Application of the Tripathy-Mandal dielectric function to the study of some properties of an electron liquid

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Using the expression for the dielectric function derived by Tripathy and Mandal in a previous paper, the pair correlation function $g(r)$ and the correlation energy of the electron liquid are calculated in the range of metallic densities. It is observed that the $g(r)$ in this case exhibits an oscillatory behavior for $r_s \geq 2$. This establishes the similarity in the behavior of the electron liquid with that of the classical liquids. Our calculated values of $g(0)$ are found to be positive up to $r_s \simeq 4$.

I. INTRODUCTION

In a previous paper[1] hereafter referred to as I, an expression for the dielectric function for an electron liquid has been obtained by Tripathy and Mandal (TM), solving the equations of motion for the double-time retarded commutator of the charge-density fluctuation operators. This method is based on a decoupling of the higher-order Green's functions, which is achieved by conserving frequency moments to an infinite order. In this theory, the expression for the dielectric function is written in the form[2]

$$\epsilon(\vec{k}, \omega) = 1 + Q_0(\vec{k}, \omega)/[1 - G(\vec{k}, \omega)Q_0(\vec{k}, \omega)], \quad (1.1)$$

where $Q_0(\vec{k}, \omega) = -v(\vec{k})\chi_0(\vec{k}, \omega)$, $\chi_0(\vec{k}, \omega)$ is the usual free-electron polarizability[3] and $v(\vec{k}) = 4\pi e^2/k^2$. The function $G(\vec{k}, \omega)$ represents the local-field correction, which takes into account the short-range correlations arising from both exchange and Coulomb effects. Numerical values of $G(\vec{k}, 0)$ as a function of k have been given in I. As one can see, an interesting feature of this $G(k)$ is that it has a very sharp peak around $k = 2k_F$, which is in contrast to the results of other existing theories. The other important result of the TM theory is that it satisfies the compressibility sum rule,[4] that is, one finds

$$\lim_{k\to 0} k^2\epsilon(\vec{k}, 0) = (4\alpha r_s/\pi)(C/C_0), \quad (1.2)$$

where k has been measured in the unit of k_F, r_s is the usual density parameter, and $\alpha = (4/9\pi)^{1/3}$. In the above equation, C and C_0 denote the compressibility of the electron liquid and the free gas. The ratio C_0/C in the TM theory is given by

$$C_0/C = 1 - \gamma 4\alpha r_s/\pi, \quad (1.3)$$

where $\gamma = \frac{1}{4}$. With this value of γ, the value of the compressibility obtained by using the above formula agrees well with the compressibility data of Rice[5] for metallic densities, following his calculation of the second derivative of the ground-state energy with respect to the volume of the electron gas. It is further seen that the values of $G(k)$ obtained in the TM theory in the limit $k \to \infty$ is $\frac{1}{3}$, which agrees with the value of $G(\infty)$ evaluated in the self-consistent Hartree-Fock approximation.[6] Using the results of this $G(k)$, we have already evaluated the structure factor $S(k)$ for different values of the electron densities. In this calculation,[7] we have found that there exists a sharp peak in $S(k)$ [value of $S(k)$ at the peak exceeding unity] around $k = 2k_F$ for the entire metallic densities. This very interesting feature observed in our structure factor is not seen in the calculations followed from other theories.

In this paper, we present the result of some of the properties of the electron liquid, like the pair correlation function and the correlation energy based on the TM theory for the whole range of metallic densities, and compare them with those of the earlier theories. These calculations have been done by using the expression for the dielectric function (1.1), with $G(\vec{k}, \omega)$ taken in the static limit ($\omega = 0$). We find that our pair correlation function $g(r)$ exhibits oscillatory behavior in the whole range of densities starting from $r_s \geq 2$. Such behavior of $g(r)$ is observed in the case of classical liquids. It is seen that the positions of the peak in our $g(r)$ for a certain r_s correspond to the average interparticle spacings for the r_s concerned, and the values of $g(r)$ at the peaks increase with r_s. The other interesting result that follows from the present calculation is that the values of $g(0)$ is positive for all values of r_s up to $r_s \simeq 4$. Comparing our $g(0)$ values with those of the Toigo-Woodruff (TW) theory[8] (where the latter can be derived from the TM theory[1] by conserving the first frequency moment only), we find that our values are relatively more

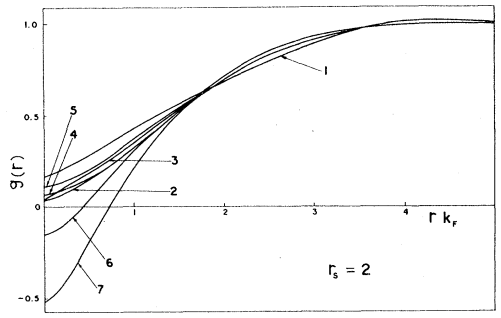

FIG. 1. Pair correlation function $g(r)$ vs rk_F for $r_s=2$. The plots 1, 2, 3, 4, 5, 6, and 7 are, respectively, from the results of the present work, Refs. 12, 8, 11, 10, Hubbard, and the RPA. Other figures also use the same labels.

positive for all values of r_s. This shows that our theory takes into account the short-range correlation effects to a reasonably good extent. The $g(r)$ calculated from a completely dynamic $G(k, \omega)$ may, however, show a more improved behavior.

II. CALCULATION AND DISCUSSION OF RESULTS

A. Pair correlation function

The expression for the pair correlation function $g(r)$ can be written

$$g(r)=1+\frac{3}{2r}\int_0^\infty k\sin(kr)[S(k)-1]\,dk\,, \qquad (2.1)$$

where k is expressed in units of k_F and r in units of k_F^{-1}. The structure factor $S(k)$ of the electron liquid is related to the dielectric function $\epsilon(\vec{k}, \omega)$ through the relation[9]

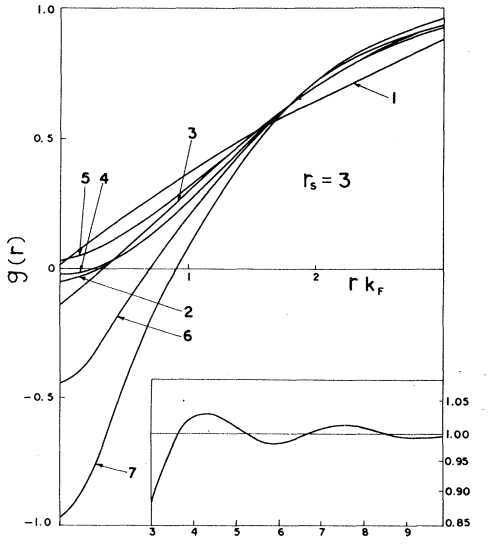

FIG. 2. Plot of $g(r)$ vs rk_F for $r_s=3$.

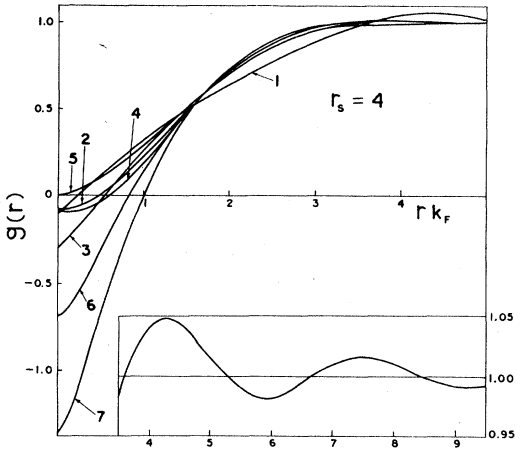

FIG. 3. Plot of $g(r)$ vs rk_K for $r_s=4$.

$$S(k)=\frac{\hbar k^2}{4\pi^2 e^2 n}\int_0^\infty \mathrm{Im}[\epsilon(\vec{k}, \omega)]^{-1}d\omega\,. \qquad (2.2)$$

Using the $G(k)$ values of the TM theory, the function $S(k)$ is calculated with the help of (1.1) and (2.2). From these numbers, the $g(r)$ is evaluated following (2.1) for various values of r_s. These results are shown graphically in Figs. 1–5 for $2\leq r_s\leq 6$. For the sake of comparison, we have also given the corresponding plots of $g(r)$ vs r of Singwi *et al.*[10-12] and of TW,[8] along with those of Hubbard and the random-phase approximation (RPA). It is to be noted that in the present theory $g(r)$ at $r=0$ remains positive up to $r_s\simeq 4$. It may be mentioned here that in all the earlier theories, the $g(0)$ becomes negative for $r_s>2$, except in that of Singwi, Tosi, Land, and Sjölander (STLS),[10] where the $g(0)$ is positive up to $r_s=4$. But it is

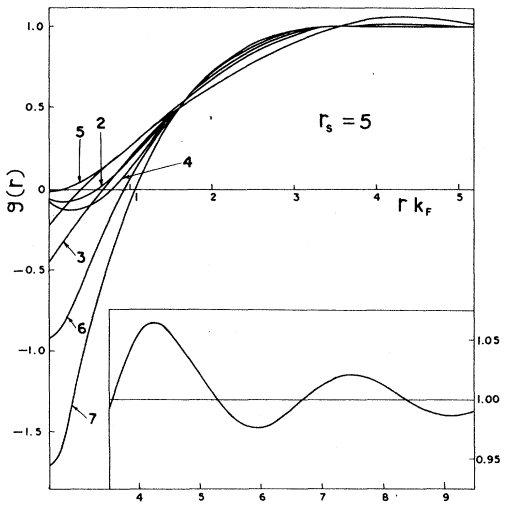

FIG. 4. Plot of $g(r)$ vs rk_F for $r_s=5$.

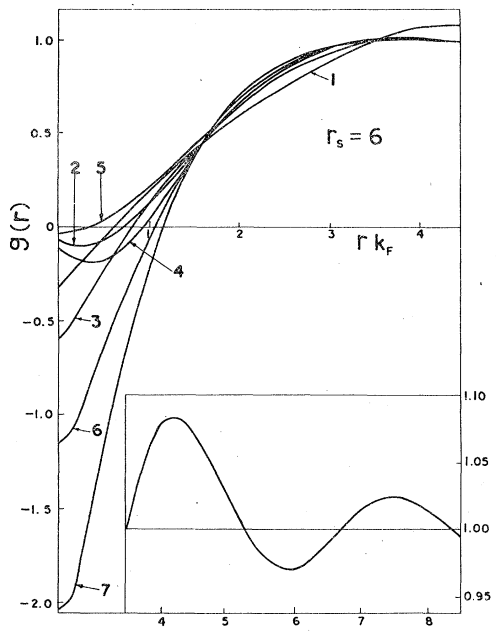

FIG. 5. Plot of $g(r)$ vs rk_F for $r_s = 6$.

known that in the STLS theory, the compressibility sum rule is badly violated. Besides, since this theory is based on an ansatz, a first-principles justification is not understood yet. In the Vashishta-Singwi (VS) theory,[12] which is a modified version of the STLS theory, though the compressibility sum rule is satisfied, the $g(0)$ turns out to be negative for $r_s > 2$. In the TW theory, which is based on a first-principles calculation, although the compressibility sum rule is satisfied, the $g(0)$ becomes negative for $r_s > 2$. Thus we see that all these theories seem to have the deficiency of simultaneously satisfying the compressibility sum rule and producing a good $g(r)$ at $r = 0$ in the range of metallic densities. This is obvious because satisfying the compressibilities sum rule only means that the small-momentum behavior of the dielectric function is good; whereas, to get a good $g(r)$, one should have the dielectric function which is to be well behaved, both in the region of small and large momenta. Using the TM theory, we have partly succeeded in overcoming the above deficiencies. This is because we have not only satisfied the compressibility sum rule, but also obtained a good $g(0)$ over a major range of metallic densities. The fact that the $g(0)$ in this case becomes negative for $r_s \geq 4$ simply means that some higher-order correlation effects are to be included in the local-field correction term $G(\vec{k}, \omega)$ of the TM theory.[1] This can be done by extending the TM theory beyond the free-particle approximation, while conserving the frequency moments to an infinite order. From the results of our $g(0)$ given in Table I, one can see that there is a consistent variation of its value in going from one r_s to the other, compared to those of other theories. For the sake of convenience, we have quoted the $g(0)$ values of the previous theories.

A very interesting feature of our $g(r)$ is that it starts to exhibit an oscillatory behavior from $r_s = 2$ and this becomes more pronounced with the increase of r_s. The values of $g(r)$ obtained by Singwi *et al.*[10] show a very small and broad peak which, even at $r_s = 6$, has a value of only 1.013. The results of Chakravarty and Woo[13] also show small peaks beyond $r_s \simeq 3.4$. The positions of the peaks in both these calculations roughly correspond to those of our first peaks and their amplitudes are much smaller than even our second peaks. The pseudopotential calculation of Dunn and Broyles[14] for $r_s \geq 5.6$ shows a peak in $g(r)$ like that of Chakravarty and Woo; even the peak positions and its heights remain almost the same in both the cases. The behavior of our $g(r)$ for the electron liquid is very similar to that observed in classical liquids, where the $g(r)$ is known to possess very pronounced narrow peaks at the average interparticle spacings, followed by many secondary peaks. The only difference in the electron liquid case is that the peak heights observed here are not so large. One can see that the position of the first peak in our $g(r)$ for a certain r_s almost coincides with the corresponding average interparticle spacings. From Figs. 1–5, it is seen that the peak heights in $g(r)$ increase with the increase of r_s. This is obvious because as one goes to low densities, the correlation among the particles becomes increasingly important. The secondary peaks observed in our $g(r)$ are relatively broadened out, as compared to the primary peaks. From this, one can conclude that like any classical liquid, the electron liquid also shows the tendency for the localization of particles. The reason why the previous theories on the electron liquid fail to show this tendency is that they all lack in accounting properly for the short-range correlation effects.

TABLE I. Values of $g(0)$ for various r_s.

r_s	2	3	4	5	6
Present theory	0.163	0.02	−0.105	−0.22	−0.327
VS	0.034	−0.04	−0.07	−0.075	−0.08
TW	0.04	−0.14	−0.31	−0.46	−0.61
SSTL (Ref. 10)	0.06	−0.02	−0.07	−0.10	−0.11
STLS (Ref. 9)	0.11	0.04	0.006	−0.02	−0.03
Hubbard	−0.16	−0.43	−0.68	−0.92	−1.14
RPA	−0.53	−0.95	−1.33	−1.70	−2.04

TABLE II. Correlation energy (Ry/electron).

r_s	1	2	3	4	5	6
Present result	−0.137	−0.103	−0.085	−0.074	−0.065	−0.059
VS	−0.112	−0.089	−0.075	−0.065	−0.058	−0.052
TW	−0.134	−0.095	−0.079	−0.068	−0.061	−0.052
SSTL	−0.124	−0.092	−0.075	−0.064	−0.056	−0.050
STLS	−0.125	−0.097	−0.080	−0.070	−0.063	−0.057
Hubbard	−0.131	−0.102	−0.086	−0.076	−0.069	−0.064
RPA	−0.157	−0.124	−0.105	−0.094	−0.085	−0.078
Nozières and Pines	−0.115	−0.094	−0.081	−0.072	−0.065	−0.060

B. Correlation energy

The expression for the total energy per particle is written as

$$E_0 = \tfrac{3}{5}\epsilon_F + \int_0^{e^2} \frac{d\lambda}{\lambda} E_{\rm int}(\lambda), \tag{2.3}$$

where λ is a parameter representing the strength of the interaction and ϵ_F is the Fermi energy. The interaction energy is given by

$$E_{\rm int}(\lambda) = -(2e^2/\pi)\bar{\gamma}(\lambda), \tag{2.4}$$

where

$$\bar{\gamma}(\lambda) = -\frac{1}{2}\int_0^{\infty} [S(k) - 1]\, dk. \tag{2.5}$$

Using (2.4) in (2.3), E_0 can be expressed in a convenient form as

$$E_0 = \frac{3}{5\alpha^2 r_s^2} - \frac{4}{\pi\alpha r_s^2}\int_0^{r_s} \bar{\gamma}(r_s')\, dr_s' \text{ Ry}. \tag{2.6}$$

Following (2.6) the correlation energy per particle is given by

$$E_{\rm corr} = \frac{0.9163}{r_s} - \frac{4}{\pi\alpha r_s^2}\int_0^{r_s} \bar{\gamma}(r_s')\, dr_s' \text{ Ry}. \tag{2.7}$$

Using our computed values of $\bar{\gamma}(r_s)$, the correlation energy has been evaluated from (2.7) and the results are given in Table II, along with those obtained by previous authors. We have given a few values of $\bar{\gamma}(r_s)$, for $r_s = 1$ to 6 in Table III. With these values of $\bar{\gamma}(r_s)$, it can be easily seen that the Ferrel condition[15] is satisfied.

TABLE III. Values of $\bar{\gamma}(r_s)$.

r_s	1	2	3	4	5	6
$\bar{\gamma}(r_s)$	0.4610	0.4978	0.5227	0.5386	0.5525	0.5640

III. CONCLUSION AND SUMMARY

In this paper, we have calculated certain properties of the electron liquid using the TM dielectric function, where the local-field correction term has been taken in the static approximation. We feel that the TM theory on which the present calculations are based has the merit of accounting for the short-range correlation effects much better than the other existing theories. This is manifest in the fact that this theory gives rise to features like the peak in $S(k)$,[7] and the oscillatory behavior in $g(r)$, which are not observed in the earlier theories. With all these properties, it is a little surprising that the TM theory does not produce a positive value for $g(0)$ for $r_s \geq 4$. This may be due to the lack of some higher-order correlation effects in the local-field correction term. However, one can not be sure of this unless one includes the dynamic dependence in $G(k)$ and looks for the new $g(0)$ values. At any rate, it will be nice to see whether the inclusion of higher-order correlation effects at all upset the trend of the present result. One of the possible ways of accounting for the higher-order correlation effects is to go beyond the free-particle approximations in the TM theory, while conserving the frequency moments. It is our feeling that when these higher-order correlation effects are included, it will result in more numbers of oscillations in $S(k)$, and thereby it will establish the similarity between the behavior of electron liquid and the classical liquid without any ambiguity. What we mean by this is that the peaks in $g(r)$ will be more pronounced, followed by many secondary peaks. We are now investigating these in detail.

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