PHYSICAL REVIEW B VOLUME 24, NUMBER 12 15 DECEMBER 1981

Analytic expression for the dielectric screening function of strongly coupled electron liquids at metallic and lower densities

Setsuo Ichimaru and Kenichi Utsumi
Department of Physics, University of Tokyo, Bunkyo-ku, Tokyo 113, Japan
(Received 26 June 1981)

We propose a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities which accurately reproduces the recent Monte Carlo results as well as those of the microscopic calculations and which satisfies the self-consistency conditions in the compressibility sum rule and the short-range correlation.

The frequency- and wave-number-dependent, longitudinal dielectric function[1] $\epsilon(q,\omega)$ is an essential quantity for description of the electronic properties of metals and related substances such as the laser-compressed plasmas and the interiors of heavy planets. The electrons (with number density n) in such a system usually form a strongly coupled system in that the Coulomb coupling constant $r_s \equiv (3/4\pi n)^{1/3} me^2/\hbar^2$ is greater than unity. The standard Lindhard function[2] based on the random-phase approximation[1] (RPA) is not applicable in these circumstances; theories[3] proposed to go beyond the RPA description thus far have failed to satisfy consistency requirements or exact boundary conditions (see below for details). In this Report we wish to present a simple fitting formula for the dielectric function of strongly coupled degenerate electron liquids, which satisfies a number of self-consistency conditions and which accurately reproduces the recent Monte Carlo results[4] as well as those of the latest microscopic calculations.[5] The result should be of use to numerical studies of the strong coupling effects involving degenerate electron liquids.

Following the polarization-potential approach,[6] we take account of the strong-coupling effects through the local-field correction $G(q)$, so that the dielectric function is expressed as

$$\epsilon(q,\omega)=1-\frac{v(q)\chi_0(q,\omega)}{1+v(q)G(q)\chi_0(q,\omega)} . \tag{1}$$

Here, $v(q) = 4\pi e^2/q^2$, and

$$\chi_0(q,\omega)=\frac{2}{\hbar}\int \frac{d\vec{k}}{(2\pi)^3} \times \frac{F(\vec{k})-F(\vec{k}+\vec{q})}{\omega-(\hbar/2m)(2\vec{k}\cdot\vec{q}+q^2)+i\eta} \tag{2}$$

is the Lindhard polarizability of the free electrons,[1,2] with $F(\vec{k})$ representing the Fermi step function. Three essential ingredients that we shall evoke for determination of $G(q)$ are: (1) Monte Carlo data of Ceperley and Alder[4] for the correlation energy, (2) the ladder diagram calculation of the short-range correlations by Yasuhara[7], and (3) the self-consistent dielectric formulation of Utsumi and Ichimaru.[5]

We begin by noting the long-wavelength behavior ($q << q_F$, the Fermi wave number),

$$G(q)\to\gamma_0 Q^2 \quad (Q\equiv q/q_F) , \tag{3}$$

where the coefficient γ_0 is connected to the correlation energy $E_c(r_s)$ in rydbergs per electron via the compressibility relation,[1,5]

$$\gamma_0=\frac{1}{4}-\frac{\pi\alpha}{24}r_s^5\frac{d}{dr_s}\left[r_s^{-2}\frac{d}{dr_s}E_c(r_s)\right] , \tag{4}$$

with $\alpha\equiv(4/9\pi)^{1/3}$. Vosko, Wilk, and Nusair[8] carried out a Padé approximate fitting of Ceperley and Alder's Monte Carlo data on $E_c(r_s)$ at six values of r_s. For an electron liquid in the paramagnetic state, which we are here concerned with, their fitting formula reads

$$r_s\frac{dE_c(r_s)}{dr_s}=b_0\frac{1+b_1x}{1+b_1x+b_2x^2+b_3x^3} \qquad (x\equiv\sqrt{r_s}) , \tag{5}$$

where $b_0 = 0.0621814$, $b_1 = 9.81379$, $b_2 = 2.82224$, and $b_3 = 0.736411$. We use (5) in (4) to determine the long-wavelength behavior (3) as a function of r_s.

According to Kimball's analysis[9] on the dielectric function of the form (1), the short-wavelength behavior of $G(q)$ is related to the radial distribution function $g(r)$ as

$$\lim_{q\to\infty} G(q)=1-g(0) . \tag{6}$$

The short-range correlation can be described by the electron-electron ladder interactions, through a consideration of which Yasuhara[7] derived an expression,

$$g(0)=\frac{1}{8}\left[\frac{z}{I_1(z)}\right]^2 , \quad z\equiv 4(\alpha r_s/\pi)^{1/2} \tag{7}$$

where $I_1(z)$ is a modified Bessel function of the first order. Use of (7) in (6) thus determines the short-wavelength behavior of $G(q)$.

Recent advances in the microscopic formulation of the dielectric function enable us to set up a set of nonlinear integral equations, through a numerical solution of which both the exchange and Coulomb-correlational effects in the local-field correction have been evaluated.[5,10] Internal consistency and accuracy of the theory have been examined and ascertained through comparison with the Monte Carlo and variational results.[4,11,12] To simulate the numerical results of the microscopic theory as well as to accommodate the boundary conditions (3) and (6), we find it appropriate to express

$$G(q)=AQ^4+BQ^2+C+[AQ^4+(B+\tfrac{8}{3}A)Q^2-C]\times\frac{4-Q^2}{4Q}\ln\left|\frac{2+Q}{2-Q}\right| , \tag{8}$$

where

$$A=0.029 \quad (0\le r_s\le 15) , \tag{9}$$

$$B=\tfrac{9}{16}\gamma_0-\tfrac{3}{64}[1-g(0)]-\tfrac{16}{15}A , \tag{10}$$

$$C=-\tfrac{3}{4}\gamma_0+\tfrac{9}{16}[1-g(0)]-\tfrac{16}{5}A . \tag{11}$$

Equations (10) and (11) derive from (3) and (6). Equation (9) is adopted so that Eq. (8) closely simulates the results of the microscopic theory[5,10]; Fig. 1 shows such a comparison at $r_s = 4$ and 10. For $r_s > 15$, A begins to decrease gradually from 0.029.

Equation (8) coupled with (4), (5), (7), (9), (10), and (11) is the principal result in this paper; the dielectric screening function is calculated according to (1). Following the standard procedure[1,5] involving the use of the fluctuation-dissipation theorem, one can then proceed to calculate various fundamental quantities such as the correlation energy and the radial distribution function. For internal consistency of the theory represented by (8), the values of γ_0 and $g(0)$ so calculated should reproduce those input values derived from (5) and (7). The former is the requirement known as the compressibility sum rule; the latter is the self-consistency requirement for the short-range correlation. The balance of this paper is devoted to examination of the extent to which these requirements are satisfied and investigation of a salient feature in (8).

In Fig. 2, we exhibit the correlation energy computed from (1) and (8), together with Vosko, Wilk, and Nusair's fitting formula [i.e., the input values of (5)] and Ceperley and Alder's data ; good agreement observed here indicates that Eqs. (1) and (8) satisfy the compressibility sum rule to a good degree of accuracy. We also compute the correlation-energy contributions $E_c(q;r_s)$ from different regions of momentum transfer[1] as defined by

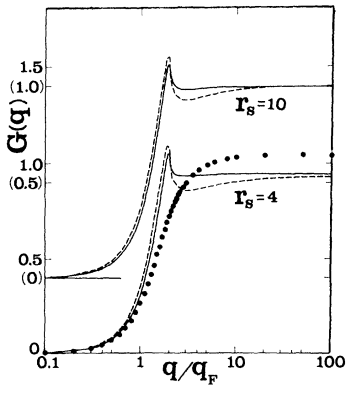

FIG. 1. Local-field correction $G(q)$ at $r_s = 4$ (below) and $r_s = 10$ (above). The solid curves represent the present fitting formula, the dashed curves, the calculations of Utsumi and Ichimaru (Ref. 5), and the dots, those of Vashishta and Singwi (Ref. 3).

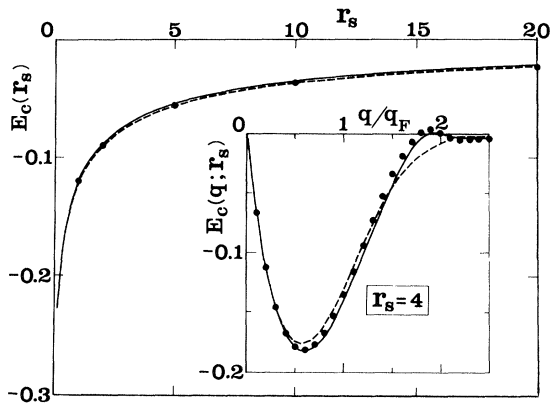

FIG. 2. Correlation energy $E_c(r_s)$ in rydbergs per electron. The solid curve refers to the present result [Eq. (9) has been used throughout], the dashed curve, the fitting formula of Vosko, Wilk, and Nusair (Ref. 8), and the dots, the Monte Carlo results of Ceperley and Alder (Ref. 4). In the inset, the correlation-energy contributions $E_c(q;r_s)$ from different regions of momentum transfer at $r_s = 4$ are shown [see Eq. (12) for the definition]. The solid curve refers to the present theory, the dashed curve, the FHNC calculations of Zabolitzky (Ref. 12) and the dots, the calculations of Utsumi and Ichimaru (Ref. 5).

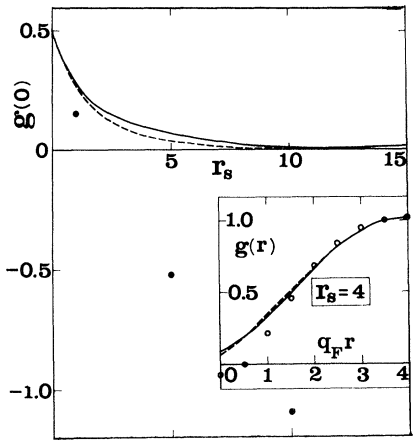

FIG. 3. Values of $g(0)$. The solid curve represents the present theory, the dashed curve, Yasuhara's formula (Ref. 7) Eq. (7), and the dots, the results obtained on the basis of Eq. (13). In the inset, the radial distribution function $g(r)$ at $r_s = 4$ is shown. The solid curve refers to the present theory, the dashed curve, the calculations of Utsumi and Ichimaru (Ref. 5), the open circles, those of Vashishta and Singwi (Ref. 3).

$$E_c(r_s)=\frac{2}{\pi\alpha r_s q_F}\int_0^\infty dq\; E_c(q;r_s)\;. \tag{12}$$

The $E_c(q;r_s)$ values predicted in the present theory at $r_s = 4$ are compared in the inset of Fig. 2 with the Fermi hypernetted chain (FHNC) calculations carried out by Zabolitzky.[12]

The values of $g(0)$ computed from (1) and (8) are compared with those of Yasuhara's formula (7) in Fig. 3. Here again we find that the self-consistency requirement is well satisfied ; notably the positivity condition $g(0)\geq 0$ is maintained. In Table I, we additionally list and compare numerical values for $g(0)$ at metallic densities predicted in various theories. In the inset of Fig. 3 we show the function $g(r)$ at $r_s = 4$ evaluated in this and other theoretical schemes.

A notable feature in (8) is its involvement of the logarithmic singularity at $q=2q_F$ and the accompanying peak at $q\simeq 1.9q_F$ (see, e.g., Fig. 1). Some of the local-field corrections proposed in the past,[3] on the contrary, do not exhibit such a feature. To simulate the latter situation one may adopt a form,

$$G(q)=a_0Q^2/(Q^2+a_1)\;, \tag{13}$$

in place of (8); the coefficients, a_0 and a_1, are to be determined from (3) and (6). In Fig. 3, the values of $g(0)$ calculated from a substitution of (13) in (1) are also plotted. We find that the value of $g(0)$ in the scheme (13) quickly goes into the negative

TABLE I. Values of $g(0)$ in various theories.

	Ref.	$r_s=1$	$r_s=2$	$r_s=3$	$r_s=4$	$r_s=5$	$r_s=6$
Present theory		0.279	0.181	0.128	0.094	0.070	0.052
Utsumi and Ichimaru	5	0.276	0.168	0.107	0.070	0.046	0.031
Yasuhara	7	0.266	0.150	0.088	0.053	0.033	0.021
Vashishta and Singwi	3	0.19	0.034	−0.04	−0.07	−0.075	−0.08
Lantto	11	0.27		0.10		0.04	
Zabolitzky	12	0.304	0.202	0.143	0.105	0.081	

domain and that the self-consistency condition is violated with a wide margin. It appears that a local-field correction of the form (13) cannot adequately accommodate those exact boundary conditions.

In conclusion we have shown that the fitting formula (8) accurately reproduces the recent Monte Carlo results as well as those of the microscopic calculations; it satisfies the self-consistency conditions in the compressibility sum rule and the short-range correlation. The formula may thus provide a simple and useful analytic description of the static correlations and screening properties of degenerate electron liquids at metallic and lower densities. Since the local-field correction (8) does not take account of the frequency-dependent effects, however, the resulting dielectric function (1) should be less accurate in describing the dynamic properties such as the detailed features in the spectral function of the density-fluctuation excitations.[13]

We wish to thank Professor D. Pines for stimulating conversations on this and related subjects, and Dr. J. G. Zabolitzky for sending the numerical data of his FHNC calculations which enabled us to make a comparison as shown in the inset of Fig. 2. This work has been supported in part by the Japanese Ministry of Education, Science, and Culture through the Research Grants Nos. 56380001 and 56580003.

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