_{\uparrow}N_{\downarrow} \quad (37)$$

Writing  $N_{\uparrow}$  and  $N_{\downarrow}$  in terms of the total number of electrons  $N = N_{\uparrow} + N_{\downarrow}$ , the polarization  $p = (N_{\uparrow} - N_{\downarrow})/N$ , and ignoring unity compared to  $N_{\uparrow}$  and  $N_{\downarrow}$ , one obtains

$$E_x \propto - \left[ \frac{N}{2} \right]^2 (1 + p^2)$$

and

$$E_c \propto - \left[ \frac{N}{2} \right]^2 (1 - p^2) \quad (38)$$

This shows the total exchange energy is reduced by polarizing the electrons, which yields an enhancement of  $\chi$ . However the correlation energy is increased by polarization and this reduces  $\chi$ .

A quantitative result for  $\chi$  is obtained by extending Hartree-Fock theory to include a local correlation potential. The effective potential felt by an electron due to an external magnetic field,  $H \cos \vec{q} \cdot \vec{r}$ , is given by

$$U_{\uparrow H} = \mu_B H + v[(1 - 2G_X)\Delta n_{\uparrow} + (1 - 2G_C)\Delta n_{\downarrow}] \quad (39)$$

and

$$U_{\downarrow H} = -\mu_B H + v[(1 - 2G_C)\Delta n_{\uparrow} + (1 - 2G_X)\Delta n_{\downarrow}] \quad (40)$$

The density responses are given by usual relations, Eq. (15). Solving for the susceptibility, one finds

$$\chi \equiv \frac{\mu_B(\Delta n_{\uparrow} - \Delta n_{\downarrow})}{H} = \frac{\chi_0}{1 - (G_X - G_C)Q} = \frac{\chi_0}{1 - G_- Q} \quad (41)$$

where  $\chi_0 = \mu_B^2 \Pi^0$  is the  $q$ -dependent Pauli susceptibility-

ty obtained from Hartree theory. We note that  $\chi$  depends only on  $G_- \equiv G_X - G_C$ . On the other hand the charge-response function  $\Pi$ ,  $\epsilon \equiv 1 + v\Pi$  [see Eq. (8) and the comment following Eq. (33)] depends only on  $G_+ = G_X + G_C$ ,

$$\Pi = \frac{\Pi^0}{1 - G_+ Q} \quad (42)$$

Equivalent expressions for  $\chi$  and  $\Pi$  have been obtained previously,<sup>4,7-9</sup> but it is worthwhile to emphasize that this comparison shows that correlation (more precisely antiparallel spin correlation) enhances the charge response, but reduces the spin response.

### V. SCREENING BY THE LATTICE

In a real metal, the compensating background of positive charge is not uniform and rigid, but is discrete and deformable. Specifically, the lattice ions are charged and can move in response to a charge perturbation. This problem of a coupled electron-lattice system has been considered by many previous investigators,<sup>10</sup> notably by Fröhlich<sup>2</sup> and by Bardeen<sup>11</sup> who found that lattice screening can lead to the attractive effective interaction between electrons which is required for superconductivity. We extend the previous theory to include the effects of exchange and correlation. We do this by a self-consistent field treatment of the coupled electron-ion system.

We consider a simple model for the lattice which neglects all effects associated with the periodicity of the ions. The lattice is regarded as a plasma of positive ions of mass  $M$  and charge  $e$ . The bare ion-ion and electron-ion interactions are denoted by  $V_{ii}^{\text{bare}}$  and  $V_{ei}^{\text{bare}}$ . The bare test-charge-ion interaction is taken as equal to  $V_{ei}^{\text{bare}}$ . In the jellium approximation both of these are equal to the bare Coulomb interaction. To define our notation we first consider the system to be perturbed by a weak external potential  $V_{\text{ext}} = v\rho_{\text{ext}}$ , which induces a density response  $\Delta n$  in the electron gas and  $\Delta n_{\text{ion}}$  in the ions.

The effective potentials felt by an electron and an ion are

$$V_{ei} = v[\rho_{\text{ext}} + (1 - G_+) \Delta n] - V_{ei}^{\text{bare}} \Delta n_{\text{ion}} \quad (43)$$

and

$$V_{\text{ion}} = -V_{ei}^{\text{bare}}(\rho_{\text{ext}} + \Delta n) + V_{ii}^{\text{bare}} \Delta n_{\text{ion}} \quad (44)$$

As usual,  $\Delta n = -\Pi^0 V_{ei}$ . The relation between  $\Delta n_{\text{ion}}$  and  $V_{\text{ion}}$  is obtained by considering the equation of motion for the ion displacement,  $\mu(r, t) \propto e^{i(\mathbf{q} \cdot \mathbf{r} - \omega t)}$ ,

$$M \ddot{\mu} = -\nabla V_{\text{ion}} \quad (45)$$

or

$$-M \omega^2 \mu = -iq V_{\text{ion}} \quad (46)$$

where  $\omega$  is the frequency of the perturbing charge density  $\rho_{\text{ext}}$ . The ionic density response is given by the divergence of the displacement.

$$\Delta n_{\text{ion}} = -N \text{div} \mu = -iq N \mu,$$

where  $N$  is the average-ion density. This yields the required relation

$$\Delta n_{\text{ion}} = \frac{N}{M} \left( \frac{q}{\omega} \right)^2 V_{\text{ion}} \quad (47)$$

With this result, Eqs. (43) and (44) are completely specified.

The usual phonon frequencies are obtained by setting  $\rho_{\text{ext}}$  equal to zero. A finite response is allowed even in the absence of an external perturbation if the frequency and wave vector obey

$$\begin{aligned} \omega_q^2 &= \frac{Nq^2}{M} \left[ V_{ii}^{\text{bare}} - \frac{(V_{ei}^{\text{bare}})^2}{v} + \frac{(V_{ei}^{\text{bare}})^2}{v\epsilon} \right] \\ &\equiv \omega_0^2 + \frac{Nq^2 (V_{ei}^{\text{bare}})^2}{M v \epsilon} \end{aligned} \quad (48)$$

This is the same result obtained in Eqs. (5)–(30) of Ref. 10. The first term  $\omega_0^2 \equiv (s_0 q)^2$ , represents the deviations from pure Coulomb interactions.  $s_0$  is the sound velocity of the ion background in the absence of Coulomb forces. The linear dependence of  $\omega_0$  on  $q$  (at small  $q$ ) arises because the divergences in  $V_{ii}^{\text{bare}}$  and  $V_{ei}^{\text{bare}}$  ( $\propto q^{-2}$ ) just cancel. For pure Coulomb interactions  $\omega_0 = 0$ . The second term simply represents the ionic plasma screened by the electron-gas dielectric function. It is the extension of the Bohm-Staver result to include exchange and correlation. The potential felt by an electron is

$$V_{ei} = \frac{v\rho_{\text{ext}}}{(1 - G_+ Q)\epsilon} \left( \frac{\omega^2 - \omega_0^2}{\omega^2 - \omega_q^2} \right) \quad (49)$$

and the potential felt by an ion is

$$V_{\text{ion}} = -\frac{V_{ei}^{\text{bare}} \rho_{\text{ext}}}{\epsilon} \left( \frac{\omega^2}{\omega^2 - \omega_q^2} \right) \quad (50)$$

The potential felt by an ion is the sum of an electrostatic potential and an additional potential due to the non-Coulombic ion-ion interactions. Another test charge would only feel the electrostatic potential. The ion potential is zero at  $\omega = 0$ , because the ions have no kinetic energy and move to minimize the potential.

If one assumes pure Coulomb interactions ( $\omega_0 = 0$ ) and neglects exchange and correlation ( $G_+ = 0$ ),  $V_{ei}$  and  $V_{\text{ion}}$  become identical and also equal to the electron-electron interaction. This limit reproduces the well-known Fröhlich interaction.<sup>2,11</sup>

### A. Electron-electron interaction with lattice screening

We now treat the electron-electron interaction explicitly including exchange and correlation. We consider the system to be perturbed by an electron with spin up. The coupled equations that determine the response of the electrons ( $\Delta n_{\uparrow}$  and  $\Delta n_{\downarrow}$ ) and the ions ( $\Delta n_{\text{ion}}$ ) are

$$\tilde{V}_{\uparrow\uparrow} = v[(1-2G_X)\rho_{\uparrow} + (1-2G_X)\Delta n_{\uparrow} + (1-2G_C)\Delta n_{\downarrow}] - V_{ei}^{\text{bare}}\Delta n_{\text{ion}}, \quad (51)$$

$$\tilde{V}_{\downarrow\downarrow} = v[(1-2G_C)\rho_{\downarrow} + (1-2G_C)\Delta n_{\downarrow} + (1-2G_X)\Delta n_{\uparrow}] - V_{ei}^{\text{bare}}\Delta n_{\text{ion}}, \quad (52)$$

$$V_{\text{ion}} = -V_{ei}^{\text{bare}}(\rho_{\uparrow} + \Delta n_{\uparrow} + \Delta n_{\downarrow}) + V_{ii}^{\text{bare}}\Delta n_{\text{ion}}. \quad (53)$$

These equations are most simply solved by forming the sum and difference of  $\tilde{V}_{\uparrow\uparrow}$  and  $\tilde{V}_{\downarrow\downarrow}$ . This yields

$$\frac{\tilde{V}_{\uparrow\uparrow} + \tilde{V}_{\downarrow\downarrow}}{2} = \frac{v\rho_{\uparrow}}{(1-G_+Q)^2\epsilon} \left( \frac{\omega^2 - \omega_0^2}{\omega^2 - \omega_q^2} \right) - \frac{v\rho_{\uparrow}G_+}{1-G_+Q}, \quad (54)$$

with the help of Eqs. (15) and (47).  $\omega$  is the

$$V_{e\bar{\sigma}_1, e\bar{\sigma}_2} = \left( \frac{(\omega^2 - \omega_0^2)/(\omega^2 - \omega_q^2)}{(1-G_+Q)[1+(1-G_+)Q]} - \frac{G_+^2Q}{1-G_+Q} - \frac{G_-^2Q}{1-G_-Q} \bar{\sigma}_1 \cdot \bar{\sigma}_2 \right) \frac{4\pi e^2}{q^2}. \quad (57)$$

Recall that both  $\omega_q$  and  $\omega_0$  are linear in  $q$  and  $\omega_0 < \omega_q$ . The first term represents the charge disturbance which is also screened by the lattice. The second term derives from the exchange interaction with the total induced electron density ( $\Delta n_{\uparrow} + \Delta n_{\downarrow}$ ). The lattice does not have this exchange interaction. The third term is due to the interaction with the magnetization or spin polarization [ $\propto(\Delta n_{\uparrow} - \Delta n_{\downarrow})$ ] induced by the perturbing electron. The magnetic interaction is not screened by the lattice. Equation (57) is the final result of this paper. The numerator of the first term goes to 1 in the absence of ion screening.

## VI. SUMMARY

We have derived the electric- and spin-response functions of the coupled electron-lattice system using a simple model for the lattice and treating exchange and correlation in a local approximation. We have done this using a straightforward and physically intuitive extension of Hartree-Fock theory. Although this theory is based on a simple model of a metal, it is appealing because it yields explicit results and one can see how exchange, correlation and the properties of the lattice each affect the response functions. In par-

frequency of  $\rho_{\uparrow}$ ; in a scattering event  $\hbar\omega = |E(\vec{k}) - E(\vec{k} + \vec{q})|$ . We also find,

$$\frac{\tilde{V}_{\uparrow\uparrow} - \tilde{V}_{\downarrow\downarrow}}{2} = \frac{-v\rho_{\uparrow}G_-}{1-G_-Q}, \quad (55)$$

$$V_{\text{ion}} = \frac{-V_{ei}^{\text{bare}}\rho_{\uparrow}}{(1-G_+Q)\epsilon} \left( \frac{\omega^2}{\omega^2 - \omega_q^2} \right). \quad (56)$$

We note that  $\frac{1}{2}(\tilde{V}_{\uparrow\uparrow} + \tilde{V}_{\downarrow\downarrow})$  depends on the response of the ions, while  $\frac{1}{2}(\tilde{V}_{\uparrow\uparrow} - \tilde{V}_{\downarrow\downarrow})$  does not. This is because the ions respond only to electrostatic potentials and not to the induced magnetization which is proportional to  $\Delta n_{\uparrow} - \Delta n_{\downarrow}$ . Again we check the consistency of our results by using  $\Delta n_{\uparrow}$  and  $\Delta n_{\downarrow}$  to calculate  $V_{ie}$ , the electrostatic potential a test charge feels due to a perturbing electron, and this again yields  $V_{ie} = V_{ei}$ .

In order to form the scattering amplitudes, we need potentials that do not include a local approximation to the direct exchange (and correlation) of the two electrons under consideration. These local approximations are removed from Eqs. (54) and (55) by adding  $2vG_X\rho_{\uparrow}$  to  $\tilde{V}_{\uparrow\uparrow}$  and  $2vG_C\rho_{\downarrow}$  to  $\tilde{V}_{\downarrow\downarrow}$ . When this is done and reexpressed in invariant notation, the electron-electron interaction is,

ticular, it becomes obvious that correlation enhances the electric response, but reduces the spin response. The electron-electron interaction, depends on both the electric and spin responses and is spin dependent. The spin-dependent term in  $V_{e\bar{\sigma}_1, e\bar{\sigma}_2}$  arises naturally and has been previously discussed as arising from spin fluctuations or paramagnons. Its effect on superconductivity is apparent because this term is repulsive for a singlet state and attractive for a triplet. The frequency dependence of  $V_{e\bar{\sigma}_1, e\bar{\sigma}_2}$  that leads to superconductivity also affects electron-electron scattering in the normal state. Because of the Pauli principle, the only electrons that can participate in scattering must lie within  $k_B T$  of the Fermi energy and the energy transfer between them is also of the order of  $k_B T$ . At low temperatures, the energy transfer will be small compared to phonon frequencies and the lattice will be able to participate in screening. However at high temperatures, the lattice will not be able to follow the perturbation and lattice screening will no longer be effective in reducing the Coulomb repulsion. This leads to an additional temperature dependence for electron-electron scattering.

In addition to these features, one can also use our results to calculate the induced electronic charge density due to an external potential and the induced

magnetization due to an external field. Divergences in these responses signal charge and spin-density waves and ferromagnetism.

In order to use the theory in an explicit calculation, one needs to know the exchange and correlation functions  $G_X$  and  $G_C$ . We emphasize that these are the same functions needed to calculate the dielectric function and the spin susceptibility.<sup>12</sup> These functions are central to electron-gas theory and approximate calculations of them exist. We also note that this theory can be directly extended to multicarrier and spin-polarized systems.

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#### APPENDIX: SELF-CONSISTENT PERTURBATION THEORY

Our approach follows Ref. 3 where Hartree-Fock self-consistent perturbation theory was used to calculate the spin susceptibility. The first problem in calculating the electron-electron interaction is to determine what the perturbation is. The perturbation that yields the results in Sec. II is obtained by replacing one single-particle wave function,  $\varphi_{k_1} = e^{i\vec{k}_1 \cdot \vec{r}}$ , in the Slater determinant by  $\psi_{k_1}$ , an admixture of  $\varphi_{k_1}$  and  $\varphi_{k_1+q}$ ,

$$\psi_{k_1} = e^{i\vec{k}_1 \cdot \vec{r}} + \frac{1}{2}\rho e^{i(\vec{k}_1+q) \cdot \vec{r}}, \quad (58)$$

where  $\varphi_{k_1+q}$  is a previously unoccupied state. We assume that both states lie essentially on the Fermi surface  $\epsilon(k_1) \approx \epsilon(k_1+q)$ . Such an admixture arises

from the scattering event  $(k_1, k_2) \rightarrow (k_1+q, k_2-q)$ . This new wave function has a periodically modulated charge density,

$$|\psi_k|^2 = 1 + \rho \cos \vec{q} \cdot \vec{r}, \quad (59)$$

which introduces a perturbation into the theory from the Hartree term. Electrons with parallel spins will feel an additional perturbation arising from the exchange (Fock) term. If we take the perturbing charge density to have spin up ( $\rho_1$ ), the bare interaction felt by another electron  $k_2$  with spin down is

$$V_{k_2, k_1} = \frac{4\pi e^2}{q^2} \rho_1. \quad (60)$$

If the second electron has spin up, it will also feel an exchange interaction,

$$V_{k_2, k_1} = \left[ \frac{4\pi e^2}{q^2} - \frac{4\pi e^2}{|k_2 - k_1 - q|^2} \right] \rho_1. \quad (61)$$

The problem then is to calculate the response of the electrons in the Fermi sea to this perturbation.

Proceeding in Hartree-Fock theory, one obtains an integral equation for the effective potential that determines the density response. This integral equation is nontrivial because it includes the full nonlocality of the exchange operator. An analogous nonlocal equation for  $\chi(q)$  was solved numerically in Ref. 3. We do not present or attempt to solve the nonlocal problem, rather we choose to treat exchange in a local approximation. This is done by using the Dirac-Slater  $n^{1/3}$  approximation for the exchange potential in the Hartree-Fock equations. In the local approximation the exchange contribution to the perturbation is given in Eq. (11). This approximation simplifies the theory which straightforwardly leads to the coupled algebraic equations that determine the density response, Eqs. (12) and (13).

<sup>1</sup>C. A. Kukkonen and J. W. Wilkins (unpublished); and C. A. Kukkonen, Ph.D. thesis (Cornell University, 1975) (unpublished).

<sup>2</sup>H. Fröhlich, Phys. Rev. **79**, 845 (1950).

<sup>3</sup>For a similar application see D. R. Hamann and A. W. Overhauser, Phys. Rev. **143**, 183 (1966).

<sup>4</sup>L. Hedin and B. I. Lundqvist, J. Phys. C **4**, 2064 (1971).

<sup>5</sup>See, for example, Ref. 4, and other work cited there.

<sup>6</sup>Hartree-Fock theory is obtained diagrammatically by using the bare Coulomb interaction (direct and exchange terms) as the irreducible interaction and iterating the Bethe-Salpeter equation in one particle-hole channel. This procedure dresses (screens) the direct Coulomb interaction but the exchange term is left bare. The result in the other particle-hole channel, bare direct and dressed exchange, is obtained by interchanging the two electrons. The total irreducible scattering amplitude for parallel spins in the

particle-particle channel is obtained from the sum of the results in the two particle-hole channels corrected for double counting. The double counting occurs if one includes the sum of both bare exchange and screened exchange because bare interaction is the leading term in screened interaction. See the analysis in Ref. 1.

<sup>7</sup>U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).

<sup>8</sup>J. C. Stoddart, J. Phys. C **8**, 3391 (1975).

<sup>9</sup>O. Gunnarson and B. I. Lundqvist, Phys. Rev. B **13**, 4274 (1976).

<sup>10</sup>See, for example, D. Pines, *Elementary Excitations in Solids* (Benjamin, New York, 1963), p. 231, and references cited therein.

<sup>11</sup>J. Bardeen, Rev. Mod. Phys. **23**, 261 (1951).

<sup>12</sup>The values of  $G_X$  and  $G_C$  at  $q=0$  are set by sum rules. Their  $q$  dependence varies from one calculation to another. See Refs. 1 and 4 for a discussion.