Temperature dependence of short-range correlations in the homogeneous electron gas

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The temperature-dependent behavior of short-range correlations in a homogeneous three-dimensional electron gas at finite temperatures and finite degeneracies is presented. From the physical meaning of the pair distribution function for two electrons at the same location, one would expect a function which increases monotonically with the temperature. Instead, a decrease is found for small temperatures. This effect is investigated extensively within the framework of the random-phase approximation of static-local-field-corrected approaches. Moreover, by applying first-order perturbation theory the nonmonotonic behavior is proven to appear in the high-density limit also. Using a density-functional based model for short-range correlations, a physical interpretation is obtained. Finally, the results are discussed in a comprehensive way.

I. INTRODUCTION

In the course of the last decade thermodynamics and correlational properties of Fermi systems have been studied comprehensively within the framework of the electron gas model, especially in the completely degenerated[1,2] and the classical[1,3] limits. However, in a substantial number of physically interesting situations the finite degree of Fermi degeneracy cannot be neglected. Examples where an approximation by one of the above asymptotic behavior fails, are liquid metals and plasmas used in fusion experiments.

Extensive investigations on electron systems at finite temperatures within the density-functional formalism were performed both in three[4] and in two[5] dimensions. In the present paper we consider a homogeneous three-dimensional (3D) electron gas which can be characterized by two parameters: the temperature T and the electron density n, conveniently replaced by

$$\Theta = k_B T / E_F \quad \text{Fermi degeneracy parameter}\ , \tag{1}$$

$$r_s = a / a_B \quad \text{density parameter}\ , \tag{2}$$

where $a=(4\pi n/3)^{-1/3}$ is the radius of a sphere containing on the average one particle, $a_B=\hbar^2/e^2m$ is the Bohr radius, and $E_F=\hbar^2k_F^2/2m$ denotes the Fermi energy $[k_F=(3\pi^2 n)^{1/3}]$. It should be mentioned that for completely degenerate systems $\Theta \ll 1$, while for classical ones $\Theta \gg 1$. r_s is a measure for the strength of the Coulomb coupling in a degenerate system ($r_s=0$ denotes the noninteracting system).

For homogeneous three-dimensional systems static-local-field-corrected theories have been proven to give good results for the static correlations at zero temperature in the metallic density range.[6-8] In addition, they allow a largely analytical treatment of the calculations. It was the merit of Tanaka and Ichimaru to extend the $T=0$ formalism to nonzero temperatures.[9] Their detailed work includes a comprehensive description of the static correlations. Being interested in quantum corrections to a mainly classical plasma, they used the so-called plasma parameter $\Gamma = e^2/ak_BT$ for their calculations. Γ, however, combines two different properties of the system: the Coulomb coupling strength, entering Γ through a, and the kinetic energy k_BT of the electrons. In highly degenerate systems the latter has to be replaced by the Fermi energy.

The purpose of the present work is the investigation of the temperature dependence of the pair distribution function $g(r,\Theta)$, especially at zero distance $r=0$. For that reason we consider an electron system with fixed density parameter r_s and vary over Θ in order to separate the two effects stated above.

The physical meaning of $g(0,\Theta)$ can be expressed by an integral over the region where the Coulomb repulsion of an electron exceeds the kinetic energy. Since the latter is increased by heating up the system, one would expect an enlarged probability for electronic tunneling through the Coulomb-barrier, and thus an increase of $g(0,\Theta)$. Instead, the result is a function $g(0,\Theta)$ having a negative gradient for small Θ's, which is rather unexpected at first sight. At a temperature $\Theta_{\min}$ $g(0,\Theta)$ reaches a minimum and then increases monotonically for higher Θ's.

This paper is organized as follows. In Sec. II the basic formalism for the calculations of the static correlations is presented and the temperature dependence of the pair distribution function is discussed in an extensive way. Three theories, their characteristics and their influence on the results are described and compared with each other: the random-phase approximation (RPA) and two static-local-field-correlated theories; the Singwi-Tosi-Land-Sjölander[6] (STLS) and the Singwi-Sjölander-Tosi-Land[7] (SSTL) approximation. Moreover, the influence of Quantum Mechanics on Fermi systems at high temperatures is described briefly.

The question whether the effect is of physical nature or not is treated in Sec. III by making first-order theory for $r_s<1$. Finally an explanation of the nonmonotonic temperature dependence of the $g(0,\Theta)$ function is given. Section IV concludes with a discussion of the results.

II. $g(r,\Theta)$ AND $g(0,\Theta)$ WITHIN THE RPA AND THE STATIC-LOCAL-FIELD-CORRECTION FORMALISM

Before explaining the temperature dependence of the pair distribution function, a description of the formalism which is used to calculate the static correlations is given. For a more detailed discussion, we refer to Ref. 9.

The starting point of the considerations is the well-known density response function $\chi(q,\omega)$. This function can be expressed by the free-particle response function $\chi^0(q,\omega)$ and a local field correction $G(q,\omega)$:[10]

$$\chi(q,\omega)=\frac{\chi^0(q,\omega)}{1-[1-G(q,\omega)]v(q)\chi^0(q,\omega)}\ , \tag{3}$$

where $v(q)=4\pi e^2/q^2$ is the Coulomb potential in momentum space. Making use of the fluctuation-dissipation theorem we obtain the dynamic structure factor and after a Fourier transformation from ω to $t=0$ the static structure factor:

$$S(q,\Theta)=-\frac{\hbar}{2\pi n}\int_{-\infty}^{\infty}d\omega\coth\left[\frac{\hbar\omega}{2Tk_B}\right]\mathrm{Im}\chi(q,\omega)\ . \tag{4}$$

For the further evaluation of Eq. (4) two approaches can be used. In the first one, which is useful for $\Theta=0$ studies[11,12] and for $\Theta\ll 1$ considerations, the particle-hole and the plasmon contributions to $S(q,\Theta)$ are calculated. As there is no analytic expression available for the plasmon dispersion relation, its evaluation is rather laborious. Therefore, the second one proposed by Tanaka and Ichimaru[9] is favorable for the rest of the Θ range. This method derives advantage from the fact that $\chi(q,\omega)$ is separately analytic in the upper and the lower halves of the complex ω plane. The integration in Eq. (4) can be carried out using the residue theorem. Introducing the dimensionless response function $\Phi(q,\omega)\equiv -2E_F\chi(q,\omega)/3n$ one arrives at

$$S(q,\Theta)=\frac{3}{2}\Theta\sum_{\gamma=-\infty}^{\infty}\Phi(q,z_\gamma)\ , \tag{5}$$

where z_γ denotes the so-called Matsubara frequencies:

$$z_\gamma=2i\pi\gamma k_BT/\hbar,\quad \gamma=0,\pm1,\pm2,\ldots\ . \tag{6}$$

A further Fourier transformation from q to r (r describes the distance between two electrons) leads to the pair distribution function $g(r,\Theta)$. Here and in the following the dimensionless quantities $q\equiv q/k_F$ and $r\equiv rk_F$ are used:

$$g(r,\Theta)=1+\frac{3}{2r}\int_0^{\infty}dq\,q\sin(qr)[S(q,\Theta)-1]\ . \tag{7}$$

For the response function of a noninteracting system one finds[9] (cf. also with Ref. 11):

$$\Phi^0(q,0)=\frac{1}{\Theta q}\int_0^{\infty}dy\,y\left[\left[y^2-\frac{q^2}{4}\right]\ln\left|\frac{2y+q}{2y-q}\right|+qy\right]\times\frac{\exp(y^2/\Theta-\tilde{\mu})}{[\exp(y^2/\Theta-\tilde{\mu})+1]^2}\ , \tag{8}$$

$$\Phi^0(q,\gamma)=\frac{1}{2q}\int_0^{\infty}dy\frac{y}{\exp(y^2/\Theta-\tilde{\mu})+1}\times\ln\left|\frac{(2\pi\gamma\Theta)^2+(q^2+2qy)^2}{(2\pi\gamma\Theta)^2+(q^2-2qy)^2}\right|\ . \tag{9}$$

Equations (8) and (9) are obtained by replacing each step function in Lindhard's formula[13] by the Fermi function

$$n^0(q,\Theta)=[\exp(q^2/\Theta-\tilde{\mu})+1]^{-1} \tag{10}$$

which describes the momentum distribution of free particles at finite Θ. The quantity $\tilde{\mu}\equiv\mu/k_BT$ denotes the reduced chemical potential of a noninteracting system and can be obtained by solving the following equation:

$$n=(2\pi)^{-3}\int d^3q\,n^0(q,\Theta)\ . \tag{11}$$

The simplest theory within the presented formalism [cf. with Eq. (3)] is the RPA, which is a pure mean-field-theory based on $G(q,\omega)=0$. This approximation works well in the high-density limit, but gives negative and therefore unphysical results for $g(r\to 0,\Theta=0)$ for $r_s\gtrsim 0.75$. In overcoming this most striking deficiency of the RPA extended mean-field theories using $G\neq 0$, but still neglecting its ω dependence, have proved successful for metallic densities ($r_s\lesssim 6$). Assuming local equilibrium for the two-particle function Singwi *et al.*[6] ($\equiv$STLS) decoupled the classical hierarchy of equations of motion and thereby derived the following expression for the local-field $G(q)$:

$$v(q)G^{\mathrm{STLS}}(q,\Theta)=-\frac{1}{n}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\times v(q')[S(\mathbf{q}'-\mathbf{q},\Theta)-1] \tag{12}$$

or, equivalently, (in dimensionless units)

$$G^{\mathrm{STLS}}(q,\Theta)=-\frac{3}{4}\int_0^{\infty}dy\,y^2[S(y,\Theta)-1]\times\left[1+\frac{q^2-y^2}{2qy}\ln\left|\frac{q+y}{q-y}\right|\right]\ . \tag{13}$$

G and S are to be determined self-consistently. This approach has led to excellent results[3,6] for the pair correlation function of the completely degenerate electron liquid ($\Theta=0$). It suffers, however, from a violation of the compressibility sum-rule.[3,7] In the classical limit $\hbar\omega\ll k_BT$, additional minor deficiencies have been noticed,[14–16] e.g., an unsatisfactory small-coupling behavior. The latter is improved by accounting for screening in $v(q')$ in Eq. (12), as done in a later proposal by Singwi *et al.*[7] (SSTL)

$$v(q)G^{\mathrm{SSTL}}(q,\Theta)=-\frac{1}{n}\int\frac{d^3q'}{(2\pi)^3}\frac{\mathbf{q}\cdot\mathbf{q}'}{q^2}\frac{v(q')}{\epsilon(q')}\times[S(\mathbf{q}'-\mathbf{q},\Theta)-1]\ . \tag{14}$$

A different suggestion has been made by Ichimaru,[15] who uses $S(q')$ instead of the inverse dielectric function $1/\varepsilon$. In the classical system both approaches yield the correct weak-coupling expansion beyond the RPA. The SSTL approximation has the further advantage of closely fulfilling the compressibility sum rule for $T=0$, although for the classical system the conformity is less satisfactory.[17] In the low-temperature region, however, the SSTL constitutes an interesting alternative to the STLS. Additional modifications[8] and improvements of the STLS yield close to those of either STLS or SSTL, and are not considered here. It should be mentioned, however, that some of those approaches listed in Ref. 8 are based on a dynamic local field correction and therefore hold the potential of new effects arising from the additional temperature dependence of the Matsubara frequencies as can be seen from Eqs. (3) and (6) (cf. the discussion in Sec. IV).

Using one of the static-local-field-corrections stated above, $S(q,\Theta)$ is obtained from Eq. (5). To avoid numerical difficulties it is advisable to treat Eq. (5) in the way suggested in Ref. 9. It is noteworthy that for $\Theta \lesssim 0.01$ the sum over γ converges rather slowly. From the numerical point of view it is therefore much more convenient to obtain $S(q,\Theta)$ from the other method mentioned above.

Although the sum over the Matsubara frequencies cannot be simplified in general, one finds in the short wavelength limit:

$$\lim_{q\to\infty} S(q,\Theta)=1-\frac{8}{3\pi a_B k_F q^4} . \tag{15}$$

This simple relation is very important for the calculation of the large q contributions to $g(r,\Theta)$ in Eq. (7) and for Kimball's relation.[10,18] It should be noted that there is no Θ dependence left in Eq. (15). In particular, it differs from the classical limit which is expected to yield a good description of the $\Theta \gg 1$ region. The classical analogue to Eq. (15) is expressed by:[17,18]

$$\lim_{q\to\infty} S^{\mathrm{cl}}(q,\Theta)=1-\mathrm{const}/q^2 . \tag{16}$$

To explain this apparent contradiction we look at Eqs. (8) and (9). For high temperatures ($\Theta \gtrsim 100$) and q smaller than a certain wave vector $q_{\mathrm{cl}}(\Theta)$ only the static response function contributes to $S(q,\Theta)$. In that case one finds

$$\Phi^0(q \lesssim q_{\mathrm{cl}},0)=2/3\Theta . \tag{17}$$

Insertion of Eq. (17) into Eq. (3) leads to

$$S(q \lesssim q_{\mathrm{cl}},\Theta)=\left[1+\frac{n}{k_B T}[1-G(q)]v(q)\right]^{-1} , \tag{18}$$

This is the classical result obtained by Berggren.[17] It follows from Eqs. (8) and (9) that $q_{\mathrm{cl}}(\Theta)$ is a monotonically increasing function. The region where the quantum character is crucial for the system and where the dynamics of the response function becomes important is therefore continually restricted to higher temperatures. For the pair distribution function this means that the exchange and correlation hole is smeared out with increasing Θ. In the $\Theta \to \infty$ limit only $g(0,\Theta)$ has to be calculated within the quantum mechanical formalism.

We now return to the calculation of the pair distribution function. Making use of the formalism discussed above we first obtain $g(r,\Theta)$ in the RPA. In Fig. 1 the result for $r_s=2$ is depicted. Here the effect described in the introduction arises: at $r=0$ the $g(r,\Theta_1=0)$ exceeds the corresponding result for $\Theta_2=1$. For large values of r these functions show the opposite behavior, i.e., in this limit $g(r,\Theta_1)>g(r,\Theta_2)$. This is a consequence of the sequential relation, which is a normalization condition for $g(r,\Theta)$:

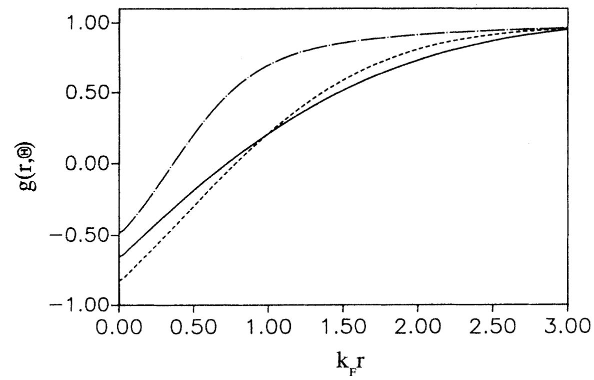

FIG. 1. Pair distribution function $g(r,\Theta)$ of Eq. (7) in RPA as a function of r and for $r_s=2$. Solid line, $\Theta=0$; dashed line, $\Theta=1$; dash-dotted line, $\Theta=5$.

$$\int d^3r[g(r,\Theta)-1]=-3\pi^2 . \tag{19}$$

Extensive calculations show that this nonmonotonic Θ dependence exists in the whole density range up to $r_s=10$, even in the high-density limit, and there is no obvious reason why it should vanish for lower densities. However, as the RPA violates Kimball's relation[18]

$$\frac{g'(0,\Theta)}{g(0,\Theta)}=\frac{1}{a_B} \tag{20}$$

it is not a good theory for small distances r. In the RPA the connection between $g'(0,\Theta)$ and the short wavelength limit of $S(q,\Theta)$ derived first by Niklasson[10] leads to

$$g'(0,\Theta)=\frac{1}{a_B} . \tag{21}$$

A theory which satisfies Eq. (20) is the STLS scheme.[9] Here the effect of the nonmonotonic Θ dependence of $g(0,\Theta)$ appears again, even in this excellent approximation. To make this transparent, we plot $g(0,\Theta)$ as a function of Θ. This is done in Fig. 2. Two important facts can be stated. Firstly, the minimum of $g(0,\Theta)$ tends towards higher values of Θ with increasing r_s. Secondly, $\Theta_{\mathrm{min}}^{\mathrm{STLS}}$ is higher than $\Theta_{\mathrm{min}}^{\mathrm{RPA}}$. Moreover, an analytical expression can be obtained for the temperature derivative of $g(0,\Theta)$ at $\Theta=0$:

$$\left.\frac{\partial g(0,\Theta)}{\partial\Theta}\right|_{\Theta=0}=0 , \tag{22}$$

Equation (22) is valid for all static-local-field approaches. In addition the behavior of the pair distribution function within the SSTL approach was studied. For $\Theta=0$ the

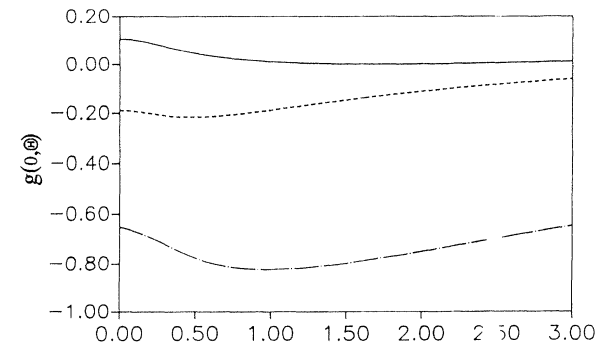

FIG. 2. Pair distribution function $g(0,\Theta)$ as a function of Θ for fixed value $r=0$ and $r_s=2$ calculated in various theories. Solid line: STLS, dashed line: SSTL, dash-dottted line: RPA.

compressibility sum rule is fulfilled in this theory for $r_s \cong 3.5$ and can thus be assumed to hold for small temperatures in the density range investigated. Here a completely different trend is observed: $\Theta_{\rm min}^{\rm SSTL}$ decreases as a function of r_s and becomes zero for $r_s \cong 6$. In order to elucidate the properties of $g(0,\Theta)$, the comparison of $\Theta_{\rm min}^{\rm STLS}$, $\Theta_{\rm min}^{\rm SSTL}$, and $\Theta_{\rm min}^{\rm RPA}$ for several values of r_s is given in Table I.

Here the question arises: is the minimum in the $g(0,\Theta)$ function only a failure of the static-local-field-corrected theories or does it reflect a physical property of the electron gas which has not been reported yet? The latter assumption in conjunction with the definition of $g(0,\Theta)$ which has been given in Sec. I implies a temperature dependence of the effective exchange and correlation potential. In order to decide whether this hypothesis is valid or not, the $r_s \ll 1$ limit is investigated, since this density range is accessible by perturbation theory.

III. PHYSICAL INTERPRETATION OF THE Θ DEPENDENCE OF $g(0,\Theta)$

For weakly coupled systems the calculation of $g(0,\Theta)$ is based on evaluating expectation values of pair operators to lowest order in the interaction only. Starting point is the static structure factor,

$$S(q,\Theta)=\frac{1}{N}\sum_{\mathbf{k},\mathbf{k}'}\langle C_{\mathbf{k}}^{\dagger}C_{\mathbf{k}-\mathbf{q}}C_{\mathbf{k}'}^{\dagger}C_{\mathbf{k}'+\mathbf{q}}\rangle$$
$$=S^0(q,\Theta)+\Delta S(q,\Theta)\ . \qquad (23)$$

Leaving detailed calculations to the appendix, ΔS is found to be formally the same as derived by Kimball[19,20] for $\Theta=0$ [cf. Eq. (A4)]; the Θ dependence enters only via

TABLE I. $\Theta_{\rm min}^{\rm RPA}$, $\Theta_{\rm min}^{\rm STLS}$, and $\Theta_{\rm min}^{\rm SSTL}$ for several values r_s.

Theory/r_s	0.1	0.5	1.0	2.0	3.0	4.0	5.0	6.0
RPA	0.6	0.8	0.9	1.0	1.1	1.2	1.3	1.4
STLS	0.8	1.0	1.3	1.7	2.3	3.4	4.9	6.7
SSTL	0.8	0.8	0.7	0.5	0.4	0.3	0.2	0.1

the Fermi functions. This results in the following v^1-corrections to $g(0,\Theta)$ [with $n_{\mathbf{k}}^0 \equiv n^0(k,\Theta)$, $\varepsilon_{\mathbf{k}} \equiv \hbar^2k^2/2m$ and $\alpha^3 \equiv 4/9\pi$]

$$\Delta g(0,\Theta)=-\frac{4}{N^2}\sum_{\mathbf{q},\mathbf{p},\mathbf{k}} v(q)\frac{n_{\mathbf{k}}^0 n_{\mathbf{p}}^0(1-n_{\mathbf{p}-\mathbf{q}}^0)(1-n_{\mathbf{k}+\mathbf{q}}^0)}{\varepsilon_{\mathbf{k}}+\varepsilon_{\mathbf{p}}-\varepsilon_{\mathbf{p}-\mathbf{q}}-\varepsilon_{\mathbf{k}+\mathbf{q}}}$$
$$=\frac{9\alpha r_s}{32\pi^4}\int d^3k\int d^3p\int d^3q\frac{1}{q^2}\frac{n_{\mathbf{k}}^0 n_{\mathbf{p}}^0(1-2n_{\mathbf{p}+\mathbf{q}}^0)}{(\mathbf{p}-\mathbf{k}-\mathbf{q})\cdot\mathbf{q}}\ . \qquad (24)$$

Equation (24) has been integrated numerically, the result is shown in Fig. 3. Again $g(0,\Theta)$ first *decreases* with increasing temperature. It can thus be concluded that the nonmonotonic Θ dependence of $g(0,\Theta)$ is an exact property of the electron gas system, at least in the $r_s \ll 1$ regime. Furthermore, it should be noted that in contrast to the previous section this result is not based on the assumption of a static-local-field correction, but is consistent with the dynamic first-order local-field corrections described in Refs. 21 and 22.

A possible criticism of the perturbational approach might arise from the fact that for dynamic properties a nonphysical behavior is found at the boundaries of the particle-home continuum. These effects and possibilities for their renormalization have been discussed extensively in Refs. 21–24. Therefore static quantities like $S(q,\Theta)$ and $g(0,\Theta)$ can be considered to be exact to $O(r_s^1)$ and the above result gives strong evidence that the nonmonotonic Θ behavior of $g(0,\Theta)$ is a property of the exact system, too.

In order to understand the physical origin of this effect one has to take into account temperature-dependent screening, too, which can be investigated best within a simple, density-functional based model for the short-range correlations: The probability of finding two electrons at the same location can be estimated by one-particle scattering in an effective potential. Thus we write the pair correlation function at zero particle separation

$$g(0;\Theta|V)\simeq\frac{1}{2}\frac{\rho(0,\Theta|V)}{\rho_0} \qquad (25)$$

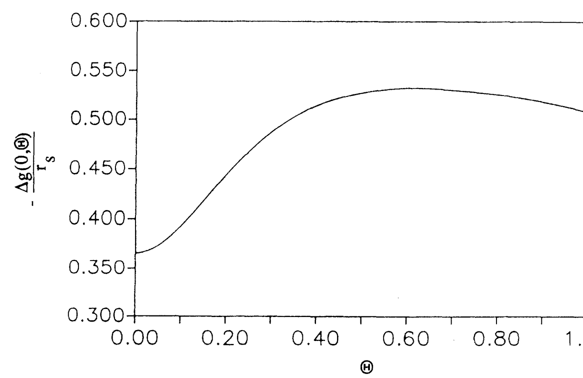

FIG. 3. Pair distribution in first-order perturbation theory. Here the r_s-independent correction of Eq. (24) is plotted as a function of Θ.

as a functional of the effective scattering potential $V(r;\Theta)$. Here, $\rho(r;\Theta|V)$ is the one-particle density

$$\rho(r;\Theta|V) \equiv \sum_{\mathbf{k},\sigma} n_{\mathbf{k}}^{0}(\Theta)|\varphi_{\mathbf{k}\sigma}(r|V)|^2 , \qquad (26)$$

where the $\varphi_{\mathbf{k}\sigma}$ are the normalized solutions of Schrödinger's equation with potential V. $\rho_0 \equiv \rho(r;\Theta|0)$ is the mean density of electrons in the gas. Because the effect investigated here is also present within pure first-order perturbation theory, we can confine these calculations to first order in the scattering potential, too. Consequently, we linearize the functional given by Eq. (26) with respect to V using Born's first approximation, which leads to

$$g(0,\Theta|U) \simeq \frac{1}{2}\left[1-3(\alpha r_s)^2\int_0^\infty dx\, U(x)\int_0^\infty dk\, k\, \sin(2kx) n_k^0(\Theta)\right] + O(U^2) , \qquad (27)$$

where we are using the common dimensionless variables; furthermore, the potential $U(x)$ is measured in Rydbergs. In order to close this model we remember the physical interpretation of $U(x)$ as an effective scattering potential caused by one electron at the origin plus the surrounding "screening cloud." Therefore Poisson's equation

$$\Delta U = -\frac{4\pi}{\alpha r_s}\left[\delta(x) - \frac{1-g(x)}{3\pi^2}\right] \qquad (28)$$

with the well-known solution

$$U(x|g) = \frac{1}{\alpha r_s x}\left[1-\frac{4}{3\pi}\left[\int_0^x ds\, s^2[1-g(s)] + x\int_x^\infty ds\, s[1-g(s)]\right]\right] \qquad (29)$$

is used. Being again interested only in first-order contributions, we replace the pair correlation function $g(s)$ in the functional [cf. Eq. (29)] by the interaction free $g^0(s)$ whose temperature dependence is known exactly. From Eq. (29) the physical origin of the negative slope in $g(0,\Theta)$ becomes quite clear: In the ground state (i.e., $\Theta=0$ the brace tends to zero for large x, which means that the pure Coulomb interaction is replaced by a screened one of shorter range [cf. Fig. (4)]. For $\Theta \to \infty$ the pair function $g^0(x,\Theta)$ becomes one and the screening terms vanish. Thus we find two competing effects contributing to the temperature behavior of the short-range correlations: On the one hand, raising Θ increases the mean kinetic energy of the particles and consequently also the tunneling probability through the potential barrier surrounding the "target" electron [cf. Eq. (27)], but on the other hand, according to Eq. (29), the width of this barrier is increased too. As it is seen from Fig. 5 the latter effect is dominant in the range of low temperatures, while for high Θ, i.e., when $g^0 \approx 1$, only the "broadening" of the momentum distribution $n^0(k,\Theta)$ remains relevant. So this mechanism turns out to satisfactorily explain the observed temperature dependence of the short-range correlations.

IV. SUMMARY AND DISCUSSION

In the electron liquid, short-range many-body correlations lead to a reduction of the bare Coulomb potential on account of the Pauli principle and due to screening. The resulting effective potential exhibits a strong temperature dependence, caused by the according Θ-induced rearrangement of the exchange and correlation hole. In particular, the latter is smeared out with increasing Θ, thus enhancing the effective strength of the barrier. This determines the small Θ behavior of the short-range pair correlations and leads to a decrease of the tunneling probability. At some temperatures $\Theta_{\min}$ the increase in the potential is compensated by the gain in the mean kinetic energy, which finally dominates the high-temperature regime.

While the RPA yields the minimum of $g(0,\Theta)$ only modestly raising with r_s at $\Theta_{\min} \approx 1$, in STLS a very shallow structure with a strongly r_s-dependent $\Theta_{\min}$ is observed. This can again be qualitatively explained by using Eq. (29) (although, strictly speaking, the latter is valid only for $r_s \ll 1$). Compared to g^{RPA}, the change of g^{STLS} with r_s is rather weak, resulting in a correspondingly smaller modification of the effective potential. As a consequence, the position of $\Theta_{\min}$ is shifted towards higher values for growing r_s.

The SSTL approximation gives less satisfactory results for the pair function at zero distance. It proves, however, that the decrease of $g(0,\Theta \ll 1)$ cannot be due to the violation of the compressibility sum rule and thus supports the quality of the STLS results. Further improvement could be obtained by calculating $g(0,\Theta)$ with use of

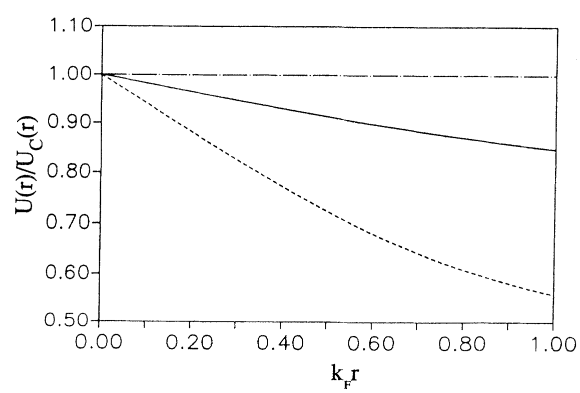

FIG. 4. Effective potential in the density-functional based model described by Eqs. (25)–(29) as a function of r. Solid line: temperature-dependent effective potential of Eq. (30) at $\Theta=1$. Dashed line: effective potential at $\Theta=\infty$ (smallest screening effect), dash-dotted line: effective potential at $\theta=0$ (largest screening effect).

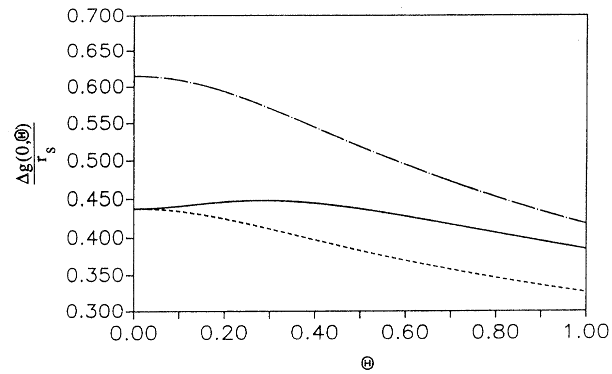

FIG. 5. Pair distribution function in the density-functional based model. The r_s-independent correction term to the result obtained in a noninteracting system is depicted as a function of Θ. Solid line: correction term of Eq. (28). Dashed line, correction term obtained by using $U(r,\Theta=0)$; dash-dotted line, correction term obtained by using $U(r,\Theta=\infty)$.

a dynamic local-field correction. As already mentioned above these approximations contain the Matsubara frequencies. They have therefore the advantage of describing the influence of the temperature-dependent effective potential on $g(0,\Theta)$ in an even better way than the STLS does.

In addition, the cusp condition given by Eq. (20) implies the following limiting behavior for a static $G(q)$

$$G(q\to\infty)=1-g(0,\Theta)\ . \tag{30a}$$

It is stressed again that both the STLS and the SSTL approach satisfy Eq. (30a) and thus ensure that Kimball's relation has been properly accounted for. A useful $G(q,\omega)$ should, of course, comply with Kimball's relations, too. The corresponding sum rule reads[10,25]

$$G(q\to\infty,\omega)=2/3[1-g(0,\Theta)]\ . \tag{30b}$$

It should be noted that Eq. (30b) is based on Niklasson's convention[10] of evaluating $\chi^0(q,\omega)$ in Eq. (3) with the fully interacting momentum distribution. The contrast between Eq. (30a) and Eq. (30b) gives again strong evidence for the mutual dependence of $g(0,\Theta)$ and dynamic correlations.

An investigation of the dynamic local-field correction presented by Devreese and Brosens[22] and by Holas, Aravind, and Singwi[21] appears promising since it provides the possibility of independently studying the finite temperature effects on the interacting momentum distribution and those on the vertex correction of the polarization. The local-field correction of Dabrowsky,[26] based on an interpolation between exact limiting forms of $G(q,\omega)$ known from sum rules, or the dynamical version of the STLS, a theory that yields $g(0)>0$ up to $r_s=20$ at $\Theta=0$, and other dynamic local fields presented in the literature[1,2,27,28] provide interesting alternatives. Further work towards this direction is in progress.

Independently of the method chosen, a detailed study of the temperature dependence of the screening potential in the electron gas and an exact evaluation of the crossover temperature $\Theta_{\min}$ appear to be of high interest. In addition, being a property of the exact system, $\Theta_{\min}$ could be used as a means for testing the quality of certain approximations.

In summary, arising from the competition between the increase of both the effective potential and the kinetic energy, a nonmonotonic temperature dependence is found for the zero-distance pair correlations in an electron liquid. Moreover, the crossover temperature $\Theta_{\min}$ is a characteristic property of the exact system.

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APPENDIX

In order to obtain the v^1 contributions to $S(q)$, the expectation value of two pairs of $C^\dagger C$ operators must be evaluated in first-order perturbation theory. The free-fermion system is determined by

$$\begin{aligned}\langle C_1^\dagger C_2^\dagger C_{2'} C_{1'}\rangle^0 &= \langle C_1^\dagger C_{1'}\rangle^0 \langle C_2^\dagger C_{2'}\rangle^0 \\ &\quad - \langle C_1^\dagger C_{2'}\rangle^0 \langle C_2^\dagger C_{1'}\rangle^0 \\ &= n_1^0 n_2^0[\delta_{11'}\delta_{22'}-\delta_{12'}\delta_{21'}]\ .\end{aligned} \tag{A1}$$

The interaction gives rise to two types of corrections to (A1). Firstly, the Fermi functions $n_k^0 \equiv n^0(k,\Theta)$ are modified according to

$$n_{\mathbf{k}}^{(1)}=n_{\mathbf{k}}^0+\beta n_{\mathbf{k}}^0(1-n_{\mathbf{k}}^0)Vol^{-1}\sum_{\mathbf{q}} v_{\mathbf{q}}\left[n_{\mathbf{k}-\mathbf{q}}^0-\frac{\int d^3p\, n_{\mathbf{p}}^0(1-n_{\mathbf{p}}^0)n_{\mathbf{p}-\mathbf{q}}^0}{\int d^3p\, n_{\mathbf{p}}^0(1-n_{\mathbf{p}}^0)}\right] \tag{A2}$$

($\beta\equiv 1/k_BT$). Though contributing to $S(q,\Theta)$ and $g(r,\Theta)$, however, these corrections have no influence on the zero-distance pair correlation and are thus omitted in the following. The remaining additions to (A1) have been evaluated, e.g., by Gasser and Fischer[20] and can be written in the following form:

$$\Delta\langle C_1^\dagger C_2^\dagger C_{2'} C_{1'}\rangle = \delta_{\mathbf{k}_1+\mathbf{k}_2,\mathbf{k}_{1'}+\mathbf{k}_{2'}}[v(1'-1)\delta_{\substack{\sigma 1,\sigma 1'\\ \sigma 2,\sigma 2'}} - v(2'-1)\delta_{\substack{\sigma 1,\sigma 2'\\ \sigma 2,\sigma 2'}}]\frac{n_{1'}^0 n_{2'}^0(1-n_2^0)(1-n_1^0)-(1-n_{2'}^0)(1-n_{1'}^0)n_1^0 n_2^0}{\varepsilon_{1'}+\varepsilon_{2'}-\varepsilon_2-\varepsilon_1}\ . \tag{A3}$$

Obviously, (A3) describes transitions from the (occupied) states $(1',2')$ to the empty states $(1,2)$ and the reverse process, the appropriate excitation energy being given in the denominator. Insertion of Eq. (A3) into the expression (23) for the static structure factor yields a result derived previously[19] for $\Theta=0$, namely,

$$\Delta S(q,\Theta)=-\frac{2}{N}\sum_{\substack{\mathbf{k},\mathbf{p}\\ \sigma,\sigma'}}[v(q)-\delta_{\sigma\sigma'}v(\mathbf{k}-\mathbf{p})]\frac{n^0_{\mathbf{k}-\mathbf{q}/2}n^0_{\mathbf{p}+\mathbf{q}/2}(1-n^0_{\mathbf{p}-\mathbf{q}/2})(1-n^0_{\mathbf{k}+\mathbf{q}/2})}{\varepsilon_{\mathbf{k}-\mathbf{q}/2}+\varepsilon_{\mathbf{p}+\mathbf{q}/2}-\varepsilon_{\mathbf{p}-\mathbf{q}/2}-\varepsilon_{\mathbf{k}+\mathbf{q}/2})}\ . \tag{A4}$$

The evaluation of $\Delta g(0,\Theta)$ is then easily performed.

In order to elucidate the point that the results obtained in the first part of Sec. III have not been restricted to the use of a static-local-field correction, an alternative way of deriving Eq. (A4) is briefly sketched now. The starting point is the first-order contribution to the dynamic local-field correction,[22] identical to the expression for the first-order parts of the proper polarization.[21] In the following Π^{SE} and Π^{EX} denote the self and exchange part of first-order polarization, while $G_1(q,\omega)$ and $G_2(q,\omega)$ are defined as

$$G_1(q,\omega)=\frac{\Pi^{SE}(q,\omega)}{v(q)[\chi^0(q,\omega)]^2},\quad G_2(q,\omega)=\frac{\Pi^{EX}(q,\omega)}{v(q)[\chi^0(q,\omega)]^2}\ . \tag{A5}$$

According to Refs. 21 and 22 the following expression holds:

$$\Pi^{SE}(q,\omega)+\Pi^{EX}(q,\omega)=\sum_{\substack{\mathbf{k},\mathbf{p},\\ \sigma,\sigma'}}\delta_{\sigma\sigma'}\mathrm{v}(\mathbf{k}-\mathbf{p})\frac{(\mathrm{n}^0_{\mathbf{k}-\mathbf{q}/2}-\mathrm{n}^0_{\mathbf{k}+\mathbf{p}/2})(\mathrm{n}^0_{\mathbf{p}-\mathbf{q}/2}-\mathrm{n}^0_{\mathbf{p}+\mathbf{q}/2})}{\omega-\mathbf{p}\cdot\mathbf{q}/m}\left[\frac{1}{\omega-\mathbf{p}\cdot\mathbf{q}/m}-\frac{1}{\omega-\mathbf{k}\cdot\mathbf{q}/m}\right]\ . \tag{A6}$$

The static structure factor can then be obtained by making use of Eq. (4). In doing so, Eq. (A6) is supplemented by the RPA, i.e., the direct contributions in v^1, which are conveniently grouped together with the last term in the above formula. The frequency integration then immediately yields

$$-\frac{1}{N\pi}\int_0^\infty d\omega\coth\left[\frac{\beta\omega}{2}\right]\mathrm{Im}\{v(q)[\chi^0(q,\omega)]^2+\Pi^{EX}(q,\omega)\}$$
$$=-\frac{1}{N}\sum_{\substack{\mathbf{k},\mathbf{p},\\ \sigma,\sigma'}}[v(q)-\delta_{\sigma\sigma'}v(\mathbf{k}-\mathbf{p})]\frac{(n^0_{\mathbf{k}-\mathbf{q}/2}-n^0_{\mathbf{k}+\mathbf{q}/2})(n^0_{\mathbf{p}-\mathbf{q}/2}-n^0_{\mathbf{p}+\mathbf{q}/2})}{\varepsilon_{\mathbf{k}-\mathbf{q}/2}-\varepsilon_{\mathbf{k}+\mathbf{q}/2}-\varepsilon_{\mathbf{p}-\mathbf{q}/2}+\varepsilon_{\mathbf{p}+\mathbf{q}/2}}\coth\left[\frac{\beta\mathbf{p}\cdot\mathbf{q}}{2\cdot m}\right]\ . \tag{A7}$$

The properties of the Fermi function given by Eq. (10) imply the identity of Eqs. (A7) and (A4). Again additional contributions to $S(q)$ arising from $\Pi^{SE}(q,\omega)$ have no influence on $g(0,\Theta)$ and are therefore of no relevance.

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