Analytical expressions for the local-field corrections in double-layer electron systems

B. TANATAR

Department of Physics, Bilkent University, Bilkent 06533 Ankara, Turkey

We develop an extension of the sum-rule version of the Singwi, Tosi, Land, and Sjölander (STLS) scheme applied to a double-layer electron system. We present analytical expressions for the intralayer and interlayer static structure factors and corresponding local-field corrections which agree quite well with the full STLS calculations. Some applications of our basic results and further generalizations of our method are discussed.

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1. Introduction

The many-body exchange and correlation effects in homogeneous quantum electron liquids is a mature field of research and of continuing interest because of current applications. The electron system interacting via the $1/r$ Coulomb potential provides a suitable model for metals and doped semiconductors, as well as a testing ground for various many-body theories. Through the recent technological advances it is now possible to manufacture lower dimensional systems (quantum-wells and quantum-wires) with interesting experimental results, which in turn stimulate further theoretical work. The random-phase approximation [1] (RPA) has been very successful in describing the dielectric properties of the interacting electron system in the high density limit. As the density of the electron liquid is lowered, the exchange and correlation effects become increasingly important leading to many interesting physical phenomena. An approximation scheme to study the correlations in interacting electron systems is provided by Singwi *et al.* [2] (STLS) in terms of the local-field factors. The local-fields take the repulsion hole around an electron into account to describe the correlation effects. The method has been extensively applied to a number of physical problems with great success [2–4].

A sum-rule version of the STLS approximation, using the long- and short-wavelength limiting behavior of the local-field corrections, is formulated by Gold [5] for a charged Bose gas at zero temperature, and subsequently by Gold and Calmels [6, 7] for electron liquids in various dimensions. This approach largely circumvents the fully numerical solution of the original STLS scheme, by introducing analytical forms to the static structure factor and local-field correction. In this paper we present an extension of the sum-rule method [6, 7] to study the density response of a double-layer electron gas to a weak external electric field. We demonstrate that the sum-rule version yields qualitatively and quantitatively similar results as the full STLS equations, by calculating the static structure factors, local-field corrections, and pair-distribution functions.
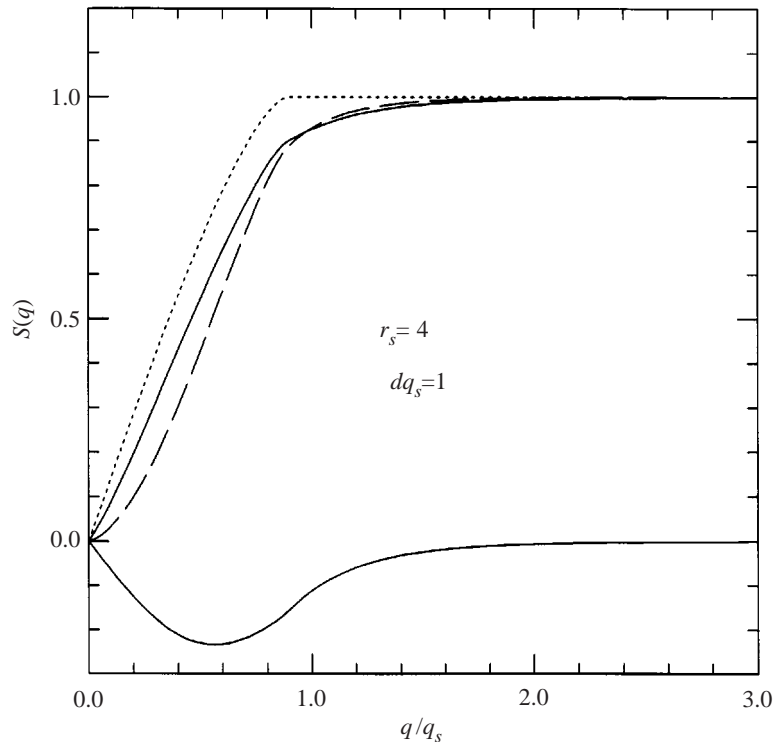
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Fig. 1. The intralayer (upper solid line) and interlayer (lower solid line) static structure factors, within the sum-rule version of the STLS approach for a double-layer electron system, at $r_s = 4$ and $dq_s = 1$. The dashed line shows $S(q)$ for a single layer at the same density (from Ref. [6], and the dotted line shows $S_0(q)$.

A double-layer electron system serves as a model for coupled quantum-well structures of recent experimental interest [8]. The effect of correlations beyond the RPA, on the ground-state of the double-layer system and superlattices has been investigated by many researchers [9, 10]. There also exists Monte Carlo simulation results for double-layer electron systems [11]. The strength of correlations are found to be significantly increased in the presence of more than one layer, because the electrons in one layer act as a polarizable background for electrons in the other one. The interlayer correlations are more pronounced as the layer separation decreases.

2. Theory and model

In the many-body description of homogeneous electron liquids, the wavevector- and frequency-dependent density response function $\chi(q, \omega)$ plays a central role, characterizing the response of the system to external longitudinal perturbations. Within the STLS approximation, the response to an external field is formulated as that of a noninteracting system responding to an effective potential, which in the equal-density double-layer electron system become $\varphi_{ij}(q) = v_{ij}(q)[1 - G_{ij}(q)]$. Here, i and j label the layers, $v_{11}(q) = 2\pi e^2/\epsilon_0 q$, and $v_{12}(q) = v_{11}(q)e^{-qd}$, denote the intralayer and interlayer Coulomb interactions, respectively. We assume that two equal density two-dimensional (2D) electron gases are kept at a parallel distance d. The densities are measured by the parameter $r_s = (\pi n a_B^2)^{-1/2}$, where a_B is the Bohr radius. The local-field factors $G_{ij}(q)$ describing the short-range correlation effects neglected by the RPA, are given in Ref. [9]. The integral
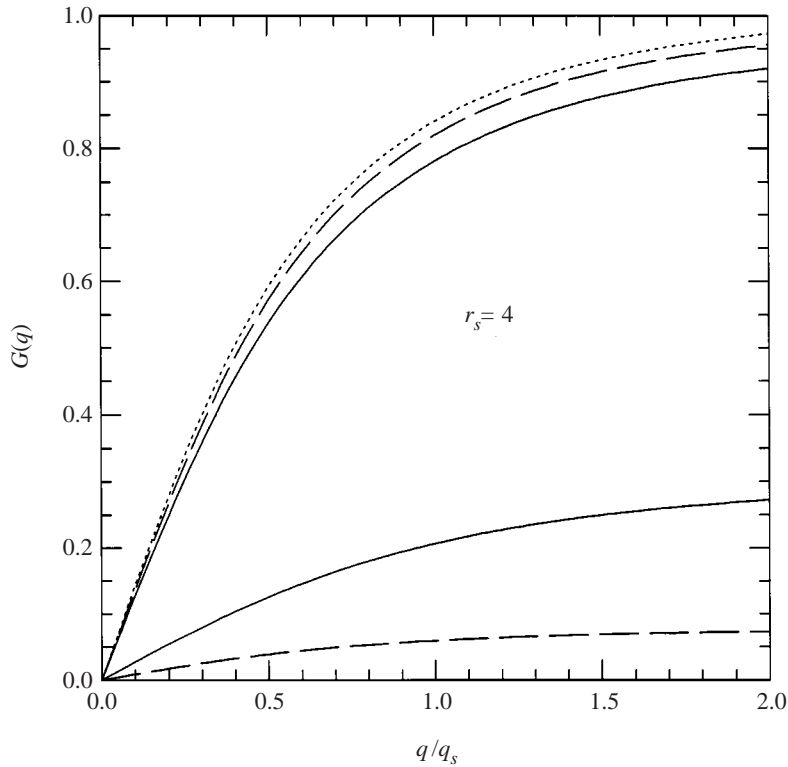
Fig. 2. The intralayer (upper curves) and interlayer (lower curves) local-field factors, for a double-layer electron system at $r_s = 4$, $dq_s = 1$ (solid lines), and $dq_s = 2$ (dashed lines). The dotted line shows $G(q)$ for a single layer from Ref. [6].

expressions for $G_{ij}(q)$ involve the static structure factors $S_{ij}(q)$, which follow from the assumption that the two-particle distribution function may be decoupled as a product of two one-particle distribution functions multiplied by the pair-correlation function [2].

The formulation of the sum-rule version of STLS scheme proceeds as follows. We replace the noninteracting response function in the response matrix [9] of the double-layer system, by the mean-spherical approximation result $\chi_0^{\mathrm{MSA}}q, \omega) = 2n\epsilon_q/[\omega^2 - (\epsilon_q/S_0(q))^2]$, where $\epsilon_q = q^2/2m$, and $S_0(q)$ is the static structure factor of the noninteracting electron gas in 2D. In χ_0^{MSA} the particle–hole pair continuum is approximated by a collective mode with energy $\epsilon_q/S_0(q)$, similar to the Feynman excitation spectrum for bosons [12]. Solving for the collective modes from the matrix expression [9] of $\chi(q, \omega)$, and identifying them with the excitation spectrum of the Feynman type, we obtain

$$S_{11,12}(q) = \frac{1}{2}\left[\frac{1}{[1/[S_0(x)]^2 + ([1-G_{11}] + e^{-x\tilde{d}}[1-G_{12}])/x^3]^{1/2}} \right.$$
$$\left. \pm \frac{1}{[1/[S_0(x)]^2 + ([1-G_{11}] - e^{-x\tilde{d}}[1-G_{12}])/x^3]^{1/2}} \right], \qquad (1)$$

where $x = q/q_s$, $q_s = 2/(r_s^{2/3}a_B)$ being the screening wavenumber [6] and $\tilde{d} = dq_s$. The above equations provide closed-form expressions for the static structure factors in terms of the local-field corrections. They are the generalization of the results of Gold [5] and Calmels [6] to double-layer electron systems, and may

be regarded as generalized MSA expressions using the terminology of Iwamoto *et al.* [12]. In the sum-rule version of the STLS scheme as introduced by Gold [5] and Gold and Calmels [6, 7] the long- and short-wavelength limits of the local-field factors $G_{ij}(q)$ are taken to simplify the full integral expressions, and the following parametric representations are assumed

$$G_{11}(x) = \frac{C_1(r_s, d)x}{[[C_2(r_s, d)]^2 + x^2]^{1/2}}, \quad \text{and} \quad G_{12}(x) = \frac{D_1(r_s, d)x}{[[D_2(r_s, d)]^2 + x^2]^{1/2}}. \tag{2}$$

The above forms of G_{ij} are motivated by similar expressions within the Hubbard approximation which is a simplified attempt to go beyond the RPA, taking only the exchange effects into account by considering the Pauli hole around each electron. The coefficients $C_i(r_s, d)$ and $D_i(r_s, d)$ are now determined by the nonlinear equations

$$\frac{C_1(r_s, d)}{C_2(r_s, d)} = r_s^{2/3} \int_0^\infty dx [1 - S_{11}(x)], \tag{3}$$

$$C_1(r_s, d) = 2r_s^{2/3} \int_0^\infty dx\, x [1 - S_{11}(x)], \tag{4}$$

$$\frac{D_1(r_s)}{D_2(r_s)} = -r_s^{2/3} \int_0^\infty dx\, S_{12}(x) e^{-x\tilde{d}}, \tag{5}$$

$$D_1(r_s) = -2r_s^{2/3} \int_0^\infty dx\, x\, S_{12}(x) e^{-x\tilde{d}}. \tag{6}$$

3. Results

We solve the self-consistent equations set out above to obtain the r_s- and d-dependent parameters. These coupled integral equations are much easier to solve than the full STLS equations as noted by Gold and Calmels [6, 7] who investigated the density response of single component electron liquids. We summarize our results in Table 1, for the coefficients $C_i(r_s, d)$ and $D_i(r_s, d)$, tabulating them for various r_s and d values. Once the r_s-dependent coefficients in the parametrized model of the local-field factors $G_{ij}(q)$ are determined, we can investigate various physical quantities of interest. The intralayer and interlayer static structure factors are depicted in Fig. 1. For a double-layer electron system, $S_{12}(q)$ is negative, and becomes nearly zero for $q/q_s > 2$. Also shown in the figure is the static factor of a single layer calculated within the same model [6]. We observe that the intralayer structure factor $S_{11}(q)$ is close to the single layer result [6]. Figure 2 shows the local-field corrections at $r_s = 4$, $dq_s = 1$ and $dq_s = 2$. We find that the interlayer local-field factor $G_{12}(q)$ is affected more than the intralayer local-field factor $G_{11}(q)$ when the layer separation d is decreased. These results are in rather good qualitative and quantitative agreement with the full STLS calculations of Liu *et al.* [9]. A closer inspection of $G_{12}(q)$ of Liu *et al.* [9] shows a slower increase with q before more rapid growth and leveling off. On the other hand, the analytic form assumed for $G_{12}(q)$ [cf. eqn (2)] follows from the small and large q expansions of the full STLS local-field expression. We believe that a closer look at the numerical calculation of the local-fields is necessary to reconcile the apparent differences. In any case, such discrepancies should be of minor importance in the calculation of other physical quantities which use the local-field factors as input. As a further test of the predictions of our sum-rule calculations, we turn to the pair distribution function. The pair distribution functions $g_{ij}(r)$ give the probability of finding an electron at a distance r in layer i when there is another electron at the origin in layer j. From the knowledge of $S_{ij}(q)$, we obtain $g_{ij}(r)$ by the Fourier transform

$$g_{ij}(r) = 1 + \frac{1}{n} \int \frac{d^2q}{(2\pi)^2} e^{i\boldsymbol{q}\cdot\boldsymbol{r}} [S_{ij}(q) - \delta_{ij}]. \tag{7}$$

Table 1: The parameters $C_i(r_s)$ and $D_i(r_s)$ ($i = 1, 2$) for the local-field corrections in a double-layer electron gas various values of r_s and d.

r_s	$C_1(r_s, d)$	$C_2(r_s, d)$	$D_1(r_s, d)$	$D_2(r_s, d)$
$d = a_B$ and $L = a_B$				
0.5	0.621591	1.56553	0.00186182	0.584962
1	0.748785	1.22093	0.0152008	0.876296
1.5	0.831497	1.08069	0.0481206	1.03937
2	0.881013	0.992698	0.101763	1.12466
2.5	0.909966	0.930316	0.172447	1.16501
3	0.927368	0.883047	0.254116	1.17979
4	0.948396	0.817942	0.426518	1.17171
5	0.965889	0.775890	0.584717	1.14269
6	0.980215	0.740654	0.716929	1.10712
7	0.994355	0.712191	0.822103	1.06912
8	1.00719	0.688625	0.903696	1.02813
9	1.01816	0.667151	0.966262	0.988152
10	1.02752	0.647799	1.01366	0.949189
$d = 2a_B$ and $L = a_B$				
0.5	0.622291	1.56162	0.000217664	1.47769
1	0.754038	1.21673	0.00194289	0.516871
1.5	0.846002	1.07533	0.00719900	0.669911
2	0.907310	0.985283	0.0181665	0.786725
2.5	0.947411	0.918889	0.0365974	0.871395
3	0.972995	0.867250	0.0635110	0.937680
4	0.997518	0.791471	0.142625	0.993342
5	1.00487	0.741645	0.248281	1.01344
6	1.00701	0.706462	0.366487	1.01233
7	1.00924	0.679739	0.484160	1.00263
8	1.01317	0.658767	0.593076	0.987118
9	1.01719	0.638231	0.690698	0.971461
10	1.02223	0.620713	0.775608	0.951821
$d = 5a_B$ and $L = a_B$				
0.5	0.622406	1.56172	0.0000107515	1.49134
1	0.754806	1.21450	0.0000928279	1.46907
1.5	0.848554	1.07069	0.000341877	0.296732
2	0.913911	0.981631	0.000888797	1.40333
2.5	0.958626	0.909151	0.00190822	0.430985
3	0.990905	0.853883	0.00361414	0.491409
4	1.03119	0.769561	0.0101083	0.597764
5	1.05237	0.707758	0.0225303	0.680708
6	1.06265	0.661073	0.0429485	0.741550
7	1.06618	0.625045	0.0729224	0.783482
8	1.06550	0.597239	0.113198	0.810440
9	1.06237	0.575725	0.163429	0.826454
10	1.05802	0.558751	0.222248	0.833228

Table 1: Continued.

r_s	$C_1(r_s, d)$	$C_2(r_s, d)$	$D_1(r_s, d)$	$D_2(r_s, d)$
		$d = 2a_B$ and $L = 2a_B$		
0.5	0.587470	1.84907	0.000262017	0.495051
1	0.707167	1.33940	0.00227857	0.501375
1.5	0.803033	1.15793	0.00822629	0.661812
2	0.871885	1.05106	0.0202842	0.771731
2.5	0.918895	0.974781	0.0401009	0.854859
3	0.949693	0.915842	0.0685457	0.912081
4	0.980471	0.830231	0.150673	0.974985
5	0.991135	0.773722	0.258286	0.996672
6	0.995839	0.734077	0.376931	0.998001
7	1.00036	0.704045	0.493970	0.990037
8	1.00589	0.679157	0.602036	0.978415
9	1.01256	0.658703	0.698075	0.961127
10	1.01944	0.640130	0.781285	0.942455
		$d = 5a_B$ and $L = 2a_B$		
0.5	0.587615	1.84720	0.0000116567	0.499155
1	0.708336	1.33592	0.0000996819	0.496422
1.5	0.806931	1.15284	0.000364082	0.494446
2	0.880701	1.04413	0.000940237	0.367053
2.5	0.934822	0.965692	0.00200530	0.43118
3	0.974452	0.903950	0.00377800	0.491241
4	1.02488	0.810468	0.0104795	0.596023
5	1.05161	0.742091	0.0232253	0.677828
6	1.06460	0.690283	0.0440879	0.738020
7	1.06920	0.650391	0.0746194	0.779851
8	1.06878	0.619551	0.115448	0.807286
9	1.06529	0.595538	0.166302	0.822359
10	1.06051	0.576972	0.225571	0.829565

We show in Fig. 3 the pair correlation functions $g_{11}(r)$ and $g_{12}(r)$ for two electron layers of density $r_s = 4$. Layer spacings of $d = 2a_B$, $3a_B$, and $5a_B$, are denoted by solid, dashed, and dotted lines, respectively. For $d = 5a_B$, $g_{12}(r)$ is close to unity indicating that interlayer correlations are weak. In this case, the double-layer system acts as two isolated planes. As the separation distance is decreased, interlayer correlations start to build up, and a dip in $g_{12}(r)$ around the origin develops. On the other hand, the gradual increase in the interlayer correlations has very little effect on the intralayer pair distribution function $g_{11}(r)$. Our results for $g_{11}(r)$ and $g_{12}(r)$ are in very good agreement with the full STLS calculations performed by Liu *et al.* [9] on the same system.

4. Discussion

In this work we have solved the self-consistent equations for $S_{ij}(q)$ and $G_{ij}(q)$ for a double-layer electron system, within the sum-rule version of the STLS scheme. The STLS approximation provides a reasonable improvement over the RPA for small densities. Despite the fact that the pair-correlation function becomes
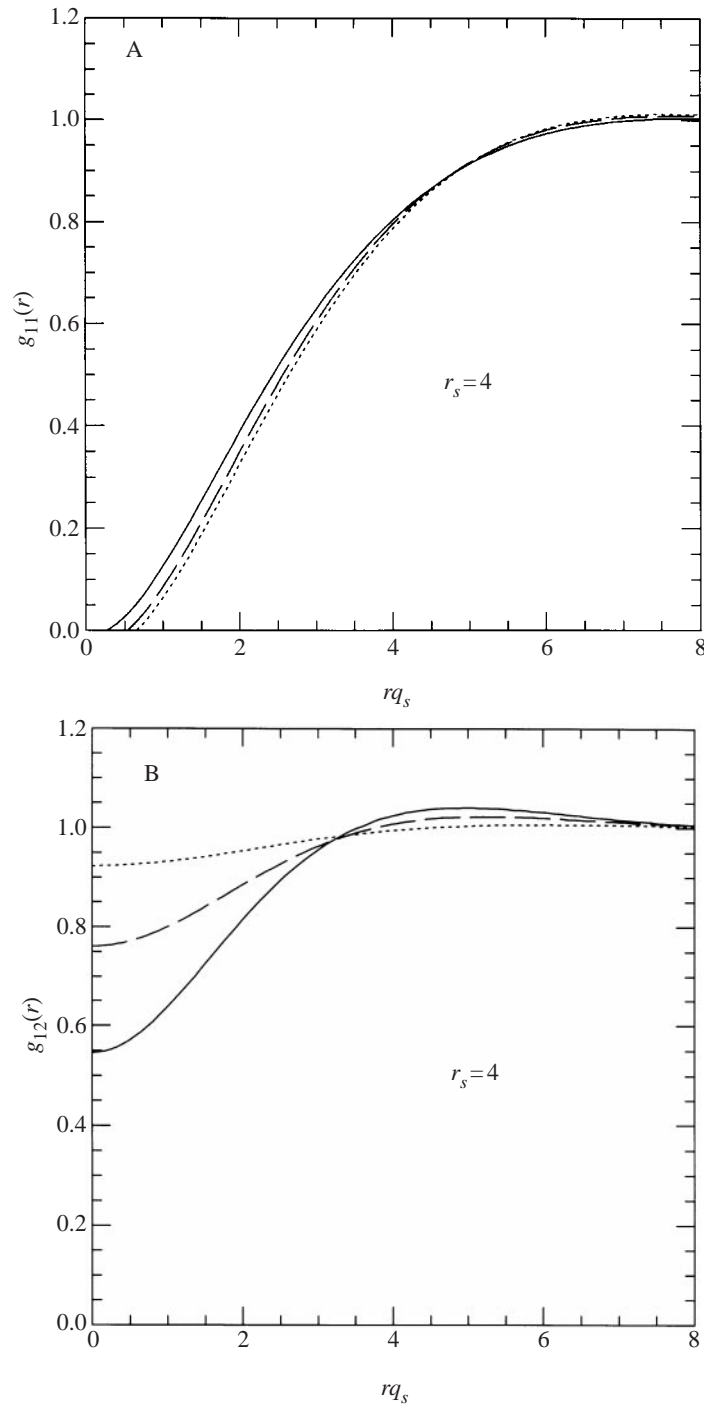
Fig. 3. The pair-distribution functions A, $g_{\uparrow\uparrow}(r)$, and B, $g_{\uparrow\downarrow}(r)$ in a double-layer electron system, at $r_s = 4$, $d = 2a_B$ (solid lines), $d = 3a_B$ (dashed lines), and $d = 5a_B$ (dotted lines).

negative for small values of r with increasing r_s, it has been found that the STLS ground-state energies are in good agreement with the Monte Carlo simulation results [11, 13] in the range $1 < r_s < 20$. The sum-rule version of the STLS approach as developed by Gold and Calmels [5–7] has the facility of reproducing most of the full STLS results with analytical expressions for the static structure factor and local-field correction. As discussed by Gold and Calmels [6], the sum-rule version works quite well, because it satisfactorily describes the transition between exchange (important for small r_s) and correlation (operative for large r_s) effects, through the model static structure factors. We have obtained a generalization of the sum-rule version of the STLS method, based on the boson-like excitation spectrum [12]. Our results compare favorably with the full STLS calculations, and thus justify our approximations and method.

These analytical approximations to the local-field factors in double-layer electron systems, provide a simple alternative to the computationally more demanding full solution of the STLS equations. A number of physically interesting situations where the correlation effects are important, such as the ground-state energy at low density, charge-density wave-induced instabilities [14], and interlayer momentum transfer phenomenon [15] can be investigated. Recently, Dong and Lei [16] utilized a similar approach to calculate the interlayer local field correlations in weakly coupled electron–electron and electron–hole layers and studied the Coulomb drag effect. It should even be possible to study the Wigner crystallization in double-layer systems using our results as input to density-functional theories [17]. Our approach lends itself to further generalizations to cover other situations as well. It should be straightforward to study double-layer electron–hole systems [9]. The finite quantum-well width effects can easily be incorporated using appropriate form factors [18] to the bare Coulomb interactions. Correlations in double-wire electron and electron–hole systems can also be investigated. We believe that our results can be used as input in more complex calculations and further applications.

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