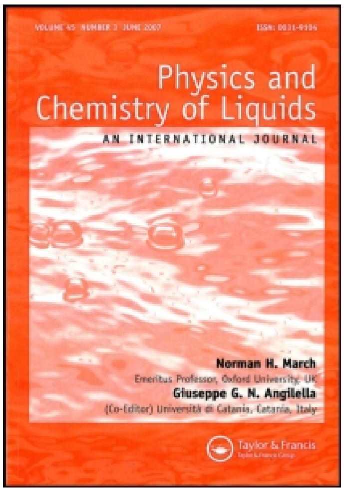

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SINGLE-PARTICLE SCATTERING APPROXIMATION FOR THE PAIR FUNCTION OF AN ELECTRON LIQUID: FULL NUMERICAL APPROACH

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The static pair correlation function of the three-dimensional homogeneous electron gas at given temperature and density is estimated by the scattering of non-interacting particles in an effective potential. The full numerical treatment of the self-consistency problem yields results that are in excellent agreement with those obtained within a generalized Thomas–Fermi approximation.

KEY WORDS: Jellium, nonzero temperature, pair function, effective interaction.

1 INTRODUCTION

In a previous paper[1] the basic principles of a *Single-Particle Scattering Approximation* (to be referred to as SPSA) for the pair function of an electron liquid have been formulated: One electron at the (arbitrarily chosen) origin of the many-electron system is the source of an effective single-particle interaction, in which the non-interacting collective is "moving". Consequently, the singled-out electron is treated as an impurity in the free Fermion system that is inducing a radial charge distribution around it. Using Poisson's equation the effective potential can be determined self-consistently together with the charge distribution.

In Ref. [1] the full self-consistency problem has been simplified by an additional approximation step, a generalized Thomas–Fermi approximation. Using this model the ground-state pair correlation function of interacting jellium at metallic densities could be calculated in excellent agreement with Monte-Carlo simulations. Furthermore, the interesting non-monotonical temperature dependence of the pair function at zero particle separation, which has been found by Schweng *et al.*[2], could also be investigated within this theory. Consequently, the main objective of the present work is to prove the validity of the generalized Thomas–Fermi approximation by numerically solving the full self-consistency problem.

This paper is organized as follows: In Section 2 the basic SPSA-equations are reformulated for full numerical treatment. Section 3 gives a brief description of the special methods necessary to obtain stable self-consistent solutions. The results obtained there are in excellent agreement with the generalized Thomas–Fermi approximation. Finally, a brief discussion in Section 4 ends this paper.

2 DESCRIPTION OF THE MODEL

Following Section 2 of Ref. [1] we can write down the basic equations for a simple SPSA:

$$\left\{\frac{\partial^2}{\partial x^2} + k^2 - \tfrac{1}{2}U(x) - \frac{l(l+1)}{x^2}\right\}u_{kl}(x) = 0 \tag{1}$$

$$n_l(x|U) = \frac{3}{2}\int_0^\infty dk\; n_k^0(\theta, \mu)\xi_l(k)\left(\frac{u_{kl}(x)}{x}\right)^2 \tag{2}$$

$$\xi_l(k)^{-1} \equiv \lim_{z\to\infty}\frac{1}{z}\int_0^z dx[u_{kl}(x)]^2 \tag{3}$$

$$n(x|U) = \sum_{l=0}^{\infty}(2l+1)n_l(x|U) \tag{4}$$

$$g(x|U) \simeq g^0(x) + \tfrac{1}{2}[n(x|U) - 1] \tag{5}$$

We are using the dimensionless units and symbols of Ref. [1] here too; in particular $x \equiv k_F r$, where k_F denotes the Fermi momentum. Eqs. (1)–(4) are the exact expressions for the local density of a pair-interaction free electron gas in the presence of a single-particle potentional $\frac{1}{2}U(x)$, expanded in terms of the radial density components. $n_k^0(\theta, \mu)$ denotes the free Fermi distribution at reduced temperature θ and chemical potential μ. Furthermore, the ansatz Eq. (5) provides a connection between the density of the inhomogeneous system and the approximated pair function of the homogeneous electron gas. It is this equation that characterizes the concrete realization of a SPSA. The replacement of Eq. (5) by a more sophisticated ansatz is possible, but beyond the scope of the present work. All together Eqs. (1)–(5) define the pair correlation function as a complex functional of the effective interaction $U(x)$.

To close the theory we interpret $U(x)$ as the electrostatic potential around a singled-out electron that is given by Poisson's equation (Eq. (1) of Ref. [1]). We can write down its most general solution as (for $x \leq \Lambda$)

$$f(x|g) = \frac{4}{3\pi}\int_x^\Lambda ds\{1 - g(s)\}s(s - x) + c_1(\Lambda) + c_2(\Lambda)x, \tag{6}$$

where the *screening factor* $f(x)$ is defined as $U(x)$ divided by the bare Coulomb potential:

$$U(x) \equiv \frac{2\alpha r_s}{x} f(x) \tag{7}$$

[r_s denotes the usual density parameter, and $\alpha \equiv (4/9\pi)^{1/3}$].

The cutoff-parameter Λ has been introduced for numerical reasons. Its physical interpretation is that of a 'system radius", outside whose sphere $f(x)$ is set to zero. A more sophiscated way to handle the asymptotic large $-x$ range is to use Eq. (6) for $x \leq \Lambda$ and the Thomas–Fermi approximation Eq. (21) of Ref. [1] for $x > \Lambda$. The numerical analysis, however, shows that this does not lead to any relevant improvement as long as Λ is chosen sufficiently large ($\Lambda \gtrsim 30$ for $\theta \lesssim 5$). Consequently, we write down the boundary conditions

$$f(0) = 1 \quad \text{and} \quad f(\Lambda) = 0 \tag{8}$$

and obtain from Eq. (6) the corresponding values for c_1 and c_2:

$$c_1(\Lambda) = 1 - \frac{4}{3\pi} \int_0^\Lambda ds\, s^2\{1 - g(s)\} \tag{9a}$$

$$c_2(\Lambda) = -\frac{c_1(\Lambda)}{\Lambda} \tag{9b}$$

3 NUMERICAL APPROACH

The combination of Eqs. (6) and (9) defines the screening factor $f(x)$ as a functional of the pair function $g(x)$. Since the numerical methods necessary to successfully evaluate the functional $g(x|U)$ [Eqs. (1)–(5)] have been discussed already in Section 4 of Ref. [1], we can concentrate here on the problem of how to determine $g(x|U)$ self-consistently with $f(x|g)$.

The solution of two coupled, nonlinear functional equations is indeed one of the most challenging problems in numerical analysis. It is well-known from, e.g., calculations within the Kohn–Sham density functional formalism[3] that the straight iteration method fails in most practical situations. This is caused by the occurrence of instabilities during the iteration cycle that are driving the algorithm into divergence. This is also true for the present case.

Among the various methods to damp oscillations during the iterative process Anderson's mixing[4,5] provides a good tradeoff between convergence enhancement and calculational effort. Following the work by Johnson[6] we characterize the m-th iteration step by inserting an "input" density distribution $n_i^{(m)}$ into Eq. (5), combining it with Eq. (6), and then calculating an "output" density $n_o^{(m)}$ from the resulting potential, using Eqs. (1)–(4). The "input" density for the next step is then calculated as

$$n_i^{(m+1)} = (1-\gamma)\bar{n}_i^{(m)} + \gamma\bar{n}_o^{(m)}, \tag{10}$$

where

$$\bar{n}_{i(o)}^{(m)} \equiv (1-\beta)n_{i(o)}^{(m)} + \beta n_{i(o)}^{(m-1)}. \tag{11}$$

Therein the parameter $\gamma \in [0, 1]$ is chosen empirically, but an *optimal* value for β can be obtained for each iteration step from a simple functional of the numerical "distances" between the "input" and "output" densities (confer Eq. (4) of Ref. [6]). It is also noteworthy that for a fixed $\beta = 0$ this algorithm reduces to the well-known so called "simple mixing" method.

Adopting Anderson's mixing algorithm for the present problem yields rapid and stable convergence for all interesting values of the parameters r_s and θ. On the average about 10 iterations are necessary to obtain sufficiently accurate results at metallic densities (using $\gamma = 0.1$). In the contrary, the "simple mixing" methods needs typically over 100 iterations and is rather unstable, i.e. small changes in the parameters can cause it to fail at all.

In Figure 1 the resulting pair correlation function for $r_s = 3$ is compared with the generalized Thomas–Fermi approximation from Ref. [1]. It is seen that the largest differences appear in the ground-state, while at $\theta = 3$ the two curves are

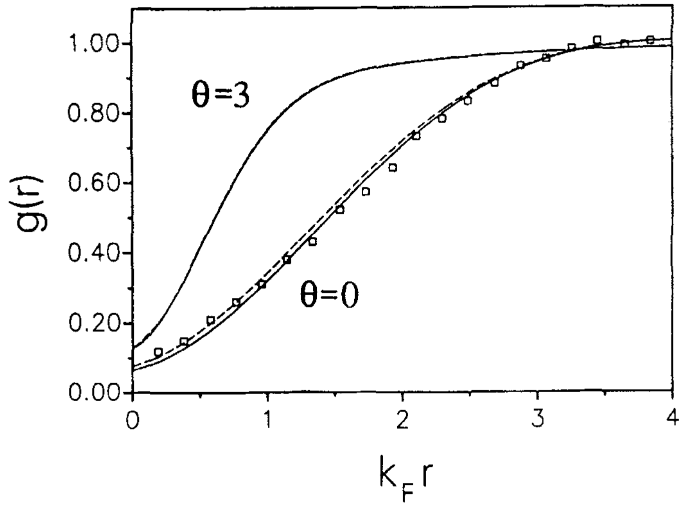

Figure 1 The pair correlation function $g(r)$ versus $k_F r$ for $r_s = 3$ and two reduced temperatures θ. The results of the full self-consistency problem (full lines) are compared with those of the generalized Thomas–Fermi approximation[1] (dashed lines). The squares are the result of a ground-state Monte-Carlo simulation; the data have been taken from Figure 3 of Ref. [9].

almost identical within the thickness of the lines. The corresponding screening factors $f(x)$ are compared in Figure 2. The deviations of the full numerical analysis from the approximated one are more significant in this case, but still do not provide a basis for serious criticism. Finally, a plot of $g(0)$ versus r_s for various approaches is seen in Figure 3.

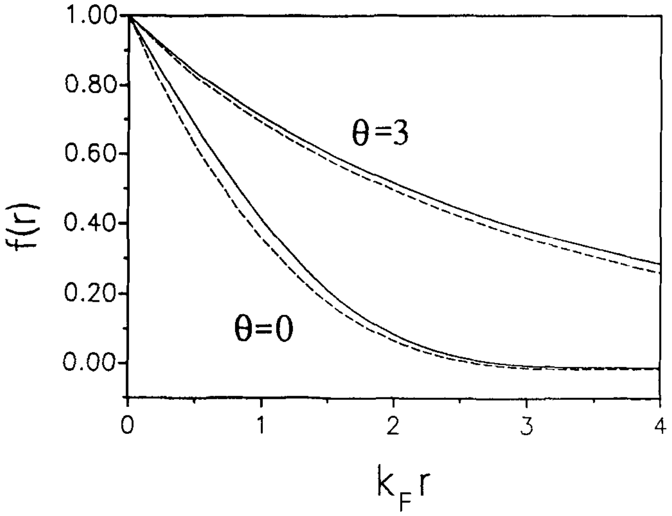

Figure 2 The screening factor $f(r)$ [confer Section 2] versus $k_F r$ for $r_s = 3$ and two reduced temperatures θ. The results of the full self-consistency problem (full lines) are compared with those of the generalized Thomas-Fermi approximation[1] (dashed lines).

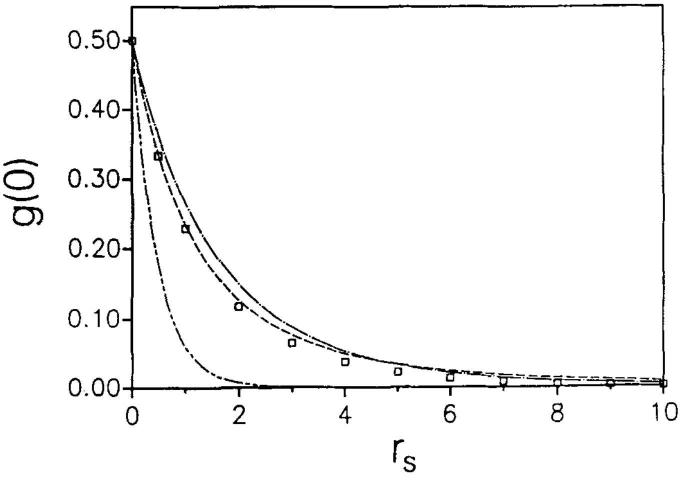

Figure 3 The pair correlation function $g(r = 0)$ at zero temperature versus r_s. The present full numerical solution (squares) is compared with the generalized Thomas-Fermi approximation[1] (dashed line), the estimation Eq. (13) (dash-double-dotted line), and the result of Yasuhara's theory[7] (dash-dotted line).

4 CONCLUSIONS

It was the main objective of the present paper to numerically prove the quantitive validity of the generalized Thomas–Fermi approximation, which has been used in Ref. [1] to simplify the self-consistency problem within the *Single-Particle Scattering Approximation* presented there. Taking into account that the effective potential more or less is only an auxiliary quantity, and consequently concentrating on the pair correlation function, the conformity indeed is excellent.

With this important result the intentions of Ref. [1] and the present work have been, on principle, fulfilled. Nevertheless, there are many questions remaining, and the perhaps most intriguing one among them simply is: How does it actually work, which means, how can such a complex many-particle quantity like the pair correlation function be modeled in such a realistic way by a relatively simple concept like the SPSA? From my point of view the answer most probably is that many aspects of the static correlations, even in a quantum liquid, are more simple than one would expect at first glance. A short calculation may confirm this standpoint:

The basic principle of a SPSA is to represent the pair correlation function by a tunneling probability. Consequently, one can tentatively simplify the scenario to an absolute minimum by just calculating the transmission coefficient of an electron through the (bare) Coulomb barrier of another one. Within WKB-approximation the result is simply given by

$$|T|^2 \simeq \exp\left[-2\int_0^{x_t} dx\, P(x)\right] \tag{12a}$$

with

$$P(x) \equiv [U(x) - E]^{1/2}. \tag{12b}$$

$U(x)$ is the potential barrier, E the energy of the scattered electron (both in units of the Fermi energy), and x_t denotes the classical turning point $P(x_t) = 0$. Now, setting E equal to the mean kinetic energy per particle of the free system ($E = \frac{3}{5}E_F$), substituting $\frac{1}{2}$ of a bare Coulomb potential for $U(x)$, and modeling $g(0)$ as $\frac{1}{2}$ of the transmission probability (to include Pauli's principle), one finally arrives at

$$g(0) \simeq \tfrac{1}{2}\exp\left(-\pi\sqrt{\tfrac{5}{3}}\alpha r_s\right) \simeq \tfrac{1}{2} - 1.057\cdot r_s + \mathcal{O}(r_s^2). \tag{13}$$

The plot of Eq. (13) is shown in Figure 3 together with the present SPSA—result and $g(0)$ obtained by Yasuhara's theory[7]. It is seen that Eq. (13) significantly overestimates the short-range correlations, which is, e.g., expressed by the fact that the absolute value of the linear expansion coefficient in Eq. (13) is by a factor of 3 too high, when compared with the exact result obtained by Kimball[8]. Nevertheless, even this extremely reduced form of a SPSA yields a more appropriate description of $g(0)$ than, e.g., the *Random Phase Approximation*, when going to metallic densities.

Of course, introducing screening effects into $U(x)$ of Eq. (13) would again improve the model towards the direction of the more sophisticated SPSA discussed in the preceding sections. However, the reader should also be aware of the fact that the WKB-approximation in Eq. (13) is used beyond its range of validity, which is given by the condition

$$(E_F)^{1/2}\cdot\left|\frac{dP}{dx}\right| \ll P(x)^2. \qquad (14)$$

The inequality Eq. (14) is not fulfilled when x tends to zero.

Nevertheless, the only purpose for presenting the crude approximation Eq. (13) was to confirm the conclusion that the static correlations described by the pair function are dominated by *single-particle* processes. This is perhaps the most important result that has been obtained within the present concept. However, it is quite probable that there are more subtle properties of the static correlations that *cannot* be modeled satisfactorily within a SPSA. It will be left to future investigations to assess what those properties might be.

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