Finite-temperature electron correlations in the framework of a dynamic local-field correction

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The quantum-mechanical version of the Singwi-Tosi-Land-Sjölander (STLS) approximation is applied to finite temperatures. This approximation has two main advantages. First, it includes a dynamic local-field correction and second, it gives positive values for the pair-distribution function in the short-range region at zero temperature. This is even valid for rather low densities. After a description of the numerical difficulties arising with the use of a dynamic approximation, the results for the static-structure factor and the pair-distribution function are discussed thoroughly. Detailed work is performed on the static part of the local-field correction, with special emphasis put on the investigation of its structure. A peak is found at a wave vector $q \approx 2.8$ (in units of the Fermi wave vector) for small temperatures, which tends towards higher values of q with increasing temperature. This peak causes an attractive particle-hole interaction in a certain q region and thus gives rise to the appearance of a charge-density wave. A parametric description is given for the static local-field correction in order to simplify further applications. Furthermore, the exchange-and-correlation free energy is considered. The results are compared with the STLS results and with the modified convolution approach.

I. INTRODUCTION

In the course of the past decades the model of the electron gas has been shown to be a good description of interacting electron systems for many applications. Among the most prominent examples are the conduction electrons in metals,[1] which recently attracted renewed experimental interest,[2] liquid metals,[3] and plasmas in astrophysical situations.[1,3]

Whereas countless investigations have been performed for zero or infinitely high temperatures, little is known about the finite-temperature Fermi gas. The random-phase approximation (RPA) (Ref. 4) has been thoroughly studied by Gupta and Rajagopal. They calculated the exchange-and-correlation potential (defined as the functional derivative of the free energy[4,5]) for the Hartree-Fock (HF) case and from a summation of ring diagrams.[6] Panat and Amritkar[7] have further simplified this approach in the spirit of a temperature-dependent Thomas Fermi theory. Additional detailed investigations of the HF and RPA properties as a function of temperature have been performed by Dharma-wardana and Taylor.[8] They obtained fitting formulas for both the exchange and the ring contribution to the free energy as functions of the temperature and the density of the system.

Many improvements on the RPA have been suggested for the ground state,[1] specifically by including static local-field corrections (LFC's). It was the merit of Tanaka and Ichimaru[9] and of Dandrea, Ashcroft, and Carlsson[10] to extend this formalism to finite temperatures. Apart from studying the Singwi-Tosi-Land-Sjölander (STLS) approximation,[11] Tanaka and Ichimaru[9] performed extensive investigations in the so-called "modified convolution approach" (MCA).[12] For this latter theory they also fitted the free energy in the density-temperature plane, although with a somewhat different form than Perrot and Dharma-wardana.[5] Additionally, the spin-dependent quantities were investigated in detail and the phase diagram was constructed.[12]

To the best of our knowledge, however, no attempt has been made to include dynamic effects into the local-field correction G at finite temperatures. At zero temperature the importance of the frequency dependence of G has been demonstrated by a number of authors.[13–20] In general it can be stated that many of the dynamic approximations show a pronounced peak structure, while most of the static ones do not. It thus appears of interest to investigate a local-field correction which accounts for this possibility and simultaneously yields favorable results for the static properties of the system. Such an approximation is the fully quantum-mechanical version[18] of the STLS, the investigation of which is the main purpose of this work.

The homogeneous three-dimensional electron gas is characterized by two parameters, the temperature T and the density n, conveniently replaced by

$$\theta = k_B T/\varepsilon_F \quad \text{(degeneracy parameter)}, \tag{1}$$

$$n = \frac{3}{4\pi}(a_B r_s)^{-3} \quad \text{(density parameter)}. \tag{2}$$

Here a_B is the Bohr radius and ε_F denotes the Fermi energy. The electron gas retains its fundamentally quantum nature over a substantial temperature range. The description of a classical one-component plasma[1,3] can be used for $\theta \gg 1$ only. In the region of $\theta \approx 0.5 \ldots 10$ both the quantum and the temperature effects have been demonstrated to be of considerable importance.[21]

This work is organized as follows. Section II gives a short description of the finite T formalism with the special emphasis lying on the new dynamic LFC. In Sec. III the static-structure factor $S(q,\theta)$ and the pair-distribution function $g(r,\theta)$ are discussed. Section IV deals with the static part of the local-field correction and

the possibility of a charge-density wave. The temperature dependence of the exchange-and-correlation energy is given in Sec. V. The results are compared with those of the usual STLS which are known to give results close to the Monte Carlo energies[22] at low temperatures. The comparison is also done in the high-temperature region. Finally, the results are discussed in Sec. VI.

In this work dimensionless quantities will be used. Specifically, all wave vectors are measured in $k_F=(3\pi^2 n)^{1/3}$ and the response function Φ includes a factor $(-2\varepsilon_F/3n)$.

II. FORMALISM

The static pair correlations of the finite-temperature system are conveniently obtained via the fluctuation-dissipation theorem[9,23] from a sum of the dynamical response function $\Phi(q,\omega)$ over its Matsubara frequencies z_γ,

$$S(q,\theta)=\frac{3\hbar}{4\pi\varepsilon_F}\int_{-\infty}^{\infty}d\omega\coth\left[\frac{\hbar\omega}{2k_BT}\right]\mathrm{Im}\Phi(q,\omega)$$
$$=\tfrac{3}{2}\theta\sum_{\gamma=-\infty}^{\infty}\Phi(q,z_\gamma)\,,\quad z_\gamma=2i\pi\gamma k_BT/\hbar \tag{3}$$

(where ω is the frequency and $\gamma=0,\pm1,\pm2,\ldots$). In the metallic density range the so-called "generalized mean-field approaches" have proved successful for the response function[1,24]

$$\Phi(q,\gamma,\theta)=\frac{\Phi^0(q,\gamma,\theta)}{1+[1-G(q,\gamma,\theta)]v(q)\Phi^0(q,\gamma,\theta)} \tag{4}$$

This is an exact expression defining the LFC $G(q,\gamma,\theta)$. In the units used here the Coulomb potential is given by $v(q)=4r_s\alpha/\pi q^2$ [with $\alpha=(4/9\pi)^{1/3}$]. The free response function has to be calculated numerically from[9]

$$\Phi^0(q,\gamma,\theta)=\frac{1}{2q}\int_0^\infty dp\,pn^0(p,\theta)$$
$$\times\ln\left|\frac{(2pq+q^2)^2+(2\pi\gamma\theta)^2}{(2pq-q^2)^2+(2\pi\gamma\theta)^2}\right|\,. \tag{5}$$

This expression is obtained from Lindhard's formula[25] by replacing each step function with the momentum distribution of free particles at finite θ, namely,

$$n^0(p,\theta)=[\exp(p^2/\theta-\tilde{\mu})+1]^{-1}\,. \tag{6}$$

The quantity $\tilde{\mu}\equiv\mu/k_BT$ denotes the reduced chemical potential of a noninteracting system and is obtained from the normalization condition

$$\frac{4\pi}{3}=\int d^3p\,n^0(p,\theta)\,. \tag{7}$$

Concerning the choice of the dynamic local-field correction we propose the use of the so-called "quantum STLS" (QSTLS) or "Hasegawa-Shimizu" approach[18,19] for the following reasons. First of all, it is the obvious generalization of the static STLS and it is thus most suitable for comparison. It also has the advantage of yielding reasonable results[18,19] throughout the metallic density range at $\theta=0$, where its pair correlations remain positive to at least the value of $r_s=10$ (this is in contrast to most other self-consistent theories). In addition, $G(q,\gamma=0,0)$ shows a distinct peak structure leading to the possibility of a charge-density wave. For that reason the temperature-dependent behavior of the peak appears to be an interesting question.

In the QSTLS approximation the dynamic local-field correction is given by (for a short recapitulation of the derivation cf. Appendix)

$$I(q,\gamma,\theta)\equiv v(q)G(q,\gamma,\theta)\Phi^0(q,\gamma,\theta)$$
$$=-\frac{1}{N}\sum_{q'}\Phi^0(\mathbf{q},\mathbf{q}',\gamma,\theta)v(q')[S(\mathbf{q}'-\mathbf{q},\theta)-1]\,, \tag{8}$$

where the generalized Lindhard function is defined as

$$\Phi^0(\mathbf{q},\mathbf{k},\gamma,\theta)=-\frac{2\varepsilon_F}{3N}\sum_p\frac{\mathbf{n}^0(\mathbf{p}-\mathbf{k}/2,\theta)-n^0(\mathbf{p}+\mathbf{k}/2,\theta)}{z_\gamma-\varepsilon(\mathbf{p}+\mathbf{q}/2)+\varepsilon(\mathbf{p}-\mathbf{q}/2)}\,. \tag{9}$$

This quantity can be further evaluated with the result

$$\Phi^0(\mathbf{q},\mathbf{k},\gamma,\theta)=\Phi^0(q,\mathbf{q}\cdot\mathbf{k},\gamma,\theta)$$
$$=\frac{1}{2q}\int_0^\infty dp\,pn^0(p,\theta)$$
$$\times\ln\left|\frac{(2pq+\mathbf{k}\cdot\mathbf{q})^2+(2\pi\gamma\theta)^2}{(2pq-\mathbf{k}\cdot\mathbf{q})^2+(2\pi\gamma\theta)^2}\right|\,. \tag{10}$$

As in the case of $\Phi^0(q,\gamma,\theta)$ it is convenient[9] to perform an additional partial integration for the case of zero frequency in order to remove the singularity of the logarithmic term,

$$\Phi^0(q,\mathbf{q}\cdot\mathbf{k},0,\theta)=\frac{1}{\theta q}\int_0^\infty dp\,p\left\{\left[p^2-\left[\frac{\mathbf{k}\cdot\mathbf{q}}{2q}\right]^2\right]\ln\left|\frac{2pq+\mathbf{k}\cdot\mathbf{q}}{2pq-\mathbf{k}\cdot\mathbf{q}}\right|+p\frac{\mathbf{k}\cdot\mathbf{q}}{q}\right\}\frac{\exp(p^2/\theta-\tilde{\mu})}{[\exp(p^2/\theta-\tilde{\mu})+1]^2}\,. \tag{11}$$

with the help of these expressions the angular integration in Eq. (8) leads to the following result for the dynamic local-field factor in the QSTLS:

$$I(q,\gamma,\theta)/v(q)=-\tfrac{3}{8}\int_0^\infty dk[S(k,\theta)-1]\int_0^\infty dp\,pn^0(p,\theta)\int_{q^2-kq}^{q^2+kq}dt\frac{1}{2t+q^2-k^2}\ln\left|\frac{(2pq+t)^2+(2\pi\gamma\theta)^2}{(2pq-t)^2+(2\pi\gamma\theta)^2}\right| \tag{12}$$

[the result for $\gamma=0$ takes an analogous form corresponding to Eq. (11)]. In the region of small wave vectors one can

further show that

$$G(q\to 0,\gamma,\theta)=-\frac{3q^2}{4\Phi^0(0,\gamma,\theta)}\int_0^\infty dk[S(k,\theta)-1]\int_0^\infty dp\, n^0(p,\theta)\frac{p}{k}\left\{\ln\left|\frac{(2p+k)^2-z_\gamma^2/q^2}{(2p-k)^2-z_\gamma^2/q^2}\right|\right.$$
$$\left.-2\int_0^1 d\xi\,\xi\ln\left|\frac{(2p+k\xi)^2-z_\gamma^2/q^2}{(2p-k\xi)^2-z_\gamma^2/q^2}\right|\right\}. \quad (13)$$

For nonvanishing Matsubara frequencies this leads immediately to

$$G(q\to 0,\gamma\neq 0,\theta)=-\frac{q^2}{2}\int_0^\infty dk[S(k,\theta)-1]=q^2\pi\alpha r_s f^{\rm int}/4\ , \quad (14)$$

where $f^{\rm int}$ denotes the interaction energy in rydbergs per electron. In the case of $\gamma=0$ Eq. (13) results in

$$G(q\to 0,0,\theta)=\frac{6q^2}{\Phi^0(0,0)}\int_0^\infty dk[S(k,\theta)-1]\int_0^\infty dp\, n^0(p,\theta)\left[\frac{p^2}{k^2}-\frac{p^3}{k^3}\ln\left|\frac{2p+k}{2p-k}\right|\right]. \quad (15)$$

At $\theta=0$ this expression reduces to a result reported by Holas and Rahman.[19]

III. STATIC CORRELATION FUNCTIONS

In the calculation of the static-structure factor the unperturbed quantity is conveniently extracted from the frequency summation

$$S(q,\theta)=S^0(q,\theta)-\frac{3\theta}{2}v(q)\sum_{\gamma=-\infty}^{\infty}\frac{[1-G(q,\gamma,\theta)]\Phi^0(q,\gamma,\theta)^2}{1+[1-G(q,\gamma,\theta)]v(q)\Phi^0(q,\gamma,\theta)}\ . \quad (16)$$

The finite-temperature free structure factor is given by

$$S^0(q,\theta)=1+\frac{3\theta}{2q}\int_0^\infty dp\, n^0(p,\theta)\ln\left|\frac{1-\exp[-(q^2+2pq)/\theta^2]}{1-\exp[-(q^2-2pq)/\theta^2]}\right|. \quad (17)$$

It already has been pointed out by Tanaka and Ichimaru[9] that the sum in Eq. (16) is not rapidly convergent. For numerical computations it is thus necessary to split off the asymptotic form of $\Phi^0(q,\gamma,\theta)$, namely,

$$\Phi^0_\infty(q,\gamma,\theta)\equiv\frac{4}{3}\frac{q^2}{q^4-z_\gamma^2}\quad (q \text{ or } \gamma\to\infty)\ . \quad (18)$$

The final expression for $S(q,\theta)$ then reads

$$S(q,\theta)=S^0(q,\theta)-\frac{3\theta}{2}v(q)\sum_{\gamma=-\infty}^{\infty}[1-G(q,\gamma,\theta)]\left[\frac{[\Phi^0(q,\gamma,\theta)]^2}{1+[1-G(q,\gamma,\theta)]v(q)\Phi^0(q,\gamma,\theta)}-[\Phi^0_\infty(q,\gamma,\theta)]^2\right]$$
$$-\frac{v(q)}{3\theta}[1-G(q,\infty,\theta)]\left[\frac{1}{\sinh^2(q^2/2\theta)}+\frac{2\theta}{q^2}\coth\frac{q^2}{2\theta}\right]$$
$$-\frac{3\theta}{2}v(q)\sum_{\gamma=-\infty}^{\infty}[G(q,\infty,\theta)-G(q,\gamma,\theta)][\Phi^0_\infty(q,\gamma,\theta)]^2\ . \quad (19)$$

The second term vanishes for large q,γ with q^{-6},γ^{-6}. It is noteworthy that in contrast to static local-field corrected theories,[9] Eq. (19) contains an additional γ sum given by the last term of this equation. This is caused by the frequency dependence of $G(q,\gamma,\theta)$. Figure 1 demonstrates that $G(q,\gamma,\theta)$ varies rather weakly with γ and quickly reaches its limit $G(q,\infty,\theta)$. Therefore Eq. (19) can be evaluated by using a suitable cutoff parameter $\vartheta(r_s,q,\theta)$ in the fourth term. The number of γ's which have to be considered decreases with increasing temperature. This is consistent with the mainly classical behavior of the system in the high-temperature limit, where only the static contribution survives.

The static-structure factor obtained this way from Eq. (19) is plotted in Fig. 2. A Fourier transformation leads from $S(q,\theta)$ to the pair-distribution function $g(r,\theta)$:

$$g(r,\theta)=1+\frac{3}{2r}\int_0^\infty dq\,\sin(qr)[S(q,\theta)-1]\ . \quad (20)$$

$g(r,\theta)$ is depicted in Fig. 3 for several combinations of r_s and θ.

With increasing r_s the pair-distribution function takes negative (and thus unphysical) values for small r, a deficiency inherent in self-consistent approaches[1] relating $S(q,\theta)$ and $G(q,\omega,\theta)$. The validity range of these approximations is determined by the smallest positive

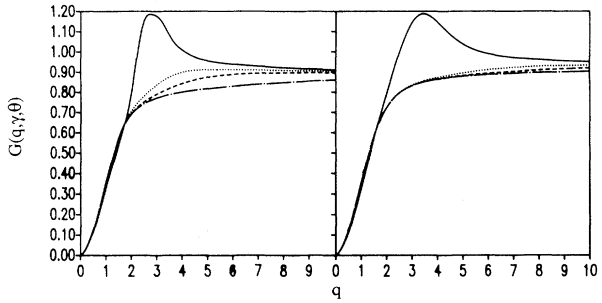

FIG. 1. Dynamic local-field correction $G(q,\gamma,\theta)$ as a function of q at $r_s=2$ for several Matsubara frequencies z. The convergence of increasing γ together with the faster convergence with increasing temperature is demonstrated. Solid line, $\gamma=0$; dotted line, $\gamma=10$; dashed line, $\gamma=20$; dash-dotted line, $\gamma=\infty$; left figure, $\theta=0.1$; right figure, $\theta=0.5$.

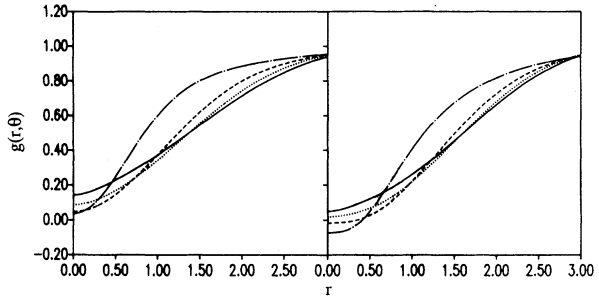

FIG. 3. Pair-distribution function $g(r,\theta)$ as a function of r for several θ's. Solid line, $\theta=0.1$; dotted line, $\theta=0.5$; dashed line, $\theta=1$; dash-dotted line, $\theta=3$; left figure, $r_s=2$; right figure, $r_s=5$.

$g(r=0,\theta)$. As it is shown in Ref. 21 this minimum is found at a finite temperature and not at $\theta=0$.

In the QSTLS the two-particle dynamics is taken into account via the momentum dependence of the Wigner functions, as manifested in the generalized Φ^0. This improves significantly the short-range pair correlations compared to the standard STLS. Thus for most practical purposes the QSTLS can be considered of sufficient quality.

IV. STATIC LOCAL FIELD $G(q,0,\theta)$

A. Peak structure and charge-density wave (CDW)

In contrast to static LFC's like STLS (Ref. 11) and MCA (Ref. 12) G^{QSTLS} shows an interesting peak structure, even for small r_s. This peak possessing a magnitude ≥ 1 is found[19] at $q\approx 2,8$ at $\theta=0$. For $\theta<0.04$ our static LFC does not change within the accuracy of our calculations and agrees with the result reported by Holas and Rahman in Ref. 19. For higher θ the position of the peak tends towards larger q values with increasing temperature. Furthermore, the width of the peak increases while its magnitude decreases slightly with θ. This is clearly shown in Fig. 4. The variation of this structure with q and θ for low densities is illustrated best in a three-dimensional plot (Fig. 5).

One of the most important consequences of this peak is the possibility of a CDW. Such an instability of the electron liquid occurs when the static response function diverges[26] because in this case electrons can be excited by an infinitesimally small external field. We therefore look for a solution of

$$1+[1-G(q,0,\theta;r_s)]r_s\frac{4\alpha}{\pi q^2}\Phi^0(q,0,\theta)=0\ . \tag{21}$$

In the q region, where a CDW is expected, $G(q,0,\theta)$ varies rather weakly with r_s, provided the coupling strength is sufficiently large. The density dependence of Eq. (21) is therefore mainly governed by the explicit appearance of r_s. We thus follow the suggestion of Ref. 19 in neglecting the r_s dependence of G beyond a certain r_s value. We found that the use of $r_s=20$ yields reliable results for $\theta\leq 1$. Equation (21) is therefore rewritten as

$$r_s=\left[[G(q,0,\theta;r_s=20)-1]\frac{4\alpha}{\pi q^2}\Phi^0(q,0,\theta)\right]^{-1}\ . \tag{22}$$

For high temperatures correspondingly higher r_s have to be chosen. It is obvious from Eq. (22) that a CDW can only occur for $G(q,0,\theta)\geq 1$. The lowest r_s value for which Eq. (22) has a solution and the corresponding q value q_{CDW} is presented in Table I for several tempera-

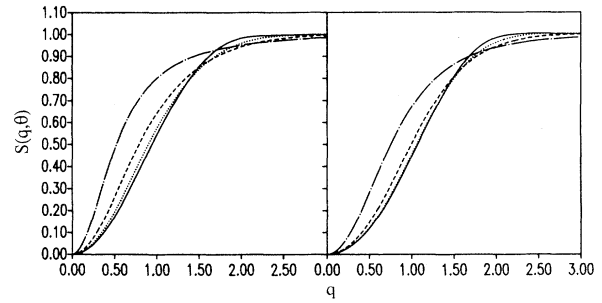

FIG. 2. Static-structure factor $S(q,\theta)$ as a function of q for several θ's. Solid line, $\theta=0.1$; dotted line, $\theta=0.5$; dashed line, $\theta=1$; dash-dotted line, $\theta=3$; left figure, $r_s=2$; right figure, $r_s=5$.

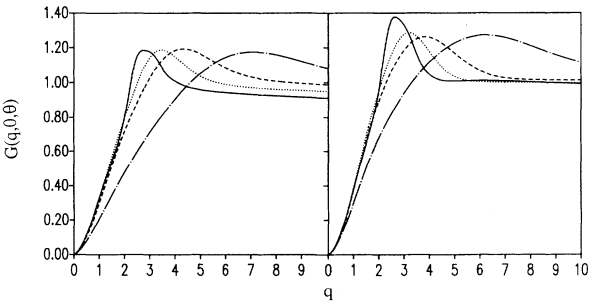

FIG. 4. Static local-field correction $G(q,0,\theta)$ as a function of q for several θ's. Solid line, $\theta=0.1$; dotted line, $\theta=0.5$; dashed line, $\theta=1$; dash-dotted line, $\theta=3$; left figure, $r_s=2$; right figure, $r_s=5$.

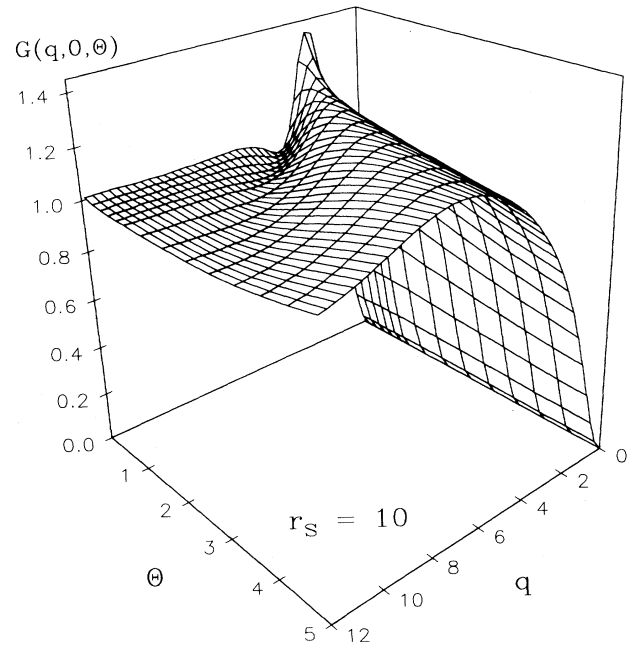

FIG. 5. Static local-field correction $G(q,0,\theta)$ as a function of q and θ for $r_s=10$.

tures (the $\theta=0$ result is taken from Holas and Rahman[19]). Furthermore, the coupling parameter $\Gamma=2\alpha^2 r_s/\theta$ is given.

Discussion

If the temperature is fixed q_{CDW} becomes larger for higher r_s. For increasing temperature the critical r_s tends towards higher values. This effect can be compared with the fact that for $\theta\rightarrow\infty$ the system behaves mainly classically in the q region considered.[21] By construction, the static part of the QSTLS LFC must tend towards the STLS results, which are always smaller than one and therefore yield no CDW. So the solution of Eq. (22) has to vanish in QSTLS for $\theta\rightarrow\infty$. This argument also explains why the magnitude of the peak decreases with increasing θ. In contrast to the r_s value and to the peak position the value q_{CDW} is almost independent of the temperature. Moreover it is seen from Table I that the influence of the temperature on the critical r_s is important even for small θ's.

TABLE I. Smallest r_s value for a charge-density wave and corresponding q position for several temperatures [$\Gamma=2\alpha^2 r_S/\theta$, $\alpha=(4/9\pi)^{1/3}$].

θ	r_s	Γ	q
0.0	60	∞	2.3
0.1	68	369	2.3
0.5	142	154	2.2
1.0	240	130	2.2

B. Fitting formula for $G(q,0,\theta)$

The static local field $G(q,0,\theta)$ has various applications. Specifically to be mentioned is its role in recent developments of weighted density-functional theory[27] and in the study of freezing of quantum liquids.[28] In order to avoid the numerically demanding calculation it is worth giving a fitting formula of $G(q,0,\theta)$. In contrast to this quantity which has a nonanalyticity at $q=2$ and $\theta=0$ and a numerically critical behavior for small θ's there, the expression $J(q,0,\theta):=G(q,0,\theta)\Phi^0(q,0,\theta)$ is a smooth function of q. We therefore construct a fit for $J(q,0,\theta)$. Some information on the fit parameters can be derived from the limiting behavior of $G(q,0,\theta)$ and $\Phi^0(q,0,\theta)$:

$$\lim \Phi^0(q,0,\theta) = \frac{\theta^{1/2}}{2}\int_0^\infty dq\, q^{-1/2}[\exp(q^2/\theta-\tilde{\mu})+1]^{-1}\,, \tag{23}$$

$$\lim \Phi^0(q,0,\theta)=\frac{4}{3q^2}\,, \tag{24}$$

$$\lim G(q,0,\theta)=1-g(0,\theta)\,. \tag{25}$$

The small-q expression for $G(q,0,\theta)$ is given by Eq. (15).

TABLE II. Fitting parameters for $\theta=0.1$, 0.5, and 1.0 for several densities.

	$\theta=0.1$	$\theta=0.5$	$\theta=1.0$
		(a) $r_s=1$	
a_1	$4.019\,90\times10^{-1}$	$2.960\,74\times10^{-1}$	$1.787\,17\times10^{-1}$
a_2	$-1.284\,37\times10^{-2}$	$-1.015\,06\times10^{-3}$	$6.638\,38\times10^{-4}$
a_3	$2.971\,60\times10^{-3}$	$5.732\,68\times10^{-4}$	$1.386\,42\times10^{-5}$
b_1	$3.542\,34\times10^{-1}$	$4.760\,54\times10^{-1}$	$5.477\,22\times10^{-1}$
b_2	$1.001\,30\times10^{-1}$	$4.984\,99\times10^{-2}$	$1.209\,39\times10^{-2}$
b_3	$-1.125\,43\times10^{-3}$	$5.338\,27\times10^{-3}$	$4.153\,61\times10^{-3}$
b_4	$2.541\,49\times10^{-3}$	$4.272\,69\times10^{-4}$	$-1.676\,10\times10^{-5}$
c_1	$-2.430\,32$	-4.3948	$-6.229\,72$
c_2	$9.497\,03\times10^{-1}$	$9.272\,90\times10^{-1}$	$8.836\,80\times10^{-1}$
		(b) $r_s=2$	
a_1	$4.303\,08\times10^{-1}$	$3.261\,65\times10^{-1}$	$2.107\,93\times10^{-1}$
a_2	$-1.906\,50\times10^{-2}$	$-3.496\,37\times10^{-3}$	$1.831\,38\times10^{-4}$
a_3	$2.645\,18\times10^{-3}$	$1.042\,41\times10^{-3}$	$1.780\,85\times10^{-4}$
b_1	$2.930\,30\times10^{-1}$	$3.715\,79\times10^{-1}$	$4.607\,09\times10^{-1}$
b_2	$9.279\,30\times10^{-2}$	$7.184\,31\times10^{-2}$	$3.293\,51\times10^{-2}$
b_3	$-2.203\,08\times10^{-3}$	$8.121\,17\times10^{-4}$	$2.241\,49\times10^{-3}$
b_4	$1.881\,14\times10^{-3}$	$7.880\,42\times10^{-4}$	$1.225\,09\times10^{-4}$
c_1	$-2.209\,30$	$-3.892\,32$	$-5.751\,37$
c_2	$8.396\,32\times10^{-1}$	$8.377\,02\times10^{-1}$	$8.002\,92\times10^{-1}$
		(c) $r_s=5$	
a_1	$4.679\,27\times10^{-1}$	$3.629\,11\times10^{-1}$	$2.473\,03\times10^{-1}$
a_2	$-3.189\,16\times10^{-2}$	$-1.314\,61\times10^{-2}$	$-4.751\,28\times10^{-3}$
a_3	$2.562\,52\times10^{-3}$	$8.749\,20\times10^{-4}$	$2.570\,89\times10^{-4}$
b_1	$1.864\,26\times10^{-1}$	$2.496\,59\times10^{-1}$	$3.173\,74\times10^{-1}$
b_2	$9.069\,33\times10^{-2}$	$6.857\,24\times10^{-2}$	$4.703\,95\times10^{-2}$
b_3	$-5.947\,08\times10^{-3}$	$-4.634\,51\times10^{-4}$	$2.218\,50\times10^{-4}$
b_4	$1.563\,48\times10^{-3}$	$5.225\,88\times10^{-4}$	$1.551\,70\times10^{-4}$
c_1	$-1.275\,70$	$-2.071\,49$	$-6.000\,93$
c_2	$7.588\,82\times10^{-1}$	$7.738\,07\times10^{-1}$	$8.123\,19\times10^{-1}$

The fit must meet the requirements for an application on a wide range of r_s and θ. It therefore turned out to be useful to divide the q range into two parts. $0 \le q \le 6$ contains the structured part with the peak, while the region $q \ge 6$ is mainly proportional to q^{-2}. Taking all this into account we choose a parametric description of the following form:

$$J(q,0,\theta)=\frac{a_1 q^2+a_2 q^4+a_3 q^6}{1+b_1 q^2+b_2 q^4+b_3 q^6+b_4 q^8}\ , \quad q \le 6\ , \tag{26a}$$

$$J(q,0,\theta)=\frac{1}{c_1+c_2 q^2}\ , \quad q \ge 6\ . \tag{26b}$$

The fitting parameters $a_1 - c_2$ are calculated by using a nonlinear optimization method on the basis of least-squares fitting. The error made by the discrepancy between the two fitting formulas at $q=6$ is less than 5×10^{-3}. This is suitable for most applications. The values for the fit coefficients are given in Table II for several r_s and θ. The fit is valid for $q \le 12$.

V. THERMODYNAMIC CONSIDERATIONS

The calculation of the excess free energy f_{xc} in the RPA has been discussed by several authors.[4–6,8,29] Here we give a short description of the calculation when LFC's are used.

The exchange-correlation part Ω_{xc} of the grand potential Ω is obtained from an integration over the coupling strength λ of the interaction part H_1 of the Hamiltonian[29] (T is the temperature, μ is the chemical potential, and V is the volume):

$$\Omega_{xc}(\mu,V,T)=\int_0^1 d\lambda\,\lambda^{-1}\langle\lambda H_1\rangle_\lambda=\frac{k_B T}{2}\sum_{\mathbf{q}}\left[\sum_{\gamma=-\infty}^{\infty} v(q)\Phi^0(q,\gamma,T)-1\right]$$
$$+\frac{k_B T}{2}\sum_{\mathbf{q}}\left[\sum_{\gamma=-\infty}^{\infty}\int_0^1\frac{d\lambda}{\lambda}\frac{\lambda^2[1-G(q,\gamma,T;\lambda)][v(q)\Phi^0(q,\gamma,T)]^2}{1+\lambda v(q)[1-G(q,\gamma,T;\lambda)]\Phi^0(q,\gamma,T)}-1\right]. \tag{27}$$

Here the first term denotes the exchange part, while the second one describes the correlation contribution to Ω_{xc}. It should be mentioned that in many cases it is useful to separate the exchange from the correlation part, e.g., for RPA calculations.[4,5] In contrast to the RPA, the local-field correction $G(q,\gamma,T;\lambda)$ in Eq. (27) prohibits an analytical solution of the λ integration.

As a next step this formalism is applied to the electron gas with fixed μ, V, and T. Under the assumption that $\mu/\mu^0 \approx 1$ a Taylor expansion leads to[8]

$$n f_{xc}(n,V,T)=\Omega_{xc}(\mu^0,V,T)/V\ . \tag{28}$$

Thus $\Omega_{xc}(\mu^0,V,T)$ for fixed values (μ^0,V,T) essentially equals the exchange-and-correlation free energy.

The effective potential $V_{xc}^{eff}=\delta(n f_{xc})/\delta n$ is discussed in Refs. 5 and 6. Again, the coupling strength integration leading to V_{xc}^{eff} can be performed analytically for the RPA only.[4,5]

According to Eqs. (27) and (28) f_{xc} can be obtained directly from the interaction energy per volume as defined in Eq. (14) via an integration over the coupling strength. As stated above this integral has to be solved numerically, where λ is conveniently replaced by r_s. Note that this only effects the interaction-dependent terms, not all density-dependent quantities like the reduced temperature $\theta(r_s)$. We therefore obtain for the exchange-correlation free energy per particle in rydbergs:

$$f_{xc}[\mathrm{Ry}]=\frac{2}{\pi\alpha r_s^2}\int_0^{r_s} dr_s'\int_0^\infty dq\,[S(q,\theta;r_s')-1]\ . \tag{29}$$

The results obtained from Eq. (29) for the exchange-and-correlation free energy in the STLS and QSTLS are compared in Table III with the MCA results.[12] These results are higher than the corresponding STLS values for all temperatures. For zero temperature the STLS energies are known to be close to the Monte Carlo calculations.[22]

TABLE III. Exchange-and-correlation free energy $-f_{xc}$ in mRy. STLS refers to standards STLS approach, QSTLS to its quantal version Eq. (12), and MCA denotes results obtained by Tanaka and Ichimaru.[12] MC are the Monte Carlo results of Ceperley and Alder.[22]

	$\theta=0$				$\theta=0.1$		$\theta=0.5$			$\theta=1$	$\theta=5$	$\theta=10$
r_s	MC	STLS	QSTLS	MCA	STLS	QSTLS	STLS	QSTLS	MCA	STLS	STLS	STLS
1.0	1035	1040	1038	1042	1034	1031	940	939	942	804	415	292
2.0	548.4	550	549	553	548	547	520	520	522	464	267	195
3.0		380	379	384	380	379	367	366	371	335	205	153
4.0		293	292	296	293	292	286	286		265	170	128
5.0	239.6	239.7	238	243	240	239	235	235	238	220	146	112
6.0		203	202	206	203	203	201	200		189	129	100
10.0	128.9	128	127	130	128	127	128	127	130	123	90	72

TABLE IV. Correlation free energy $-f_{\text{corr}}$ (mRy) (notation as in Table III).

	$\theta=0.1$		$\theta=0.5$			$\theta=1$	$\theta=5$	$\theta=10$
r_S	STLS	QSTLS	STLS	QSTLS	MCA	STLS	STLS	STLS
1.0	154	151	383	383	386	455	335	251
2.0	108	107	241	241	244	289	227	174
3.0	87	86	181	181	122	219	179	139
4.0	73	72	147	146		178	150	118
5.0	64	63	124	124	127	150	130	104
6.0	57	56	108	107		131	116	93
10.0	40	39	72	71	75	88	82	68

With increasing θ the QSTLS energies quickly approach those of the standard STLS, the differences being negligible already at $\theta\approx 1$.

The fit for $f_x(r_s,\theta)$ presented in Ref. 5 is used to obtain the correlation part of the free energy from the above data for f_{xc} (Table IV). It is seen that $-f_x$ decreases faster with θ than $-f_{\text{xc}}$, leading to an increase in the correlation part for $\theta\lesssim 1$.

Finally, Table V shows the comparison with the classical results of Berggren.[30] It is known that in this limit much better approaches are available.[1,3] Therefore one might question the quality of the STLS energies with increasing θ. From the close agreement with the Monte Carlo results[22] at $\theta=0$, however, the STLS can be assumed to provide a good description to at least $\theta\approx 1$. Furthermore, even in the limit $\theta\gg 1$, the quantum system does not show the unphysical short-range behavior of the classical STLS.[21,30] One can therefore expect that the finite-temperature quantum STLS yields reasonable results throughout the intermediate regime of finite degeneracy.

VI. SUMMARY AND DISCUSSION

The use of a dynamic LFC instead of a static one in the description of a finite-temperature electron liquid allows the investigation of new physical effects. One of the most important of them is the possibility of a CDW. The smallest r_s value where such an instability appears increases with increasing θ while the corresponding wave vector remains constant. Even at small temperatures $\theta\cong 0.1$ the predictions differ considerably from the $\theta=0$ results.[19] Responsible for the existence of a CDW is a peak in the static local-field correction $G(q,\gamma=0,\theta)$.

TABLE V. High-temperature behavior of the free excess energy measured in $k_B T$. For a given Γ, f_{xc} denotes the quantum results and f_{OCP} denotes the classical results evaluated at temperature θ and with the corresponding density parameter $r_s=\theta\Gamma/(2\alpha^2)$.

	$r_S(\theta)$			f_{OCP}		$-f_{\text{xc}}(\theta)$	
Γ	$\theta=10$	$\theta=50$	$\theta=100$	f_{OCP}	$\theta=10$	$\theta=50$	$\theta=100$
0.1	1.84	9.20	18.43	0.015	0.019	0.018	0.017
0.2	3.68	18.42	36.75	0.043	0.050	0.048	0.047
0.3	5.52	27.71		0.077	0.087	0.085	
0.4	7.37			0.161	0.128		

One finds that this maximum is shifted towards larger q with increasing θ. While the peak's amplitude decreases, the width of the q region where $G(q,0,\theta)\geq 1$ increases substantially with θ.

For the static-structure factor and the pair-distribution function the QSTLS yields favorable results compared with static LFC's.[21] In particular, the short-range behavior is improved considerably.

For the exchange-and-correlation energy one detects only a small deviation from the STLS results for higher temperatures. This corresponds to the fact that the difference between STLS and QSTLS vanishes in the classical limit. We close this article with a short outlook on other theories and on the possibility to extend this work.

In order to improve the small q behavior of the QSTLS and STLS the following proposals have been made in the literature. First, in the so-called Singwi-Sjölander-Tosi-Land approach[31] the Coulomb potential in Eq. (8) is screened by the dielectric function of the system. Derived from a diagrammatic analysis,[24] this screening should be a dynamic one. Due to the lack of investigations of this fully dynamic SSTL at $\theta=0$, however, this approach cannot be assessed. Second, in the so-called "quantum Vashishta Singwi" approximation[19,20,32] the local-field correction is replaced by

$$G(q,\gamma,\theta)\rightarrow\left[1+\tfrac{1}{2}n\frac{\partial}{\partial n}\right]G^{\text{QSTLS}}(q,\gamma,\theta)\ . \tag{30}$$

At finite temperatures this requires a very high computational effort, since the derivations for every γ in Eq. (30) are numerically very sensitive. Finally, it appears promising to screen the interaction in Eq. (8) by the static-structure factor, i.e.,

$$I(q,\gamma,\theta)=-\frac{1}{N}\sum_{q'}\Phi^0(\mathbf{q},\mathbf{q}',\gamma,\theta)v(q')S(q')\times[S(\mathbf{q}'-\mathbf{q},\theta)-1]\ . \tag{31}$$

This expression has the advantage that it can be derived in analogy to the QSTLS (cf. Appendix) and that it coincides with the MCA approach investigated extensively by Ichimaru and co-workers[1,12,33,34] if the limit $\hbar\rightarrow 0$ is taken for $\Phi^0(\mathbf{q},\mathbf{q}',\gamma,\theta)$. (As mentioned in Sec. IV A this limit also transforms the QSTLS into the standard STLS.) Although Eq. (31), too, is computationally rather demanding, it can be simplified by invoking the screening in a global manner as successfully applied in Ref. 12. Further work in this direction is in progress.

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APPENDIX

For the ease of comparison with the classical case, all quantities carry their natural dimensions. The starting point is the Wigner distribution function,[1] which is defined in the following way [ψ and $\psi^\dagger$ are the creation and annihilation operators for an electron at space and time point $(\mathbf{r},t)$]:

$$f_\sigma(\mathbf{k},\mathbf{r},t)=\int d\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}}\langle \psi^\dagger_{\sigma\mathbf{r}-\mathbf{x}/2}(t)\psi_{\sigma\mathbf{r}+\mathbf{x}/2}(t)\rangle \equiv n^0(k)+\delta f_\sigma(\mathbf{k},\mathbf{r},t)\ . \tag{A1}$$

The linearized equation of motion for δf in a weak external potential $U^{\rm ext}$ can be written in the symbolic form

$$\left[\frac{\partial}{\partial t}-\frac{q}{m}\frac{\partial}{\partial \mathbf{r}}\right]\delta f_\sigma(\mathbf{k},\mathbf{r},t) =-\frac{2}{\hbar}\sin\left[\frac{\hbar}{2}\frac{\partial}{\partial \mathbf{r}_1}\cdot\frac{\partial}{\partial \mathbf{k}}\right] \times\left[U^{\rm ext}(\mathbf{r},t)n^0(\mathbf{k}) +\int d\mathbf{r}' v(\mathbf{r}-\mathbf{r}')\sum_{k'\sigma'}\delta f^{(2)}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}',\mathbf{r}',\mathbf{r},t)\right]\ . \tag{A2}$$

The subscript in the operator $\partial/\partial\mathbf{r}_1$ indicates that $\partial/\partial\mathbf{r}$ acts only on the first factor in the following products, i.e., on $U^{\rm ext}$ and $v(\mathbf{r}-\mathbf{r}')$. $\delta f^{(2)}$ denotes the deviation from the equilibrium part of the two-particle Wigner function $f^{(2)}$, defined by

$$f^{(2)}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}',\mathbf{r}',\mathbf{r},t)=\int d\mathbf{x}\, e^{-i\mathbf{k}\cdot\mathbf{x}}\int d\mathbf{x}' e^{-i\mathbf{k}'\cdot\mathbf{x}'}\langle \psi^\dagger_{\sigma\mathbf{r}-\mathbf{x}/2}(t)\psi^\dagger_{\sigma'\mathbf{r}'-\mathbf{x}'/2}(t)\psi_{\sigma'\mathbf{r}'+\mathbf{x}'/2}(t)\psi_{\sigma\mathbf{r}+\mathbf{x}/2}(t)\rangle\ . \tag{A3}$$

In order to close this hierarchy, approximations are necessary for δf. Following Singwi *et al.*,[11] Hasegawa and Shimizu[18] suggested the ansatz of local equilibrium

$$f^{(2)}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}',\mathbf{r}',\mathbf{r},t)=f_\sigma(\mathbf{k},\mathbf{r},t)f_{\sigma'}(\mathbf{k}',\mathbf{r}',t)g^{\rm eq}(\mathbf{r}-\mathbf{r}')\ . \tag{A4}$$

It should be noted that this ansatz does not fulfill the sequential relation

$$\int d\mathbf{r}'\sum_{\substack{\mathbf{k}\sigma\\ \mathbf{k}'\sigma'}} f^{(2)}_{\sigma\sigma'}(\mathbf{k},\mathbf{k}',\mathbf{r}',\mathbf{r},t)=\int d\mathbf{r}' f^{(2)}(\mathbf{r}',\mathbf{r},t)=nf(\mathbf{r},t)\ . \tag{A5}$$

In order to ensure that the pair function has the correct weight under the $\mathbf{r}'$ integral in Eq. (A2) the above ansatz has to be modified according to

$$f^{(2)}\to f^{(2)}+f_\sigma(\mathbf{k},\mathbf{r},t)n\int d\mathbf{y}\, h^{\rm eq}(\mathbf{r}-\mathbf{y}) \times h^{\rm eq}(\mathbf{y}-\mathbf{r}')f_{\sigma'}(\mathbf{k}',\mathbf{y},t)\ . \tag{A6}$$

($h^{\rm eq}$ is short for $g^{\rm eq}-1$.) Linearization around thermal equilibrium and Fourier transformation of Eq. (A2) leads to the form

$$\left[\omega-\frac{\mathbf{k}\cdot\mathbf{q}}{m}\right]\delta f_\sigma(\mathbf{k},\mathbf{q},\omega)=[n^0(\mathbf{k}-\mathbf{q}/2)-n^0(\mathbf{k}+\mathbf{q}/2)]U^H(q,\omega) +\delta\rho(\mathbf{q},\omega)\sum_{\mathbf{q}'}v(q')A(q')[n^0(\mathbf{k}-\mathbf{q}'/2)-n^0(\mathbf{k}+\mathbf{q}'/2)][S(\mathbf{q}-\mathbf{q}')-1]\ . \tag{A7}$$

$U^H=U^{\rm ext}+v\delta\rho$ denotes the Hartree potential and the "screening function" A is to be replaced by 1 for the quantum STLS. In the corrected approach of Eq. (A5) $A(q')$ is identical with the static-structure factor $S(q')$.

Equation (A7) is divided by $\omega-\mathbf{k}\mathbf{q}/m=\omega-\varepsilon(\mathbf{k}+\mathbf{q}/2)+\varepsilon(\mathbf{k}-\mathbf{q}/2)$ and summed over $\mathbf{k}$. This yields

$$\delta\rho(q,\omega)=\sum_{\mathbf{k}\sigma}\delta f_\sigma(\mathbf{k},\mathbf{q},\omega) =\chi^0(q,\omega)[U^{\rm ext}(q,\omega)+v(q)\delta\rho(q,\omega)]+\delta\rho(q,\omega)\sum_{\mathbf{q}'}v(q')A(q')\chi^0(q,q',\omega)[S(\mathbf{q}-\mathbf{q}')-1]\ . \tag{A8}$$

A comparison of Eq. (A8) with $A(q')=1$ and Eq. (4) gives the desired result of Eq. (8) while the use of $A(q')=S(q')$ leads to Eq. (31).

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