# Theory of electron liquids. I. Electron-hole pseudopotentials

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The polarization-potential theory developed by Aldrich and Pines for helium liquids is extended to electron liquids. Configuration-space pseudopotentials are introduced to describe the modifications in electron interaction at short distances brought about by charge- and spin-induced correlations. The results obtained for the compressibility and spin susceptibility by Vosko, Wilk, and Nusair from Monte Carlo calculations are combined with simple physical arguments to obtain new expressions for the wave-vector-dependent dielectric function and spin susceptibility, which reduce in the long-wavelength limit to the Monte Carlo results. The relative effectiveness of charge- and spin-induced correlations is calculated as a function of electron density, and results are compared with previous calculations for electron liquids and with the corresponding results for the helium liquids.

## I. INTRODUCTION

After almost 50 years of microscopic calculations, electron liquids continue to be a fruitful field of investigation.<sup>1</sup> While there now exist a number of satisfactory calculations of the ground-state energy, spin susceptibility, and of the static pair correlation function, many of them carried out during the past decade, there is at present no satisfactory understanding of the elementary excitation spectrum or static dielectric function in the region of metallic densities where the dimensionless coupling constant  $r_s$  lies in the strong-coupling range,  $2 \leq r_s \leq 5.5$ .

It is perhaps not surprising that this is the case. First, the influence of band structure poses problems for the interpretation of electron-energy loss and x-ray scattering experiments, while it is difficult to design an experiment which measures accurately the wave-vector dependence of the static dielectric function in metals. Second, for wave numbers comparable to or larger than  $q_F$ , the Fermi wave number, multipair excitations (which correspond to exciting at least two quasiparticles and quasiholes from the Fermi sphere) begin to play an important role for both the dynamic and static dielectric functions. It is, however, difficult to calculate with confidence the strength and characteristic energies of this part of the spectrum. Third, it is likely that as the coupling constant increases so does the effective mass of the electrons, yet to date no satisfactory calculations which take this into account for either the static or dynamic dielectric function have been carried out. Moreover, while there exist a variety of calculations of the local-field correction to the dielectric function, this quantity is not directly measurable, and no simple criterion exists which permits one to disentangle local-field corrections from, for example, multipair contributions to the static or dynamic polarizability.

In the present series of papers we seek to address the above theoretical problems in a number of ways. Our basic approach, which is closely related to the polarization-potential theory of Aldrich and Pines,<sup>2,3</sup> is to

combine the results of recent accurate Green's-function Monte Carlo calculations of the ground-state energy, and pair correlation functions<sup>4</sup> with exact sum rules and physical arguments to obtain the self-consistent fields, which determine the local-field corrections and the backflow responsible for the wave-vector-dependent particle-hole effective mass. We introduce a phenomenological spectral density for the multipair excitations and show how modemode coupling between the single-pair—plasmon branch of the spectrum and the multipair branch influences the plasmon dispersion. Because the approach we use is essentially identical to that employed by Aldrich and Pines in their treatment of elementary excitations in <sup>3</sup>He and <sup>4</sup>He, it is straightforward to compare and contrast the results obtained for the electron and helium liquids.

In this first paper we introduce electron-hole configuration-space and momentum-space pseudopotentials to describe the way in which short-range charge- and spin-induced correlations between electrons act to modify, at short distances, the influence of the Coulomb potential between electrons of parallel and antiparallel spin. Where the electron effective mass  $m^* \cong m$  (i.e., no backflow), we show that the spatial integral of these pseudopotentials is determined by the compressibility and spin susceptibility which are in turn known from the Monte Carlo calculations. Hence for a given choice of the shape (in either configuration space or momentum space), the pseudopotential is determined uniquely. In this way we arrive at a simple physical picture for the static local-field correction to the dielectric function, one which facilitates comparison of the present and previous calculations.

In the second paper<sup>5</sup> in this series we use the mean spherical (or hydrodynamic) approximation to calculate the local-field correction from the variational calculations of the static form factor S(q) and the correlation energy. We develop an interpolation procedure which enables us to pass smoothly from the low momentum transfer region, where, for example, the pseudopotentials developed in the

present paper provide a more accurate account of S(q) than do the Monte Carlo calculations, to the region of wave vectors  $(\geq q_F)$  where the latter calculations are reliable; we use this procedure to calculate the ground-state energy as well, and we compare our results with those of a calculation using our polarization potentials.

In a planned third paper<sup>6</sup> of the present series we consider the role played by multipair excitations and backflow. We use the  $\omega^3$ -sum rule to examine constraints on their spectral density and discuss the wave-vector dependence of the interplay between multipair excitations and the single-pair—plasmon branch in determining both S(q)and the static dielectric function. We introduce a simple model for multipair excitations and use this to calculate the plasmon dispersion. In the fourth paper, we use sumrule arguments to place limits on the importance of effective-mass corrections arising from backflow, and present as well a microscopic calculation of the electron self-energy.

The outline of the present paper is as follows. In Sec. II we define the polarization potentials and pseudopotentials and relate these to the response function for the electron liquid. We give in Sec. III the input parameters from Monte Carlo calculations required to determine the electron-hole pseudopotentials. In Sec. IV we give the resulting effective potentials for two choices of shape of the short-range electron-hole pseudopotential: a Yukawa form and a dielectric form. In Sec. V we compare our results with previous calculations of local-field corrections. In Sec. VI we present the nonlocal spin susceptibility. In Sec. VII we give a brief summary of principal results and conclusions. We give in the Appendixes expressions for the polarization potentials in the high-density limit and for a neutral hard-sphere Fermi gas, and present as well a discussion of local-field corrections.

## II. POLARIZATION POTENTIALS AND PSEUDOPOTENTIALS

The dielectric function of an electron liquid may be written in the form (sc denotes screened)

$$\epsilon(q,\omega) = 1 - \frac{4\pi e^2}{q^2} \chi_{\rm sc}(q,\omega) , \qquad (2.1)$$

where  $\chi_{sc}(q,\omega)$  describes the response of the electrons to the sum of an external longitudinal field,  $\phi_{ext}(q,\omega)$  [which couples to the density fluctuation  $\rho(q,\omega)$ ], and the induced polarization field,

$$\phi_{\rm pol}^0(q,\omega) = \frac{4\pi e^2}{q^2} \langle \rho(q,\omega) \rangle . \qquad (2.2)$$

If one takes for  $\chi_{sc}(q,\omega)$  the free-electron (Lindhard) response function,  $\chi^{0}(q,\omega)$ , one obtains the usual randomphase approximation (RPA) expression for  $\epsilon(q,\omega)$ , in which all effects of the Coulomb interaction are described by the polarization field, Eq. (2.2).<sup>7</sup> As is well known, the RPA is valid in the very-high-density limit,  $r_s \ll 1$ , where  $r_s$  is the interelectron spacing measured in units of the Bohr radius. As one goes to metallic ( $2 \le r_s \le 5.5$ ) and lower densities, an expression of the form (2.2) no longer provides an accurate description of the consequences of electron interaction, primarily because it fails to take into account the short-range (in space) correlations which act to keep electrons from feeling the full consequences of the field, (2.2). An approximate way to take these latter correlations into account is to modify the expression (2.2) to read

$$\phi_{\text{pol}}^{C}(q,\omega) = \left(\frac{4\pi e^2}{q^2} + f_q^s\right) \langle \rho(q,\omega) \rangle , \qquad (2.3)$$

where  $f_q^3 \langle \rho(q,\omega) \rangle$  is a frequency-independent phenomenological pseudopotential. To the extent that the characteristic frequencies associated with the short-range correlations are large compared to the frequencies for which (2.3) is applied, modeling their influence by a static field should provide a reasonable approximation. If one further assumes that the response of the electrons to the sum of the external field and the *modified* polarization field, Eq. (2.3), is given by the Lindhard function, one finds

$$\chi_{\rm sc}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - f_q^s \chi^0(q,\omega)} .$$
 (2.4)

The dielectric response of the electron liquid is a spinsymmetric response to an external field that couples to the density fluctuations. The system response to an external field that couples to spin-density fluctuations is given by the wave-number- and frequency-dependent paramagnetic (spin-antisymmetric) response function  $\chi_P(q,\omega)$ . By analogy with (2.3), we take electron interaction into account by calculating the system response to the external field plus a spin polarization field,

$$\phi_{\text{pol}}^{I}(q,\omega) = f_{q}^{a} \langle \sigma(q,\omega) \rangle , \qquad (2.5)$$

where  $\langle \sigma(q,\omega) \rangle$  is the induced spin-density fluctuation. On making the further approximation that the system responds as a gas of free electrons to the sum of the external field and the local field, (2.5), we obtain

$$\chi_P(q,\omega) = -\mu_B^2 \frac{\chi^{0}(q,\omega)}{1 - f_a^a \chi^{0}(q,\omega)} . \qquad (2.6)$$

The expressions (2.3)—(2.6) are the analog, for chargedparticle systems, of the scalar-polarization potentials introduced by Pines and Aldrich<sup>2,3</sup> to treat the consequences of short-range correlations in neutral quantum liquids. As is the case with the neutral fermion systems, the polarization potentials, (2.3) and (2.5), may be given a simple physical interpretation as spin-symmetric (and -antisymmetric) combinations of effective interactions between electrons of parallel and antiparallel spin,

$$V_q^{\dagger\dagger} = \frac{4\pi e^2}{q^2} + f_q^{\dagger\dagger} , \qquad (2.7)$$

$$V_q^{\uparrow\downarrow} = \frac{4\pi e^2}{q^2} + f_q^{\uparrow\downarrow} . \tag{2.8}$$

Thus one has

$$V_{q}^{s} = \frac{1}{2} (V_{q}^{\uparrow\uparrow} + V_{q}^{\uparrow\downarrow}) = \frac{4\pi e^{2}}{q^{2}} + f_{q}^{s} , \qquad (2.9)$$

$$V_q^a = \frac{1}{2} (V_q^{\dagger \dagger} - V_q^{\dagger \downarrow}) = f_q^a , \qquad (2.10)$$

where

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$$f_q^s = \frac{1}{2} (f_q^{\uparrow\uparrow} + f_q^{\uparrow\downarrow}) , \qquad (2.11)$$

$$f_q^a = \frac{1}{2} (f_q^{\dagger\dagger} - f_q^{\dagger\downarrow}) . \qquad (2.12)$$

To make explicit the link to the polarization potential approach to neutral Fermi liquids, we note that the spincoherent and incoherent response functions of the electron liquid take the form

$$\chi^{C,I}(q,\omega) = \frac{\chi^0(q,\omega)}{1 - V_a^{s,a} \chi^0(q,\omega)} , \qquad (2.13)$$

where the potentials  $V_q^{s,a}$  are given by Eqs. (2.9) and (2.10). Expressions of the form (2.4) and (2.6) are found in many approximate microscopic theories; the potentials  $f_a^s$ and  $f_q^{a}$  are interpreted as local-field corrections to the RPA.<sup>8-17</sup> The requirement that the response of the system to a static long-wavelength perturbation (a uniform compression) must give the correct compressibility provides a limit on the long-wavelength behavior of  $\epsilon(q,0)$ (Ref. 7) and hence  $f_q^s$ . The static long-wavelength limit of the dielectric function is given by

$$\lim_{q \to 0} \epsilon(q,0) = 1 + \frac{\omega_p^2}{s^2 q^2} , \qquad (2.14)$$

where  $\omega_p = (4\pi n e^2/m)^{1/2}$  is the plasma frequency and s, the isothermal sound velocity, is related to the compressibility by

$$\kappa = 1/mns^2 \,. \tag{2.15}$$

From Eqs. (2.1), (2.4), and (2.14) one obtains the condition

$$\lim_{q \to 0} f_q^s \equiv f_0^s = [V/N^0(0)](\kappa_0/\kappa - 1)$$
(2.16)

on making use of the result

$$\lim_{q \to 0} \chi_{\rm sc}(q,0) = -\frac{n}{ms^2} \,. \tag{2.17}$$

Here

$$N^{0}(0) = \frac{3}{2} \frac{N}{E_{F}^{0}}$$
(2.18)

is the free-particle density of states, V is the volume,  $E_F^0 = \hbar^2 q_F^2 / 2m$ , and  $\kappa_0 \equiv 1 / mns_0^2$  is the free-particle compressibility, with  $s_0 = \hbar q_F / \sqrt{3}m$ . It is convenient to introduce the dimensionless quantity

$$F^{s} = f_{0}^{s} N^{0}(0) / V . (2.19)$$

Then, Eq. (2.16) becomes

$$F^s = \kappa_0 / \kappa - 1 . \tag{2.20}$$

From Eq. (2.6) one obtains a similar constraint on  $f_q^a$ ,

$$\lim_{q \to 0} f_q^a \equiv f_0^a = [V/N^0(0)](\chi_P^0/\chi_P - 1) , \qquad (2.21)$$

where

and

$$\chi_P = \lim_{q \to 0} \chi_P(q, 0) \tag{2.22}$$

$$\chi_P^0 = -\lim_{q \to 0} \mu_B^2 \chi^0(q, 0)$$
 (2.23)

is the free-electron spin susceptibility. It is also convenient to define

$$F^{a} = f_{0}^{a} N^{0}(0) / V . \qquad (2.24)$$

Then Eq. (2.21) becomes

$$F^a = \chi_P^0 / \chi_P - 1$$
 (2.25)

Equations (2.20) and (2.25) serve as boundary conditions on the pseudopotentials  $f_q^{\uparrow\uparrow}$  and  $f_q^{\uparrow\downarrow}$ , which determine the effective interactions between electrons of parallel and antiparallel spin. The parameters  $F^s$  and  $F^a$  resemble, but are not identical to, the parameters  $F_0^s$  and  $F_0^a$  which, together with the effective-mass parameter  $F_1^s$ , describe the influence of electron interaction on  $\kappa$  and  $\chi_P$  in Landau Fermi-liquid theory.<sup>18</sup> In the present calculation the interacting electron density of states N(0), and hence  $F_1^s$ , appear nowhere because in (2.4) and (2.6) the free-electron response function enters. In Landau theory expressions of the form (2.4) and (2.6) are found; however,  $\chi^{\bar{0}}(q,\omega)$  is replaced by a long-wavelength Lindhard response function for particles and holes of effective mass  $m^*$ . The relationship between our parameters and the corresponding Landau parameters is thus  $F^{s,a} = F_0^{s,a} / (1 + F_1^s / 3)$ .

Finally we note that the dielectric function (2.1) with the screened response function of the form (2.4) satisfies the f-sum rule<sup>7</sup>

$$\lim_{p \to \infty} \epsilon(q, \omega) = 1 - \frac{\omega_p^2}{\omega^2} . \qquad (2.26)$$

An analysis of the  $\omega^3$  sum rule is given in the second paper.

#### **III. INPUT PARAMETERS**

Before constructing the polarization potentials we discuss the input parameters which determine their longwavelength limit. We determine the compressibility, and hence  $F^s$ , with the aid of an interpolation formula for the correlation energy derived by Vosko, Wilk, and Nusair (VWN).<sup>19</sup> Their formula is based on the results of recent Monte Carlo calculations by Ceperley and Alder.<sup>4</sup> The compressibility may be calculated from the correlation energy by the thermodynamic relation

$$\frac{\kappa_0}{\kappa} = 1 - \frac{\alpha}{\pi} r_s + \frac{\alpha^2}{6} r_s^4 \left[ \frac{d^2}{dr_s^2} - \frac{2}{r_s} \frac{d}{dr_s} \right] \frac{E_{\text{corr}}(r_s)}{N} , \quad (3.1)$$

where  $\alpha = (4/9\pi)^{1/3}$ , N is the total number of electrons, and  $r_s = 1/\alpha q_F a_B$ , with  $a_B$  the Bohr radius. In Table I we list the VWN compressibility for different values of  $r_s$  and compare it with the results of various microscopic theories. We see that the latter are in quite good agreement with the Monte Carlo results. Put another way, the calculated values of the compressibility are not sensitive to the particular methods of approximation used to calculate the correlation energy.

The VWN results, as well as those of other theories, lead to a compressibility which increases with  $r_s$  and becomes infinite in the vicinity of  $r_s = 5.2$ , after which it be-

rs	VWN <sup>a</sup>	$\mathbf{HF}^{b}$	RPA <sup>c</sup>	$\mathbf{H}^{d}$	NP <sup>e</sup>	STLSf	VS <sup>g</sup>	LB <sup>h</sup>	UI <sup>i</sup>
1	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83	0.83
2	0.64	0.67	0.64	0.65	0.65	0.64	0.64	0.64	0.64
3	0.45	0.50	0.45	0.46	0.46	0.45	0.43	0.45	0.46
4	0.26	0.34	0.24	0.26	0.27	0.25	0.21	0.25	0.26
5	0.05	0.17	0.03	0.06	0.07	0.05	-0.03	0.05	0.05
6	-0.16	0.005	-0.19	-0.15	-0.15		-0.29		-0.15

TABLE I. Compressibility ratio  $(\kappa_0/\kappa)$  for several values of  $r_s$  calculated from correlation energy in various theories.

<sup>a</sup>Present calculation based on the interpolation formula for correlation energy by Vosko *et al.* (Ref. 19). <sup>b</sup>Hartree-Fock approximation.

<sup>c</sup>Random-phase approximation.

<sup>d</sup>Hubbard (Ref. 8).

eNozières and Pines (Ref. 20).

<sup>f</sup>Singwi et al. (Ref. 9).

<sup>g</sup>Vashishta and Singwi (Ref. 15).

<sup>h</sup>Lowy and Brown (Ref. 16).

<sup>i</sup>Utsumi and Ichimaru (Ref. 14).

comes negative. In the actual Monte Carlo calculations, however, one assumes that the background of positive ions (in which the electrons are impressed) is infinitely rigid; hence no charge inhomogeneity will develop, and the system will remain stable. Of course, for an actual metal, at these densities [e.g., Cs ( $r_s = 5.56$ )], the positive ions are not rigid, and charge-density waves could in principle develop to stabilize the system.

VWN have used the Monte Carlo calculations of Ceperley and Alder for the correlation energy of a ferromagnetic electron liquid<sup>4</sup> to obtain an interpolation formula for the spin-dependent correlation energy. We use their "fit" (in Table 6 of Ref. 19) to the spin stiffness in order to calculate the paramagnetic spin susceptibility. The VWN results for the paramagnetic spin susceptibility are given for different values of  $r_s$  in Table II, while these are compared with other theories<sup>11,21-23</sup> and experiment<sup>24</sup> for  $r_s = 3.22$ (Li) and  $r_s = 3.96$  (Na) in Table III. From Table III one sees that the VWN values for the susceptibility are consistent with experiment. We use these values of the paramagnetic spin susceptibility to determine the static long-wavelength limit of the spin-antisymmetric polarization potential. The values of  $F^s$  and  $F^a$ , together with

$$F^{\uparrow\uparrow} \equiv F^s + F^a \tag{3.2}$$

and

$$F^{\uparrow\downarrow} \equiv F^s - F^a , \qquad (3.3)$$

calculated from Eqs. (2.20) and (2.25), are listed in Table IV and plotted in Fig. 1 for  $0 \le r_s \le 20$ .

## **IV. POLARIZATION-POTENTIAL PARAMETERS**

The general form of the pseudopotentials, (2.7) and (2.8), which describe the effective interaction between electrons of parallel and antiparallel spin, may be obtained by simple physical arguments. As we have noted earlier, the major physical effects that  $f_q^{\dagger\dagger}$  and  $f_q^{\dagger\downarrow}$  are designed to take into account are the short-range correlations that prevent electrons of parallel (antiparallel) spin from sam-

pling the full consequences of the Coulomb restoring force at short distances. These pseudopotentials must therefore be attractive (microscopically they describe particle-hole interactions) and, apart from the possible consequences of dielectric screening (see below), may be expected to have a range which is comparable to the interparticle spacing. Since short-range correlations of necessity involve comparatively high frequencies, a description of their consequences by a static field may be expected to be valid for frequencies, for example,  $\omega \leq E_F/\hbar$ .

Consider, for example, the Fourier transform of  $V_q^{\dagger \dagger}$ , (2.8);

$$V^{\dagger\dagger}(r) = \frac{1}{V} \sum_{\vec{q}} \left[ \frac{4\pi e^2}{q^2} + f_q^{\dagger\dagger} \right] e^{i \vec{q} \cdot \vec{r}}$$
$$= \frac{e^2}{r} + f^{\dagger\dagger}(r) . \qquad (4.1)$$

For small r, as a result of the Pauli principle, we might expect that  $f^{\uparrow\uparrow}(r)$  will cancel the  $r^{-1}$  singularity in  $V^{\uparrow\uparrow}(r)$ ; for large r, its effects are likely small. A simple form for  $f^{\uparrow\uparrow}(r)$  which meets these criteria is

$$f^{\dagger\dagger}(r) = -(e^2/r)\exp(-q_{\dagger\dagger}r), \qquad (4.2a)$$

TABLE II. Paramagnetic spin susceptibility for several values of  $r_s$  calculated from spin-dependent correlation energy.

r <sub>s</sub>	$\chi_P/\chi_P^{0a}$	$\chi_P \ (10^{-6})^{b}$	
1	1.15	2.99	
2	1.31	1.69	
3	1.46	1.26	
4	1.62	1.05	
5	1.79	0.93	
6	1.98	0.85	

 ${}^{a}\chi_{P}^{0}=2.59\times10^{-6}r_{s}^{-1}$  in cgs units is the noninteracting value. <sup>b</sup>In cgs units.

TABLE III. Comparison of the paramagnetic spin susceptibility ( $\times 10^6$  in cgs units) in different theories with experiment for  $r_s = 3.22$  (Li) and  $r_s = 3.96$  (Na).

	rs	$m_c/m^a$	Hp	NP <sup>c</sup>	SSTL <sup>d</sup>	VWN <sup>e</sup>	Expt. <sup>f</sup>
Li	3.22	1.66	2.62	2.09	1.76	1.99	1.98±0.04
Na	3.96	1.00	0.97	0.84	0.86	1.06	$1.07 {\pm} 0.03$

<sup>a</sup>The cyclotron mass ratio due to Ham (Ref. 21).

<sup>b</sup>Rice (Ref. 23).

<sup>c</sup>Silverstein (Ref. 22) as corrected by Rice (Ref. 23).

<sup>d</sup>Singwi, Sjölander, Tosi, and Land (Ref. 11).

<sup>e</sup>Present calculation based on the interpolation formula for spin-dependent correlation energy by Vosko *et al.* (Ref. 19).

<sup>f</sup>Kushida, Murphy, and Hanabusa (Ref. 24).

where  $q_{\uparrow\uparrow}$ , the inverse correlation (screening) length for this "exchange" hole around a given electron may be expected to be  $\sim q_F \sim r_0^{-1}$ , where  $r_0$  is the interelectron spacing. The corresponding expression for  $f^{\uparrow\downarrow}(r)$  is

$$f^{\uparrow\downarrow}(r) = -(e^2/r)\exp(-q_{\uparrow\downarrow}r) . \qquad (4.2b)$$

With the form (4.2) we find

$$\lim_{r \to 0} V^{\dagger\dagger}(r) = e^2 q_{\dagger\dagger} , \qquad (4.3a)$$

$$\lim_{r \to 0} V^{\dagger \downarrow}(r) = e^2 q_{\dagger \downarrow} , \qquad (4.3b)$$

while for large r these effective potentials are essentially unchanged from their Coulomb values. On making use of Eqs. (4.2) we find

$$f_q^{\dagger\dagger} = -\frac{4\pi e^2}{q^2 + q_{\dagger\dagger}^2} , \qquad (4.4a)$$

$$f_{q}^{\dagger \downarrow} = -\frac{4\pi e^{2}}{q^{2} + q_{1\downarrow}^{2}} .$$
 (4.4b)

We further note that the spatial integrals of the pseudopotentials,  $f^{\dagger\dagger}(r)$  and  $f^{\dagger\downarrow}(r)$ , are determined by the compressibility and spin susceptibility. More specifically, one has

$$f_0^{\dagger\dagger} = \int d^3r f^{\dagger\dagger}(r) = F^{\dagger\dagger} V / N^0(0) , \qquad (4.5a)$$

$$f_0^{\dagger\downarrow} = \int d^3r f^{\dagger\downarrow}(r) = F^{\dagger\downarrow} V / N^0(0) . \qquad (4.5b)$$

Thus for pseudopotentials which may be characterized by a single parameter (e.g.,  $q_{\uparrow\uparrow}$  and  $q_{\uparrow\downarrow}$ ), once the form of the pseudopotential is chosen, its wave-number dependence is uniquely determined. With our Yukawa pseudopotentials, Eqs. (4.2), on making use of Eqs. (4.5) we find

$$q_{\rm tt}/q_{\rm FT} = (-1/F_{\rm tt})^{1/2}$$
, (4.6a)

$$q_{\uparrow\downarrow}/q_{\rm FT} = (-1/F_{\uparrow\downarrow})^{1/2}$$
, (4.6b)

where  $q_{\rm FT} = (6\pi ne^2/E_F^0)^{1/2}$  is the Fermi-Thomas wave number. We list the ratios  $q_{\uparrow\uparrow}/q_{\rm FT}$ ,  $q_{\uparrow\downarrow}/q_{\rm FT}$ ,  $q_{\uparrow\uparrow}/q_F$ , and  $q_{\uparrow\downarrow}/q_F$  in Table V, and show  $V^{\uparrow\uparrow}(r)$  and  $V^{\uparrow\downarrow}(r)$  in Fig. 2 for  $r_s = 1$ , 5, and 20. From Table V and Fig. 2 one sees the following.

(i) For a given  $r_s$ , the inequality,  $V^{\dagger\downarrow}(r=0) > V^{\dagger\dagger}(r=0)$  holds.

(ii) For a given  $r_s$ , as r increases  $V^{\uparrow\downarrow}(r)$  goes over more rapidly to Coulomb behavior than does  $V^{\uparrow\uparrow}(r)$ .

(iii)  $V^{\uparrow\uparrow}(r)$  is almost independent of  $r_s$ , while  $V^{\uparrow\downarrow}(r)$  for  $q_F r \leq 2$  decreases with increasing  $r_s$ . An equivalent statement is that  $q_{\uparrow\uparrow}/q_F$  is nearly independent of  $r_s$ , while  $q_{\uparrow\downarrow}/q_F$  decreases rapidly with increasing  $r_s$ .

These results possess a simple physical interpretation. The short-range correlations between antiparallel spin electrons, which determine  $q_{11}$ , provide a measure of what the "unaided," short-range part of the Coulomb interaction accomplishes in creating a "correlation hole" around a given electron; this hole reduces the effectiveness of the very short-range part of the interaction, and cancels the

TABLE IV. Polarization potentials in the long-wavelength limit calculated from the compressibility and the paramagnetic spin susceptibility.

r <sub>s</sub>	$F^{s}$	F <sup>a</sup>	$F^{\uparrow\uparrow}$	$F^{\dagger\downarrow}$
1	-0.17	-0.13	-0.31	-0.04
2	-0.36	-0.23	-0.59	-0.12
3	-0.55	-0.32	-0.86	-0.23
4	-0.74	-0.38	-1.13	-0.36
5	-0.95	-0.44	-1.39	-0.51
10	-2.03	-0.65 <sup>b</sup>	-2.68	-1.38
15	$-3.18^{a}$	-0.73 <sup>b</sup>	-3.91	-2.45
20	-4.40	$-0.77^{b}$	-5.17	-3.63

<sup>a</sup>Interpolated from the values of  $F^s$  at  $r_s = 5$ , 10, and 20. <sup>b</sup>Extrapolated from the values of  $F^a$  at  $r_s = 1, 2, ..., 5$ .



FIG. 1. Polarization potentials in the long-wavelength limit. The dashed straight line indicates the Hartree-Fock value,  $F^{s}(\text{HF}) = -(\alpha/\pi)r_{s}$ .

 $r^{-1}$  singularity near the origin. For parallel spin electrons, on the other hand, it is the combined effect of the Pauli principle and Coulomb correlations which keeps electrons apart. As a result, near the origin, the strength of the effective interaction between parallel spin electrons, while the range of the "exchange plus correlation hole," which modifies the interaction between electrons of parallel spin, is greater than that of the correlation hole, which modifies the interaction between antiparallel spin electrons.

 $V^{\dagger\dagger}(r)$  is almost independent of density because the Pauli principle is quite effective in keeping electrons apart; thus the influence of the short-range Coulomb correlations on  $V^{\dagger\dagger}(r)$  is small, and could, in fact, be neglected in first approximation. The weak density dependence of  $V^{\dagger\dagger}(r)$  reflects the fact that the higher the density, the more effective is the Pauli principle in keeping electrons of parallel spin apart. The opposite (and strong) density dependence of  $V^{\dagger\downarrow}(r)$  reflects the fact that the lower the density, the more effective are the shortrange Coulomb correlations in keeping electrons apart. As one might expect, since the coupling constant which characterizes the importance of Coulomb interactions is proportional to  $r_s$ , the relative importance of Coulomb correlations increases with  $r_s$  (i.e., with decreasing electron density). Thus at  $r_s = 5$  (or 20) the ratio of the correlation hole around an electron to the interparticle spacing,  $q_F/q_{\uparrow\downarrow}$ , is considerably larger than at  $r_s \simeq 1$ . Put another way, at these lower densities, Coulomb correlations are

TABLE V. Effective wave number of polarization potentials.

r <sub>s</sub>	$q_{\dagger\dagger}/q_{\rm FT}$	$q_{\uparrow\downarrow}/q_{\rm FT}$	$q_{\uparrow\uparrow}/q_F$	$q_{\uparrow\downarrow}/q_F$
1	1.81	5.06	1.47	4.12
2	1.30	2.87	1.50	3.30
3	1.08	2.08	1.52	2.93
4	0.94	1.66	1.53	2.71
5	0.85	1.41	1.54	2.56
10	0.61	0.85	1.57	2.19
15	0.51	0.64	1.60	2.02
20	0.44	0.53	1.60	1.91



FIG. 2. Effective interactions between electrons of parallel and antiparallel spin,  $V^{\dagger\dagger}(r)$  and  $V^{\dagger}(r)$ , in units of  $e^2q_F$  for  $r_s = 1, 5$ , and 20. The dashed curve shows the bare Coulomb potential  $r^{-1}$ .

considerably more effective in keeping electrons of antiparallel spin apart, thereby preventing them from sampling the consequences of the very-short-range part of the Coulomb interaction. In general, as  $r_s$  increases,  $V^{\uparrow\downarrow}(r)$ approaches more nearly to  $V^{\uparrow\uparrow}(r)$ ; in the very-low-density limit ( $r_s \gg 20$ ), Coulomb correlations may be expected to dominate exchange correlations, and  $V^{\uparrow\downarrow}(r) \cong V^{\uparrow\uparrow}(r)$ .

It is instructive to consider the high-density limit,  $r_s \ll 1$ . We show in Appendix A that in this limit one has

$$q_{\uparrow\uparrow} = \sqrt{2}q_F [1 + (\alpha r_s / 4\pi)(\ln r_s - 1.49) + \cdots]^{-1/2},$$
 (4.7a)

$$q_{\uparrow\downarrow} = 2\sqrt{2}q_F[(\alpha r_s/\pi)(2.716 - \ln r_s) + \cdots]^{-1/2}$$
. (4.7b)

Thus in the high-density limit the ratio of the exchange hole to the interparticle spacing goes to a constant, while the strength of the interaction between parallel spins takes on the value (given in Ry)

$$V^{\dagger\dagger}(r=0) = \sqrt{2}e^2 q_F = \frac{5.43}{r_s} . \qquad (4.8)$$

On the other hand, the radius of the correlation hole shrinks to 0; in this limit, then, the role of Coulombinduced correlations between electrons of antiparallel spin is negligible, and the short-range part of their interaction goes as  $r^{-1}$  to very nearly the origin. In this limit one has, moreover,

$$f_q^{\dagger\dagger} = -\frac{4\pi e^2}{q^2 + 2q_F^2} , \qquad (4.9)$$

$$f_q^{\dagger \downarrow} = 0 , \qquad (4.10)$$

$$f_q^a = f_q^s = -\frac{2\pi e^2}{q^2 + 2q_F^2} \,. \tag{4.11}$$

The result, Eq. (4.9), is just the Hubbard local-field approximation, as modified by Geldart and Vosko.<sup>25</sup> We thus see that the modified Hubbard local-field correction, involving as it does only short-range correlations between electrons of parallel spin, is exact in the high-density limit, and that in fact Eq. (4.9) provides a good first approximation to  $f_q^{\dagger\dagger}$  for metallic electron densities. On the other hand, by the time one reaches the onset of metallic densities ( $r_s \leq 2$ ), Coulomb correlations between electrons of antiparallel spin play a significant role, and must be taken into account if one seeks a quantitative account of the dielectric function and dynamic form factor.

It is likewise illuminating to compare these results with the corresponding calculations of Aldrich and Pines<sup>3</sup> for liquid <sup>3</sup>He and with the results obtained for a dilute hardsphere Fermi gas.<sup>26</sup> In the case of liquid <sup>3</sup>He, Aldrich and Pines find  $f^{\dagger\downarrow}(r=0) > f^{\dagger\uparrow}(r=0)$ .<sup>27</sup> This means that a pair of <sup>3</sup>He particles with antiparallel spin interacts more strongly than that with parallel spin. In addition, the range of  $f^{\dagger\dagger}(r)$  ( $r_{\dagger\dagger}$  in Ref. 3) is longer than that of  $f^{\dagger\downarrow}(r)$  $(r_{\pm})$  in Ref. 3) in liquid <sup>3</sup>He. Thus in both the electron and helium liquids the Pauli principle acts to enhance the role of short-range correlations resulting from particle interaction in keeping particles of parallel spin apart and reducing the effectiveness of the very short-range part of the interaction. Moreover, in both liquids, as one increases the density, the effective interaction between particles of antiparallel spin at short distances increases, because short-range correlations become less effective in keeping particles apart.

There is, however, an important difference between the electron liquids and the <sup>3</sup>He liquid; in the latter, at all densities, the radius of the "correlation hole" is close to that of the "correlation plus exchange hole," while  $V^{\dagger\downarrow}(r=0) - V^{\dagger\uparrow}(r=0)$  is small compared to either  $V^{\dagger\downarrow}(r=0)$  or  $V^{\dagger\uparrow}(r=0)$ . In other words, for liquid <sup>3</sup>He, the influence of the Pauli principle is small compared to that of the direct particle interactions, and may, in fact, be neglected to first approximation. [As a result, the effective interaction between <sup>4</sup>He quasiparticles in liquid <sup>4</sup>He is very close to that of <sup>3</sup>He quasiparticles (of either spin) in liquid <sup>3</sup>He at the same density.] In contrast, as we have just seen, for parallel spin electrons at all densities it is the Pauli principle which plays the dominant role, with particle interaction a small correction.

The dilute hard-sphere gas, considered in Appendix B, resembles the electron liquids. The dimensionless volume integral of the effective interaction between antiparallel spin  $F^{\uparrow \downarrow}$  is proportional to  $aq_F$ ; this quantity thus provides a measure of particle correlations alone in keeping particles apart, and so reducing the overall effectiveness of the interaction, which becomes, in this limit, a weak contact potential. On the other hand, the dimensionless volume integral of the interaction between parallel spin particles is is proportional to  $(aq_F)^2$ . Pauli principle correlations thus are so effective in keeping particles of parallel spin apart that their net interaction is negligible compared to that between antiparallel spin particles.

The form we have proposed for the pseudopotentials,  $f^{\uparrow\uparrow}(r)$  and  $f^{\uparrow\downarrow}(r)$ , is not unique. For example, pseudopotentials which have a low-q behavior identical to Eqs. (4.4) but a somewhat different large-q behavior are

$$\widetilde{f}_{q}^{\dagger\dagger} = -\frac{4\pi e^2}{q^2 \epsilon_{\dagger\dagger}(q,0)} , \qquad (4.12a)$$

$$\widetilde{f}_{q}^{\uparrow\downarrow} = -\frac{4\pi e^2}{q^2 \epsilon_{\uparrow\downarrow}(q,0)} , \qquad (4.12b)$$

where the screening factors  $\epsilon_{\uparrow\uparrow}$  and  $\epsilon_{\uparrow\downarrow}$  are given by their static RPA value for densities which correspond to  $q_{\uparrow\uparrow} = q_{\rm FT}$  and  $q_{\uparrow\downarrow} = q_{\rm FT}$ , respectively:

$$\epsilon_{\uparrow\uparrow}(q,0) = 1 + \frac{q_{\uparrow\uparrow}^2}{q^2} F(q,0) ,$$
 (4.13a)

$$\epsilon_{\uparrow\downarrow}(q,0) = 1 + \frac{q_{\uparrow\downarrow}^2}{q^2} F(q,0) ,$$
 (4.13b)

where

$$F(q,0) = \frac{1}{2} + \frac{q_F}{2q} \left[ 1 - \left( \frac{q}{2q_F} \right)^2 \right] \ln \left| \frac{q + 2q_F}{q - 2q_F} \right| .$$
(4.14)

For small q, F(q,0)=1, and one recovers Eqs. (4.4); the behavior of  $f_q^{\uparrow\uparrow}$  and  $f_q^{\uparrow\downarrow}$  is, however, modified at larger q. This "dielectric" form of the pseudopotential is likewise uniquely determined by the Monte Carlo calculations of the compressibility and spin susceptibility; however, as may be seen in Fig. 3 the short-range character of the resulting effective interactions is somewhat different. The overall physical picture we have presented for the Yukawa pseudopotentials is, of course, maintained; the differences between the Yukawa and dielectric pseudopotentials is one of detail, a comparatively small quantitative difference, not a qualitative one.

#### V. LOCAL-FIELD CORRECTIONS

It is instructive to compare our results for  $f_q^s$  with previous calculations.<sup>8,9,14,15,25</sup> To do so we introduce the local-field correction



FIG. 3. Comparison of the local-field corrections, defined by Eq. (5.1), calculated with the Yukawa [Eq. (4.4)] and dielectric [Eq. (4.12)] polarization potentials for  $r_s = 2$  (dashed curves) and 4 (solid curves).

$$G(q) = -\frac{q^2}{4\pi e^2} f_q^s . (5.1)$$

The physical interpretation of G(q) and some of its properties are considered in Appendix C. Various forms of G(q) have been proposed. Among these, we may distinguish three general types of local-field corrections.

(i) Hubbard: G(q) in the Hubbard approximation<sup>8</sup> as well as the modification proposed by Geldart and Vosko<sup>25</sup> is  $r_s$  independent as a function of  $q/q_F$ . G(q) increases monotonically as a function of  $q/q_F$  and levels off at large q ( $\gg q_F$ ) with a limiting value  $\frac{1}{2}$ .

(ii) Self-consistent schemes: Singwi and his co-workers have developed several self-consistent schemes in calculating the local-field correction. In their original theory<sup>9</sup> the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) equations were truncated by assuming a form for the twoparticle correlation function, which led to a dielectric function with a form similar to Eq. (2.1) and Eq. (2.4) with G(q) expressed as a function of the static form factor S(q). On the other hand, for a given G(q), S(q) may be uniquely determined by the dielectric function via the fluctuation-dissipation theorem. Thus this link gives a method of calculating G(q) self-consistently. The G(q)thus obtained, including later variations, is similar to Hubbard's for  $q \ll q_F$ , but rises above  $\frac{1}{2}$  for large q ( $\geq q_F$ ). Our G(q) has a similar behavior.

(iii) G(q)'s with a peak structure at  $q \simeq 2q_F$ : Geldart and Taylor,<sup>12</sup> Toigo and Woodruff,<sup>13</sup> and recently Lantto *et al.*<sup>28</sup> obtained a local-field correction with a marked peak structure near  $q = 2q_F$ . This is a characteristic feature of the Hartree-Fock approximation. Utsumi and Ichimaru<sup>14</sup> incorporate this peak structure in their choice of G(q). However, whether such a peak structure survives after higher-order terms in perturbation theory are considered is not known at present and under debate.<sup>1</sup>

In Fig. 4 we compare our calculated values of G(q) with these representative calculations of G(q); those by Hubbard<sup>8</sup> (H), Singwi, Tosi, Land, and Sjölander<sup>9</sup> (STLS), Geldart and Vosko<sup>25</sup> (GV), Vashishta and Singwi<sup>15</sup> (VS), and Utsumi and Ichimaru<sup>14</sup> (UI-II). In Fig. 5 we show the

UI-11 r.=4

FIG. 4. Comparison of local-field corrections. Our G(q) is shown for  $r_s = 1$ , 4, and 20 (solid curves). The G(q)'s due to Hubbard (H: Ref. 8), Singwi, Tosi, Land, and Sjölander (STLS: Ref. 9), and Geldart and Vosko (GV: Ref. 25) are  $r_s$  independent. The G(q)'s due to Vashishta and Singwi (VS: Ref. 15) and Utsumi and Ichimara (UI-II: Ref. 14) are shown for  $r_s = 4$ .

q/q

static dielectric function  $\epsilon(q,0)$  in our polarizationpotential model [Eqs. (2.4) and (4.4)], and compare it with that in RPA for  $r_s = 2$  and 4. We see that our Yukawa model for  $f^s(r)$  leads to results for G(q) which are close to that obtained by Geldart and Vosko for small  $r_s$  ( $\leq 1$ ) and at small wave numbers ( $q \leq q_F$ ). For  $q \gg q_F$ , ours lie between those of STLS and Vashishta and Singwi. While G(q) is useful for the purpose of comparing different theoretical calculations of dielectric response, it is not a directly observable quantity; what is, in principle, observable is  $\epsilon(q,0)$  and/or  $\epsilon(q,\omega)$ . However, as noted in the Introduction, there are two reasons why one would expect the values of  $\epsilon(q,0)$  or  $\epsilon(q,\omega)$  to depart (perhaps appreciably) from those calculated using our values (or any others) of the local-field correction:

(i) Electrons in general may be expected to possess an effective mass, and the particle-hole excitations will, in general, be characterized by a q-dependent effective mass  $m_q^*$ .

(ii) Multipair excitations may contribute in an essential way to  $\chi_{sc}(q,\omega)$  and hence to  $\epsilon(q,\omega)$  and  $\epsilon(q,0)$ .

We could incorporate the first class of corrections into our calculations by introducing an effective mass  $m_q^*$  into  $\chi^0(q,\omega)$ ; however, in the absence of accurate microscopic calculations or reliable experimental measurements of  $m_q^*$ , it does not seem worthwhile to do so at this stage. We consider this question further in a planned paper<sup>6</sup>, at which time we also take up the question of how, at least phenomenologically, one can incorporate multipair excitations into the theory.

Finally we comment on the high-q behavior of G(q). It is known that the form of the dielectric function (2.1) with (2.4) leads to the relation<sup>29-31</sup>

$$\lim_{q \to \infty} G(q) = 1 - g(0) , \qquad (5.2)$$

where g(0) is the value of the pair correlation function at zero interparticle separation. This condition, however, does not provide as powerful a constraint as the compres-



FIG. 5. Static dielectric function  $\epsilon(q,0)$  in our polarizationpotential model [Eqs. (2.4) and (4.4) (solid curves)] and in RPA (dashed curves) for  $r_s = 2$  and 4.

1.C

(b) 905 sibility sum rule does at  $q \rightarrow 0$ . This is because it is in the form  $1 - f_q^s \chi^0(q, \omega)$  that the Lindhard function is modified [Eq. (2.4)]. Namely, the function  $|f_q^s| (\propto G(q)/q^2)$  drops rapidly  $(\propto q^{-2})$  for large q ( $\gg q_F$ ). In particular, since  $\chi^0(q, 0) \propto q^{-2}$  for  $\omega = 0$  and large q, the static screening property is insensitive to the values of G(q) at  $q \gg q_F$ .

### VI. NONLOCAL SPIN SUSCEPTIBILITY

It is straightforward to use the pseudopotentials derived in the preceding section to calculate the nonlocal static spin susceptibility. According to Eqs. (2.6) and (2.21) it is given by

$$\chi_P(q,0) = -\mu_B^2 \chi^I(q,0) = -\mu_B^2 \frac{\chi^0(q,0)}{1 - f_q^a \chi^0(q,0)} , \qquad (6.1)$$

where  $f_q^a$ , the spin-antisymmetric electron-hole pseudopotential, is given in Eq. (2.12). In the long-wavelength limit this equation becomes

$$\lim_{q \to 0} \chi_P(q,0) \equiv \chi_P = \frac{\mu_B^2 N^0(0) / V}{1 + F^a} .$$
(6.2)

We give in Fig. 6 a plot of  $-nf_q^a$  for several values of  $r_s$  to bring out the wave-vector dependence of  $f_q^a$  for our choice of pseudopotential, while in Fig. 7 we give our results for  $\chi_P(q,0)/\chi_P$  for some values of  $r_s$ .

We note that the q dependence of our  $f_q^a$  is chosen such that it is consistent with experimental values at  $q \rightarrow 0$ . Thus this provides an exact boundary condition for consistency check in other theories. Singwi and his coworkers have calculated  $f_q^a$  [I(q) in their notation.]<sup>10,11</sup> We compare our  $f_q^a$  with the one in their second version<sup>11</sup> in Fig. 6. We find that the q dependence of our  $f_q^a$  is, roughly speaking, similar to theirs in Ref. 11, which is a marked improvement over their first version (Ref. 10). However, note some discrepancies between their values of  $f_q^a$  and ours at  $q \rightarrow 0$ .



FIG. 6. Spin-antisymmetric pseudopotential  $f_q^a$  for  $r_s = 1, 2, 4$ , and 10. The solid curves represent our calculations and the dashed curves those of Singwi, Sjölander, Tosi, and Land (Ref. 11).



FIG. 7. Static spin susceptibility  $\chi_P(q,0)$  in our model [Eqs. (2.6) and (4.4)] for  $r_s = 2$ , 4, 10, and 20 (solid curves), and in the RPA (dashed curve) for  $r_s = 2$ . The functions are normalized by their values at q = 0 ( $\chi_P$ ).

#### VII. DISCUSSION

In the approach presented here, what is new to the calculation of the response functions of electron liquids (the dielectric function and spin susceptibility) is the introduction of simple configuration-space pseudopotentials to describe the modification in electron interaction at short distances brought about by charge- and spin-induced correlations. The advantages of the present approach are perhaps fourfold.

(i) It provides a simple (built-in) way of sorting out the role of charge-induced correlations from spin-induced (i.e., Pauli-principle-induced) correlations because one distinguishes at the outset between the interaction of parallel and antiparallel spin electrons.

(ii) It provides a simple way to incorporate in the relevant response functions the results of recent "exact" Monte Carlo calculations of static liquid properties.

(iii) It provides a useful tool for the many-body theorists who are interested in comparing the consequences of particle interaction in quite different systems.

(iv) It provides a simple physical perspective on previous calculations of the response functions of electron liquids.

On the other hand, the theory is phenomenological; it is consequently difficult to assess its validity at finite wave vectors, a question to which we return in the following papers in this series. The interested reader can perhaps take encouragement from the fact that although the various local-field corrections differ appreciably from one another (see Fig. 4), the corresponding static dielectric functions do not, while our expression for the nonlocal spin-density response function should provide a simple useful input into calculations of those metallic properties which involve this quantity.

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# APPENDIX A: POLARIZATION-POTENTIAL PARAMETERS IN THE HIGH-DENSITY LIMIT

In this appendix we derive the polarization-potential parameters in the high-density limit by using the analytic expressions for the compressibility and the spin susceptibility in the random-phase approximation (RPA). Within the RPA the correlation energy per particle has been calculated to be<sup>32-35</sup>

$$\frac{E_{\rm corr}(r_s)}{N} = \frac{2}{\pi^2} (1 - \ln 2) \ln r_s - 0.094 + 0.018 r_s \ln r_s + \cdots$$
 (A1)

From Eq. (3.1) the compressibility ratio is

$$\frac{\kappa_0}{\kappa_{\rm RPA}} = 1 - \frac{\alpha}{\pi} r_s - \frac{1}{\pi^2} (1 - \ln 2) \alpha^2 r_s^2 - 0.006 \alpha^2 r_s^3 \ln r_s$$
$$-0.003 \alpha^2 r_s^3 + \cdots .$$
(A2)

On the other hand, the paramagnetic spin susceptibility ratio in the RPA is  $^{36,37}$ 

$$\frac{\chi_P^0}{\chi_{\text{RPA}}} = 1 - \frac{\alpha}{\pi} r_s + \frac{1}{2} \left[ \frac{\alpha r_s}{\pi} \right]^2 \left[ 0.306 - \ln \left[ \frac{\alpha r_s}{\pi} \right] \right] + \cdots$$
(A3)

Then using Eqs. (A2) and (A3) in (2.20), (2.25), (3.2), (3.3), and (4.6), one obtains in the long-wavelength limit

$$q_{\uparrow\uparrow} = \sqrt{2}q_F \left[ 1 + \left( \frac{\alpha r_s}{4\pi} \right) (-1.49 + \ln r_s) + \cdots \right]^{-1/2},$$
(A4)

$$q_{\uparrow\downarrow} = 2\sqrt{2}q_F \left[ \left( \frac{\alpha r_s}{\pi} \right) (2.716 - \ln r_s) + \cdots \right]^{-1/2}.$$
(A5)

At this point the meaning of the Hubbard approximation becomes clear. The scheme used by Hubbard as modified by Geldart and Vosko<sup>25</sup> corresponds to taking

$$q_{\uparrow\uparrow} = \sqrt{2}q_F , \qquad (A6)$$

$$q_{\uparrow\downarrow} = \infty$$
 , (A7)

in the long-wavelength limit.

These expressions are obtained from Eqs. (A4) and (A5) by taking the high-density limit. Thus our scheme reduces to that of Hubbard in the long-wavelength limit at high densities, the latter of which in turn correctly reproduces the RPA results for compressibility and spin susceptibility.

## APPENDIX B: COMPARISON WITH THE LANDAU PARAMETERS OF A DILUTE HARD-SPHERE FERMI GAS

It is instructive to compare the polarization potentials of an electron liquid and those of <sup>3</sup>He with the Landau parameters of a dilute hard-sphere Fermi gas. As we shall see, there is a close similarity among the effective interactions of these systems.

From the expression for the Landau quasiparticle interaction,<sup>26</sup> one easily obtains the following Landau parameters for a dilute hard-sphere Fermi gas:

$$F_0^s = \frac{2}{\pi} a q_F \left[ 1 + \frac{4}{3\pi} (2 + \ln 2) a q_F \right] , \qquad (B1)$$

$$F_0^a = -\frac{2}{\pi} a q_F \left[ 1 + \frac{4}{3\pi} (1 - \ln 2) a q_F \right], \qquad (B2)$$

$$F_1^s = \frac{8}{5\pi^2} (7\ln 2 - 1)(aq_F)^2 , \qquad (B3)$$

$$F_1^a = -\frac{8}{5\pi^2} (2 + \ln 2) (aq_F)^2 , \qquad (B4)$$

from which

$$F_0^{\dagger\dagger} = \frac{8}{3\pi^2} (2\ln 2 + 1)(aq_F)^2 , \qquad (B5)$$

$$F_0^{\uparrow\downarrow} = \frac{4}{\pi} a q_F \left[ 1 + \frac{2}{\pi} a q_F \right] , \qquad (B6)$$

$$F_1^{\dagger\dagger} = \frac{24}{5\pi^2} (2\ln 2 - 1)(aq_F)^2 , \qquad (B7)$$

$$F_1^{\uparrow\downarrow} = \frac{8}{5\pi^2} (8\ln 2 + 1)(aq_F)^2 .$$
 (B8)

Therefore, one sees that  $F_0^{\dagger \downarrow} > F_0^{\dagger \dagger}$ . Namely, a quasiparticle pair with antiparallel spin interacts more strongly than a quasiparticle pair with parallel spin. Although these results are valid only in the weak-coupling region  $(aq_F \ll 1)$ , these features essentially reflect the Pauli principle, which reduces the particle interaction with parallel spins by keeping the two particles away from each other. Therefore, this simple model system demonstrates a common feature among the Fermi systems which we have mentioned in Sec. IV.

# APPENDIX C: THE STATIC LOCAL-FIELD CORRECTION

The influence of static local-field corrections on the dielectric function of an electron liquid is frequently expressed in the form

$$\epsilon(q,\omega) = 1 - \frac{v(q)\chi^{0}(q,\omega)}{1 + v(q)G(q)\chi^{0}(q,\omega)} , \qquad (C1)$$

where  $v(q) = 4\pi e^2/q^2$  and G(q) is the static local-field correction, which is related to  $f_q^2$  by

$$G(q) = -\frac{q^2}{4\pi e^2} f_q^s .$$
 (C2)

The corresponding expression for the density-density response function then takes the form

$$\chi(q,\omega) = \frac{\chi^{0}(q,\omega)}{1 - (4\pi e^{2}/q^{2} + f_{q}^{s})\chi^{0}(q,\omega)} = \frac{\chi^{0}(q,\omega)}{1 - (4\pi e^{2}/q^{2})[1 - G(q)]\chi^{0}(q,\omega)} .$$
 (C3)

It is instructive to develop a physical interpretation for G(q) analogous to that presented for  $f_q^s$ . Equation (C2) may be written in the configuration space as

$$\nabla^2 f^s(r) = 4\pi e^2 G(r) , \qquad (C4)$$

where G(r) is the Fourier transform of G(q). From Eq. (C4) it is apparent that the pseudopotential  $f^{s}(r)$  can be regarded as arising from a "screening" charge, eG(r), and that the effective potential,

$$V_{\text{eff}}(r) = v(r) + f^{s}(r) \tag{C5}$$

can be regarded as the solution of

$$\nabla^2 V_{\text{eff}}(r) = -4\pi e^2 [\delta(r) - G(r)] . \qquad (C6)$$

From this perspective a simple physical interpretation of the high-q limit for G(q) obtained by Shaw and Kimball, Eq. (5.2),<sup>29-31</sup> emerges. The high-q limit of the Fourier transform Eq. (C6) is thus

$$\lim_{q \to \infty} V_q^{\text{eff}} = \lim_{q \to \infty} \frac{4\pi e^2}{q^2} [1 - G(q)] = \frac{4\pi e^2}{q^2} g(0) . \quad (C7)$$

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- <sup>1</sup>For a review, see K. S. Singwi and M. P. Tosi, in *Solid State Physics*, edited by H. Ehrenreich, F. Seitz, and D. Turnbull (Academic, New York, 1981), Vol. 36, p. 177; S. Ichimaru, Rev. Mod. Phys. <u>54</u>, 1017 (1982).
- <sup>2</sup>D. Pines, in *Quantum Fluids*, edited by D. F. Brewer (North-Holland, Amsterdam, 1966), p. 257.
- <sup>3</sup>C. H. Aldrich III, Ph.D. thesis, University of Illinois (1974) (unpublished); C. H. Aldrich III and D. Pines, J. Low Temp. Phys. <u>32</u>, 689 (1978).
- <sup>4</sup>D. M. Ceperley and B. J. Alder, Phys. Rev. Lett. <u>45</u>, 566 (1980).
- <sup>5</sup>N. Iwamoto, E. Krotscheck, and D. Pines, following paper, Phys. Rev. B <u>29</u>, 3936 (1984).
- <sup>6</sup>N. Iwamoto, E. Krotscheck, and D. Pines (unpublished).
- <sup>7</sup>D. Pines and P. Nozières, *Theory of Quantum Liquids* (Benjamin, New York, 1966), Vol. I.
- <sup>8</sup>J. Hubbard, Proc. R. Soc. London, Ser. A <u>243</u>, 336 (1957).
- <sup>9</sup>K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. <u>176</u>, 589 (1968).
- <sup>10</sup>R. Lobo, K. S. Singwi, and M. P. Tosi, Phys. Rev. <u>186</u>, 470

We see that the physical content of their result is that at small distances the charge responsible for the net effective spin-symmetric interaction is given by the pair correlation function at the origin, g(0).

We have given above the spin-symmetric form of equations which obviously hold for the effective interaction between both parallel and antiparallel spin electrons. Thus one can define

$$G^{\dagger\dagger}(q) = -\frac{q^2}{4\pi e^2} f_q^{\dagger\dagger} , \qquad (C8a)$$

$$G^{\dagger\downarrow}(q) = -\frac{q^2}{4\pi e^2} f_q^{\dagger\downarrow} , \qquad (C8b)$$

so that

$$V_q^{\dagger\dagger} = \frac{4\pi e^2}{q^2} [1 - G^{\dagger\dagger}(q)] , \qquad (C9a)$$

$$V_q^{\uparrow\downarrow} = \frac{4\pi e^2}{q^2} [1 - G^{\uparrow\downarrow}(q)].$$
 (C9b)

Equation (C7) is separately satisfied for  $V_q^{\dagger\dagger}$  and  $V_q^{\dagger\downarrow}$ , according to

$$\lim_{q \to \infty} V_q^{\dagger \dagger} = \frac{4\pi e^2}{q^2} g^{\dagger \dagger}(0) , \qquad (C10a)$$

$$\lim_{q \to \infty} V_q^{\uparrow \downarrow} = \frac{4\pi e^2}{q^2} g^{\uparrow \downarrow}(0) , \qquad (C10b)$$

where  $g^{\dagger\dagger}(r)$  is the pair correlation function for electrons of parallel spin,  $g^{\dagger\downarrow}(r)$  that for electrons of antiparallel spin, and

$$g(r) = \frac{1}{2} [g^{\dagger\dagger}(r) + g^{\dagger\downarrow}(r)] .$$
 (C11)

(1969).

- <sup>11</sup>K. S. Singwi, A. Sjölander, M. P. Tosi, and R. H. Land, Solid State Commun. <u>7</u>, 1503 (1969); Phys. Rev. B 1, 1044 (1970).
- <sup>12</sup>D. J. W. Geldart and R. Taylor, Can. J. Phys. <u>48</u>, 155 (1970); <u>48</u>, 167 (1970).
- <sup>13</sup>F. Toigo and T. O. Woodruff, Phys. Rev. B <u>2</u>, 3958 (1970).
- <sup>14</sup>K. Utsumi and S. Ichimaru, Phys. Rev. B <u>22</u>, 1522 (1980); <u>22</u>, 5203 (1980).
- <sup>15</sup>P. Vashishta and K. S. Singwi, Phys. Rev. B <u>6</u>, 875 (1972); <u>6</u>, 4883(E) (1972).
- <sup>16</sup>D. N. Lowy and G. E. Brown, Phys. Rev. B <u>12</u>, 2138 (1975).
- <sup>17</sup>K. Bedell and G. E. Brown, Phys. Rev. B <u>17</u>, 4512 (1978).
- <sup>18</sup>L. D. Landau, Zh. Eksp. Teor. Fiz. <u>30</u>, 1058 (1956); <u>32</u>, 59 (1957) [Sov. Phys.—JETP <u>3</u>, 920 (1957); <u>5</u>, 101 (1957)].
- <sup>19</sup>S. H. Vosko, L. Wilk, and M. Nusair, Can. J. Phys. <u>58</u>, 1200 (1980).
- <sup>20</sup>P. Nozières and D. Pines, Phys. Rev. <u>111</u>, 442 (1958).
- <sup>21</sup>F. Ham, Phys. Rev. <u>128</u>, 2524 (1962).
- <sup>22</sup>S. D. Silverstein, Phys. Rev. <u>130</u>, 912 (1963); <u>130</u>, 1703 (1963).
- <sup>23</sup>M. Rice, Ann. Phys. (N.Y.) <u>31</u>, 100 (1965).
- <sup>24</sup>T. Kushida, J. C. Murphy, and M. Hanabusa, Phys. Rev. B <u>13</u>, 5136 (1976).
- <sup>25</sup>D. J. W. Geldart and S. H. Vosko, Can. J. Phys. <u>44</u>, 2137 (1966).
- <sup>26</sup>A. A. Abrikosov and I. M. Khalatnikov, Zh. Eksp. Teor. Fiz.

<u>33,</u> 1154 (1957) [Sov. Phys.—JETP <u>6</u>, 888 (1958)].

- <sup>27</sup>By definition the polarization potentials in Ref. 3 include the bare interaction. Therefore, the quantities  $f^{\dagger\dagger}(r)$  and  $f^{\dagger\downarrow}(r)$  defined here correspond to our  $V^{\dagger\dagger}(r)$  and  $V^{\dagger\downarrow}(r)$ , respectively.
- <sup>28</sup>L. Lantto, P. Pietiläinen, and A. Kallio, Phys. Rev. B <u>26</u>, 5568 (1982).
- <sup>29</sup>R. W. Shaw, J. Phys. C <u>3</u>, 1140 (1970).
- <sup>30</sup>J. C. Kimball, Phys. Rev. A <u>7</u>, 1648 (1973).
- <sup>31</sup>See also G. Niklasson, Phys. Rev. B <u>10</u>, 3052 (1974).

- <sup>32</sup>W. Macke, Z. Naturforsch. <u>5a</u>, 192 (1950).
- <sup>33</sup>M. Gell-Mann and K. A. Brueckner, Phys. Rev. <u>106</u>, 364 (1957).
- <sup>34</sup>D. F. DuBois, Ann. Phys. (N.Y.) 7, 174 (1959).
- <sup>35</sup>W. J. Carr, Jr. and A. A. Maradudin, Phys. Rev. <u>133</u>, A371 (1964).
- <sup>36</sup>K. A. Brueckner and K. Sawada, Phys. Rev. <u>112</u>, 328 (1958).
- <sup>37</sup>B. S. Shastry, Phys. Rev. Lett. <u>38</u>, 449 (1977); Phys. Rev. B <u>17</u>, 385 (1978).