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DAWSON–MARCH MODEL FOR THE PAIR FUNCTION OF A TWO-DIMENSIONAL ELECTRON LIQUID

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Based on the functional representation for the pair function developed by Dawson and March the ground state correlations of a two-dimensional electron gas are investigated. The method appears to produce reliable results for high and intermediate densities. Although the approach contains a linearization step using first order Born's approximation, the resulting zero-distance-correlations remain positive.

KEY WORDS: Jellium, pair correlations, effective potential, Kimball relation.

1 INTRODUCTION

The two-dimensional (2D) electron gas has been found a fruitful model for the description of electrons in MOS inversion layers as well as semi-conductor quantum wells and heterojunctions¹. There is ample evidence that in these systems the electrons are dynamically confined in a plane. The attractiveness of these structures stems from the possibility of varying the electronic density over a very large range.

From the many body point of view it is to be noted that short range correlations are much more important in the 2D than in the 3D case. This effect is usually expressed in the pair distribution function g of the system, which has therefore been studied by a variety of methods^{2–13}: Self consistent (so-called 'STLS') calculations^{2–4} have led to very accurate results for the correlation energy as compared to Monte Carlo computations^{5,6}. They suffer, however, from the well known deficiency of yielding negative values at small distances. The validity of ladder-summations^{7,8}, which remove this weakness, is restricted to very small particle separations. More refined theories such as coupled-cluster⁹ or approximative Fermi-hypernetted-chain calculations¹² require a very high computational effort. Thus a simpler and less time consuming calculation method would be desirable.

In the 3D system the heuristic approach of Dawson and March^{14,15} (DM) as evaluated by A. Schinner¹⁶ has proved to produce realistic results over a wide range

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of densities. It is based on a generalization of the free pair distribution function formula to a density functional of an effective single particle potential. The latter is determined self consistently by Poisson's equation. The aim of the present work is to adapt this procedure for the 2D system and to investigate the validity of the model in this case.

In Section 2 the ansatz of the pair distribution function is presented and a linear functional of the effective potential w is obtained for g . Section 3 gives the derivation of w as a functional of g . Finally, numerical solutions and results are discussed in Section 3.

2 DERIVATION OF THE FUNCTIONAL $g(x|w)$

Following the basic concept developed by Dawson and March¹⁴ we start from a closer inspection of the free pair distribution function in the two-dimensional jellium system

$$g^0(x) = 1 - 2 \left[\frac{J_1(x)}{x} \right]^2 \quad (1)$$

($J_1(x)$ is denoting the first order Bessel function of the first kind). Here and in the following we are using dimensionless units that are measuring distances in k_f^{-1} , momenta in k_f , and energies in Rydbergs, where k_f is the Fermi momentum. Taking advantage of the analysis by March and Murray¹⁵, we can easily write down the expression

$$n_m(x) = \frac{2n}{\pi} \int_0^{k_f} dk \xi_m(k) \frac{u_{k,m}(x)^2}{x} \quad (2)$$

for the m th radial density component of the pair-interaction-free two-dimensional electron gas under the influence of an external one-particle potential $V(x)$, and with arbitrary Fermi momentum k_f . The $u_{k,m}(x)$ are then the—not necessarily normalized—real solutions of the radial Schrödinger equation

$$\left\{ \frac{\partial^2}{\partial x^2} + k^2 - (\alpha r_s)^2 V(x) - \frac{m^2 - \frac{1}{4}}{x^2} \right\} u_{k,m}(x) = 0 \quad (3)$$

to the given $V(x)$. The $\xi_m(k)$ are defined as

$$\xi_m(k)^{-1} \equiv \lim_{\zeta \rightarrow \infty} \frac{1}{\zeta} \int_0^\zeta dx u_{k,m}(x)^2 \quad (4)$$

and take care of the correct norm of the wave function in Eq. (2). r_s in Eq. (3) is the usual density parameter that is connected to the average density n in Eq. (2) by the relation $n^{-1} = \pi(r_s a_B)^2$, where a_B stands for the Bohr radius; α is an abbreviation for $1/\sqrt{2}$.

For vanishing external potentials $V(x)$ the fundamental solutions of Eq. (3) can be

found easily

$$\begin{aligned}
 u_{k,m}^0(x) &= \left(\frac{\pi}{2} kx\right)^{1/2} \cdot J_m(kx) \\
 v_{k,m}^0(x) &= \left(\frac{\pi}{2} kx\right)^{1/2} \cdot N_m(kx).
 \end{aligned}
 \tag{5a,b}$$

J_m and N_m denote the m th order Bessel and Neumann functions¹⁷, respectively. Hence, we realize that Eq. (1) can be rewritten in terms of Eqs. (2) and (5) as

$$g^0(x) = 1 - x^{-2} \left[\frac{1}{n} \frac{\partial}{\partial k_f} n_1(x) \right]_{k_f=1}. \tag{6}$$

The basic idea within the Dawson–March approximation now is to generalize the exact result Eq. (6) to the case of the interacting Fermi fluid, where the effects of the pair interaction will be simulated by a single particle potential $V(x)$ in $n_1(x)$. Thus we interpret Eq. (6) as a functional of V

$$g(x|V) = 1 - \frac{2}{\pi x^2} \xi_1(1) u_{1,1}(x)^2 \tag{7}$$

where ξ_1 and $u_{1,1}$ must be calculated from Schrödinger’s equation (3) using the potential $-V(x)/2$ (the $-1/2$ is due to the fact that a repulsive potential should decrease $g(0)$, and that two electrons of equal masses are scattering). $V(x)$ then has the meaning of a local field corrected Coulomb potential that is globally taking into account the interaction effects of $g(x)$ via a correction of the exchange contributions in Eq. (1). This potential is determined in a self consistent way together with the pair correlation function in the next chapter. Here we end with a further simplification of the functional Eq. (7) by evaluating the wave function $u_{1,1}(x)$ within first order perturbation theory for $V(x)$. This leads us to the final result

$$\begin{aligned}
 \Delta g(x|w) &= g(x|V) - g^0(x) \\
 &= \frac{\pi r_s^2}{x^2} \left\{ J_1(x) N_1(x) \int_0^x ds w(s) J_1(s)^2 + J_1(x)^2 \int_x^\infty ds w(s) J_1(s) N_1(s) \right\} \tag{8}
 \end{aligned}$$

where we have introduced $w(x) \equiv x \cdot V(x)$.

3 EFFECTIVE POTENTIAL $w(x|g)$

The deviation of $g(x)$ from $g^0(x)$ gives essentially the probability of finding a particle at a distance x from a given particle in the origin due to exchange and correlation effects. Correspondingly Δg can be interpreted as being roughly equivalent to an induced particle density of

$$\rho^{\text{ind}}(x, z) = n \Delta g(|x|) \delta(z), \tag{9}$$

where n denotes the area density of the charge layer. Although in a real quantal system the charge distribution always has a finite width in the z -direction, the model of a strictly 2D electron gas is assumed in Eq. (9), since correlation effects are most pronounced in the latter case². The applicability of the DM model beyond the 3D system is thus most severely tested. The use of (9) in Poisson's equation immediately results in the following induced potential (in Rydbergs)

$$V^{\text{ind}}(x|\Delta g) = \frac{4}{\pi\alpha r_s} \left[\int_0^x ds \frac{s}{x} K\left(\frac{s}{x}\right) \Delta g(s) + \int_x^\infty ds K\left(\frac{x}{s}\right) \Delta g(s) \right]. \quad (10)$$

(K denotes the elliptic integral of the 1st kind).

To this the potential of the particle in the origin must be added. Limit analysis of Δg and V shows that in order to fulfill Kimball's relation¹⁸

$$g'(0) = 2\alpha r_s g(0), \quad (11)$$

the bare Coulomb potential has to be corrected by a factor a with

$$a = 3g(0). \quad (12)$$

It is interesting to note the similarity with local field corrected potentials¹², which, too, have an effective short-range Coulomb interaction modified by the value of $g(0)$ due to Niklasson's relation^{19,20} for the local field correction^{19,2} $G(q) \sim [1 - g(0)]$ for large momenta q .

The expression for the one-body potential $w = xV$ appearing in Eq. (8) for $g(x|w)$ then finally reads

$$w(x|\Delta g) = \frac{4}{\pi\alpha r_s} \left[\frac{a\pi}{2} + \int_0^x ds s K\left(\frac{s}{x}\right) \Delta g(s) + \int_x^\infty ds x K\left(\frac{x}{s}\right) \Delta g(s) \right]. \quad (13)$$

4 RESULTS AND DISCUSSION

In the 3D case Poisson's equation leads to a comparatively simple homogeneous integro-differential equation for w as presented in Ref. 16. For the 2D problem, however, the self consistent solution strategy had to be modified by iterating Eqs. (8) and (13). In order to improve convergence properties, a linear combination of the two previous steps was used as input for the next iteration. While the effective one-body potential shows some sensitivity to the numerical parameters used, the quantity of main interest, the pair distribution function, is hardly influenced by such variations.

The solutions obtained for $w(x)$ are shown in Figure 1 for three different values of r_s . As in the 3D case the structure is more pronounced with increased coupling strength. Figure 2 gives a comparison of the corresponding pair correlation functions.

Finally, the values for $g(0)$ as calculated from the DM model are compared with other theories. Short range correlations being mainly determined by two-particle scattering processes, reliable results for $g(0)$ have been obtained by summation of

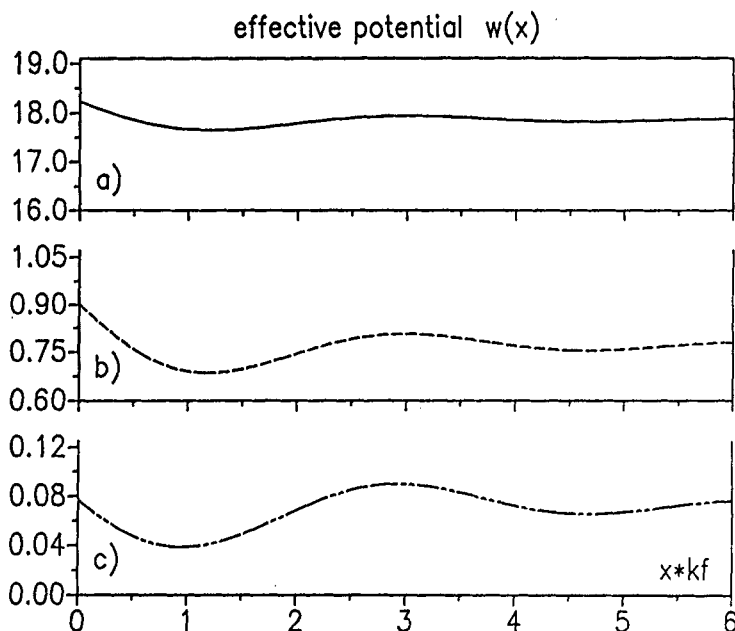


Figure 1 Results for $w(x)$ from the self consistent solution of Eqs. (8, 13). a) $r_s = 0.1$ (solid line), b) $r_s = 1$ (dashed line) and c) $r_s = 512$ (dash-dotted line).

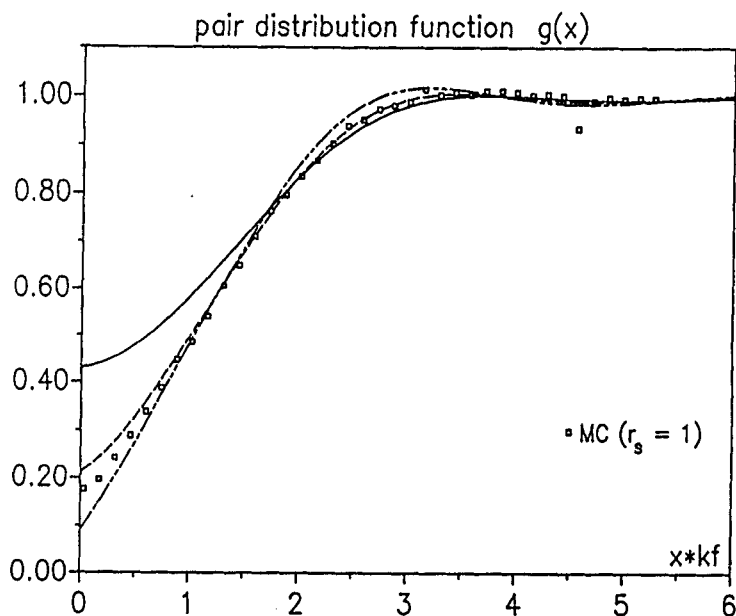


Figure 2 Self consistent results for the pair correlation function $g(x)$ for various densities: $r_s = 0.1$ (solid line), $r_s = 1$ (dashed line) and $r_s = 5$ (dash-dotted line). The squares denote the Monte-Carlo results of Ref. 6.

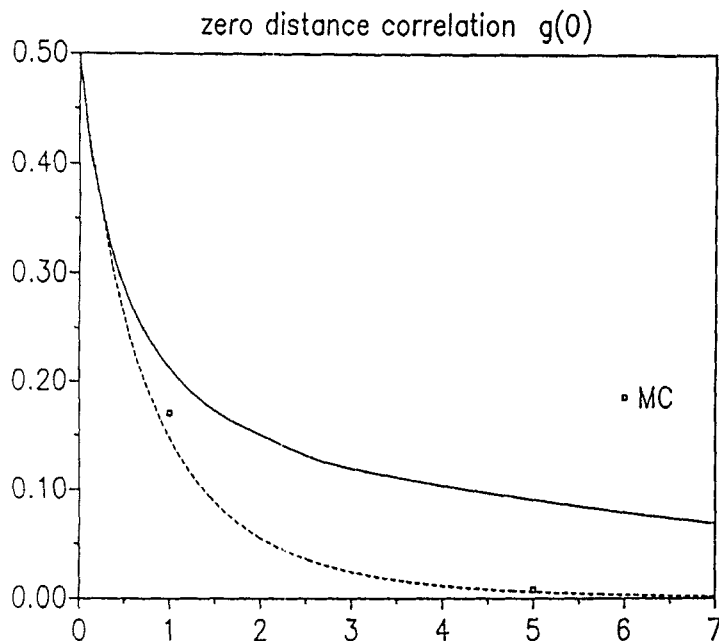


Figure 3 Zero distance pair correlation $g(x=0)$ versus r_s from the present theory (solid line) and the ladder summation, Eq. (14) (dashed line). The squares denote the Monte-Carlo results of Ref. 6.

Goldstone ladder diagrams^{7,8}. Figure 3 shows the comparison of DM with their approximate analytical evaluation⁷, i.e.

$$g(0) = 0.5[I_0(2\sqrt{\alpha r_s})]^{-2}. \quad (14)$$

Table 1 shows $g(0)$ for different values of r_s obtained in the various approaches: Dawson–March (present), first order perturbation theory (Ref. 11), STLS (Ref. 2), analytical⁷ and numerical⁸ ladder summation, coupled-cluster (Ref. 9), and finally Monte-Carlo (Ref. 6) calculations. Strictly speaking, the validity of DM is restricted to the small coupling region due to the linearization of $g(x|w)$. This explains the less satisfactory behaviour for large r_s . (In addition, the numerical effort required to obtain

Table 1 Pair distribution function at zero distance.

| r_s | DM | 1.0. | STLS | Lad(A) | Lad(N) | CCM | MC |
|-------|------|-------|------|--------|--------|------|------|
| 0.5 | 0.29 | 0.15 | 0.32 | 0.26 | 0.31 | 0.30 | — |
| 1.0 | 0.21 | -0.21 | — | 0.15 | 0.21 | 0.21 | 0.17 |
| 2.0 | 0.15 | -0.92 | — | 0.06 | 0.13 | 0.12 | — |
| 4.0 | 0.10 | -2.30 | 0.03 | 0.01 | — | 0.05 | — |

stable results is increased significantly for $r_s \gtrsim 7$). In the $r_s \ll 1$ limit

$$g(0) = 0.5 - \gamma r_s + \mathcal{O}(r_s^2) \quad (15)$$

with

$$\gamma^{1.\text{Ord}} = 0.71 \quad \gamma^{\text{DM}} = 0.82$$

the conformity is also good. While in the perturbational treatment¹¹, which is also a weak coupling approach, $g(0)$ turns negative at $r_s \approx 0.7$, the DM values appear to remain positive over the whole density range investigated. In addition, they are surprisingly good up to $r_s \approx 2$.

In summary, the DM approximation has been shown to yield satisfactory results for the 2D pair correlation function over an appreciable density range. The theory gives positive $g(0)$ values for all parameters investigated, but, as expected, tends to break down for strong coupling. The overall behaviour of the results is similar to the corresponding 3D case¹⁶.

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