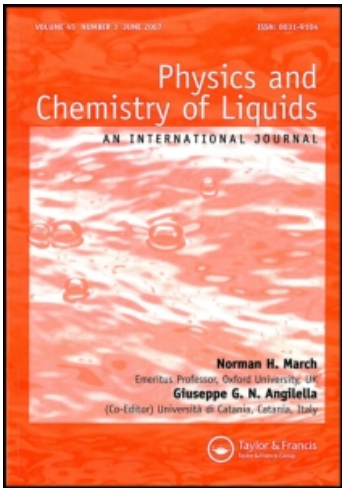

Physics and Chemistry of Liquids
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713646857

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To cite this Article Schinner, Andreas(1988) 'Numerical Solution of the Dawson-March Model for the Pair Function of an Electron Liquid', Physics and Chemistry of Liquids, 18: 2, 117 — 122
To link to this Article: DOI: 10.1080/00319108808078585
URL: http://dx.doi.org/10.1080/00319108808078585

Phys. Chem. Liq., 1988, Vol. 18, pp. 117-122
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Printed in the United Kingdom

Numerical Solution of the Dawson–March Model for the Pair Function of an Electron Liquid

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(*Received 3 February 1988*)

Reformulating the free-fermion pair correlation function, Dawson and March found an integral equation for an effective single particle potential, leading to a new approximation for interacting jellium. This equation is investigated within two regions: For $r_s \ll 1$ an exact solution can be found, for arbitrary densities numerical solutions are obtained.

Key Words: Poisson's equation, Kimball relation, jellium.

1 INTRODUCTION

An interesting new approach to determine the pair correlation function $g(r)$ of isotropic jellium was developed by Dawson and March in 1984[1]. Starting from the non-interacting Fermi liquid, they found a possibility to express the free pair function in terms of the p-component of the free electron density matrix. By then introducing an effective single particle potential $V(r)$, the pair interaction was approximately taken into account within this framework. Finally, writing down $g(r)$ as a linearized functional of V and combining this result with Poisson's equation led them to a linear integral equation for V.

In the present paper I shall first show that an exact solution for this equation can be found in the high density limit. Furthermore, the results of numerical calculations for arbitrary density values will be presented. A brief discussion of the resulting $g(r)$ ends this paper.

2 CALCULATION SCHEME AND HIGH DENSITY SOLUTION

Introducing the dimensionless variables $x \equiv k_f r$ and $V(r) \equiv Ryd \cdot u(x)/x$, one can write down Eqs (4) and (8) of Ref. 1 as

$$g(x) = g_0(x) + \tfrac{3}{8}\pi\alpha r_s \frac{u''(x)}{x} \tag{1}$$

and

$$u''(x) = -\beta r_s x^{-2}\left\{G_1(x)\int_x^\infty u(s)G_2(s)ds + G_2(x)\int_0^x u(s)G_1(s)ds\right\} \tag{2}$$

with

$$\begin{aligned} G_1(x) &\equiv x j_1^2(x) \\ G_2(x) &\equiv x j_1(x)\tilde{n}_1(x) \\ g_0(x) &\equiv 1 - \tfrac{9}{2}G_1(x)x^{-3} \end{aligned} \tag{3}$$

$$\alpha \equiv \left(\frac{4}{9\pi}\right)^{1/3} \simeq 0.52106$$

$$\beta \equiv 24\alpha/\pi \simeq 3.98062$$

$j_1(x)$ and $\tilde{n}_1(x)$ are the first-order spherical Bessel and Neumann functions, respectively; $r_s = a_B^{-1}(\frac{4}{3}\pi n)^{-1/3}$ denotes the usual density parameter.

Since Eq. (2) is linear with respect to $u(x)$, an additional normalization condition is required, in order to obtain a definite $g(x)$ from Eq. (1). As the resulting g should satisfy Kimball's relation[2]

$$g'(0) = \alpha r_s g(0) \tag{4}$$

the combination of Eqs (1) and (4) leads to

$$g(x) = g_0(x) + \alpha r_s[u^{IV}(0) - 2\alpha r_s u^{III}(0)]^{-1}u''(x)/x \tag{5}$$

$u(x)$ is now an arbitrarily normalized solution of Eq. (2).

Integrating twice, Eq. (2) can be rewritten as

$$u(x) = \int_x^\infty ds \int_s^\infty dt\ \mathrm{rhs}[u; t] + u'(\infty)x + u(\infty) \tag{6}$$

where rhs$[u; t]$ stands for the right hand side of Eq. (2). Because $V(r)$ has to vanish as $r \to \infty$, $u'(\infty)$ must be equal to zero.

It can easily be shown that

$$u''(x) = Ar_s x^{-2}H(x) + O(r_s^2) \tag{7}$$

with

$$H(x) \equiv G_1(x)\int_x^\infty G_2(s)ds + G_2(x)\int_0^x G_1(s)ds \tag{8a}$$

or, having carried out the integrals,

$$H(x) = \tfrac{1}{2}G_1(x)\{\mathrm{si}(2x) - 2j_1(2x)\} \tag{8b}$$
$$+ \tfrac{1}{2}G_2(x)\left\{\frac{\sin(2x)}{x} - \left(\frac{\sin(x)}{x}\right)^2 + \ln(x) - \mathrm{ci}(2x) + C - 1\right\}$$

solves Eq. (6) in the high density limit. (si and ci are the Sine and Cosine Integral, respectively; C denotes Euler's constant.) Inserting the expansion

$$H(x) \simeq \begin{cases} -\dfrac{x^3}{36}(\pi - x) & \text{for } x \ll 1 \\ \dfrac{\sin(2x)}{4x}\ln(x) & \text{for } x \gg 1 \end{cases} \tag{9}$$

into Eq. (5), one finds

$$g(0) = \frac{1}{2} - \frac{\pi}{2}\alpha r_s + O(r_s^2) \simeq \frac{1}{2} - 0.8184 r_s + O(r_s^2) \tag{10}$$

Comparing this result with the exact high-density expansion, obtained by Kimball[3]

$$g(0) = \tfrac{1}{2} - 0.36584 r_s - 0.032966 r_s^2 \ln(r_s) + O(r_s^2) \tag{11}$$

an at least approximate conformity is found.

3 NUMERICAL APPROACH

Using Eq. (6) with $u'(x \to \infty) = 0$, one can define the iteration scheme

$$u_{n+1}(x) = \int_x^\infty ds \int_s^\infty dt\ \mathrm{rhs}[u_n; t] + u(\infty) \tag{12}$$
$$u_0(x) \equiv u(\infty)$$

which proves itself converging very fast, especially in the metallic density range ($2 < r_s < 6$). The resulting solutions $u(x)$, normalized to $u(0) = 1$, are shown in Figure 1 for various r_s-values. The corresponding results for $g(r)$, obtained from Eq. (5), can be seen in Figure 2. Finally, the curves in Figure 3 compare $g(r = 0; r_s)$, calculated from Eqs (3) and (5), with the Yasuhara result.[4]

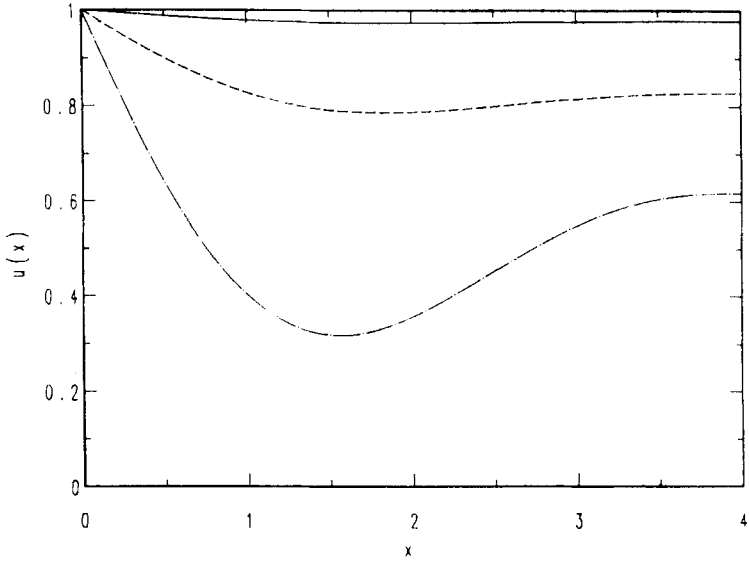

Figure 1 Numerical solutions of Eq. (2) with the initial conditions $u(0) = 1$ and $u'(x \to \infty) = 0$ for $r_s = 0.1$ (solid line), $r_s = 1$ (dashed line) and $r_s = 10$ (dash-dotted line).

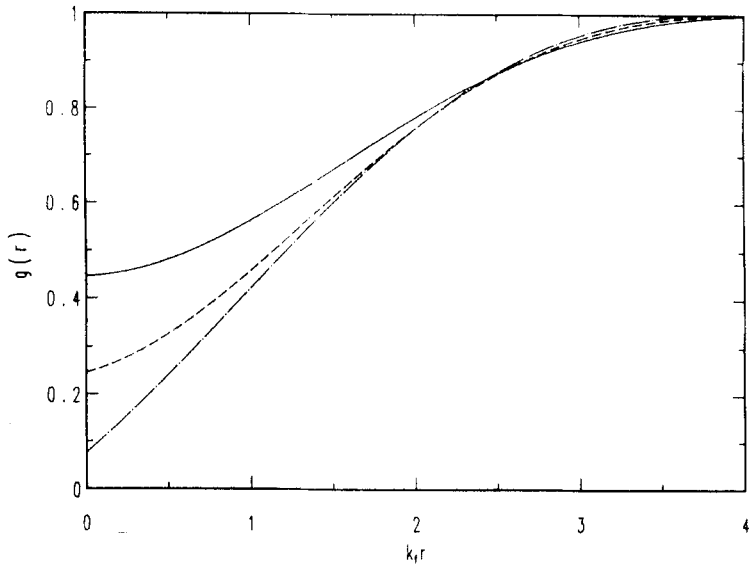

Figure 2 The pair correlation function $g(r)$ versus $k_f r$, calculated from Eq. (5), using $u(x)$ from Figure 1. The curves are corresponding to the r_s-values 0.1 (solid line), 1 (dashed line) and 10 (dash-dotted line).

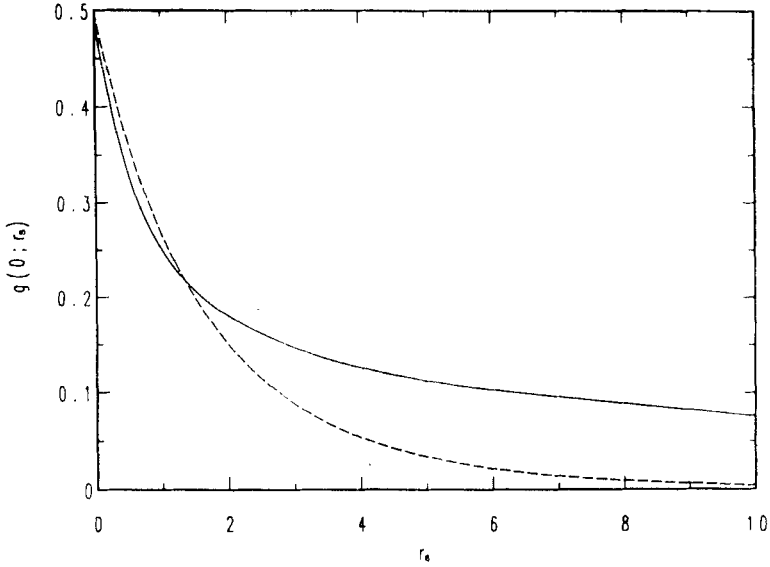

Figure 3 The pair correlation function $g(r = 0)$ versus r_s from the present results (solid line) and the Yasuhara theory[4] (dashed line).

4 CONCLUSION

The numerical results as well as the high-density solution of the Dawson-March-approximation seem to confirm the at least qualitative validity of their method. Although it is obvious from Figure 3 that $g(0; r_s \gg 1)$ is decreasing too slowly within this approximation, one has to bear in mind that the derivation of Eq. (2) already contains a linearization step, which, on principle, is limiting the theory to the case $r_s \ll 1$. But even beyond that region this method provides a positive $g(0; r_s)$, which is still comparable to the results of some much more comprehensive theories.[5] A further improvement could probably be achieved by incorporating higher order terms in Eq. (2), i.e. solving the full nonlinear model. In the present linearized theory, however, the calculation of $g(r)$ can be carried out quickly enough, so that it might be of interest, to somehow combine this method with other approximations, e.g. of the FHNC[6] or pseudoclassical[7] type. In any case it should be the most important as well as comprehensive task to deepen the understanding of the many-body principles, which are causing the *ansatz* Eqs (1) and (2) to result in such a surprisingly realistic pair correlation function.

Acknowledgements

The author wishes to thank Professors N. H. March and W. Macke for valuable and stimulating discussions.

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