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LETTER TO THE EDITOR

# Asymptotic behaviour of the equilibrium pair correlation in the classical electron gas

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**Abstract.** The non-convolution graphs, sometimes referred to as bridge graphs, which figure in the Mayer–Salpeter expansion of the potential of average force $w_2(r)$ with respect to the plasma parameter, are systematically studied. They decrease at infinity faster than the first-order Debye graph $e^{-r}/r$. An exact expression for $w_2(r)$ which allows a systematic improvement of the hyper-netted chain (HNC) approximation is obtained.

The optical diagnostics of hot and dense plasmas considered in the laser fusion programme (Chapline *et al* 1975) have recently prompted the need for an accurate knowledge of the asymptotic behaviour of the pair correlation function $g_2(r)$ of the classical one-component Coulomb gas. Recently several authors have investigated the structure of the expansion, with respect to the plasma parameter $\Lambda = U(\lambda_D)/k_B T$ with $U(\lambda_D)$ an average interaction potential at screening (Debye) distance $\lambda_D$, of the potential of average force $w_2(r)$ defined as

$$g_2(r) = \exp(w_2(r)/k_B T), \tag{1}$$

in the two-dimensional (Deutsch and Lavaud 1973) and three-dimensional (del Rio and De Witt 1969, Cohen and Murphy 1969) cases.

It is already known (authors cited above, Mitchell and Ninham 1968) that the longest convolution chains built from $c$ $(=0, \ldots, n)$ Debye chains and $(n-1)$ simple bubbles (two Debye chains curved together) provide the most important contribution to the asymptotic behaviour of $g_2(r)$ as far as the convolution graphs of order $n$ in $\Lambda$ are considered. Also, Cooper (1973), Springer *et al* (1973) and Ng (1974) have been able to reproduce the Monte Carlo data for $g_2(r)$ (Brush *et al* 1963, 1966, Hansen 1973) with the aid of the HNC equation with an amazing accuracy for nearly all values of $\Lambda$. These results appear as very comforting if one remembers that the sum of the Fourier transforms of the convolution chains with simple bubbles for all $n$ reproduces the content of the HNC equation (del Rio and De Witt 1969). All these calculations have had to assume from the beginning that the HNC approach with only the convolution graphs retained (Van Leeuwen *et al* 1959) is the correct one. They then suffer from the lack of knowledge of the asymptotic behaviour of the bridge graphs systematically neglected in the derivation of the HNC equation.

With the purpose of justifying that the above conjecture is correct, we rely ourselves upon the Mayer–Salpeter expansion (Salpeter 1958) of $w_2(r)$ recently used in the two-dimensional case (Deutsch and Lavaud 1973). In order to handle easily the asymptotic behaviour of higher-order graphs ($n \geqslant 3$) without spurious difficulties associated with the short-range behaviour, we may replace, whenever necessary, the classical Coulomb interaction $r^{-1}$ with an effective one, taking into account the diffraction correction ($\hbar = 0$), ie $r^{-1}(1-e^{-Cr})$ with $C \sim$ (thermal De Broglie wavelength)$^{-1}$.

A graph of order $n$ is given (Salpeter 1958) by its $l$ Debye bonds and its $k$ nodal points where at least three bonds merge in with $l-k = n$. The first non-convolution and strongly connected graph is known to appear with $n = 3$ and their number together with the number of convolution chains and of mixed chains (Mitchell and Ninham 1968) increases rapidly with $n$. The $n$th-order bridge graphs, generated by joining any two points (including the root points), a line and a point, or a line and a line in the $(n-1)$th-order bridge graphs, may all be derived from the third-order bridge graph. The Fourier transform convolution methods (del Rio and De Witt 1969, Cohen and Murphy 1969, Deutsch and Lavaud 1973, Mitchell and Ninham 1968), applied to the graphs containing at least one articulation point, have clarified that (i) at infinity they decrease more slowly than the $p$-bubbles ($2 \leqslant p \leqslant n$, $k = 0$) or the bridge graphs building them and that (ii) the dominant graph at infinity in this category for given $l \geqslant 2(n-1)$ and $k$ is the longest convolution chain with $(n-1)$ 2-bubbles and $c$ $(=0, 1, \ldots, n)$ Debye lines in between. On the other hand, it may be easily shown that the graphs with $n \leqslant l \leqslant 2(n-1)$ contribute most significantly to the $r \to 0$ range, while their asymptotic behaviour is controlled by $p$-bubbles with $p \geqslant 3$. Their topological structure is already present at lower orders. Therefore they differ from the corresponding graphs by one or more lines only and their asymptotic decrease is faster. We are thus led to study the asymptotic behaviour of the bridge graphs. Using a method exploited by Mitchell and Ninham (1968) and its extended versions (Deutsch *et al* 1975, Furutani and Deutsch 1975), we have been able to describe the Fourier transforms of the third- and fourth-order bridge graphs in the form $A-Bk^2$ for $|k|^2 \ll 1$ ($k$ is the conjugate to $r$) with $AB > 0$. The asymptotic behaviour of a given bridge $(l, k)$ graph is then written as

$$\lim_{r\to\infty} \text{bridge} \simeq C\beta e^{-\alpha r}/r \tag{2}$$

where $\beta = A^2/B$, $\alpha = (A/B)^{1/2} > 1$ and

$$C = (-1)^l\Lambda^n[8\pi^7/(2\pi^2)^n] \quad \text{or} \quad (-1)^l\Lambda^n[2\pi^7/(2\pi^2)^{n-1}],$$

according as no or one double bond is present. The result $\alpha > i$ which we have numerically obtained shows that these graphs decrease at infinity much faster than the first Debye term $e^{-r}/r$. This result checks the HNC hypothesis for $n = 4$. The same techniques will apply again for $n = 5$, but it seems very difficult to proceed farther for $n \geqslant 6$. We therefore address ourselves to an extension to the present situation of a remark due to Riddel and Uhlenbeck (1953) for short-range interactions which provides (Deutsch *et al* 1975, Furutani and Deutsch 1975)

$$\lim_{r\to\infty} |\text{bridge graph } (l, k)| \leqslant \frac{l\Lambda^n}{(4\pi)^k}\frac{e^{-(I-1)r}}{r}, \qquad \text{for all } n \tag{3}$$

where $I$ = degree of convection, defined as a minimum number of nodal points to remove in order that a given connected graph be disconnected with respect to the root points. Equation (3) allows us to disregard in the asymptotic range not only the numerous multiply connected structures present at all $l$ values, but also the shorter chains with the corresponding bridge graphs. The longest convolution chains made of

$c$ $(=0, 1, \ldots, n)$ Debye chains and $(n-1)$ 2-bubbles with $l \geqslant 2(n-2)$ show the characteristic behaviour $(b+c = k+1)$

$$\lim_{r\to\infty} |\text{convolution graph } (l, k)| \simeq \frac{\Lambda^n n!}{(n-c)!c!} \frac{1}{2^{2(n-1)}} \frac{(r/2)^{c-1}\mathrm{e}^{-r}}{(c-1)!}. \tag{4}$$

The comparison of equations (3) and (4) clearly shows the asymptotic pre-eminence of the convolution chain over all graphs with the same $l \geqslant 2(n-1)$ and $k$, ie in all subclasses $(l, k)$ of importance for $\lim_{r\to\infty} w_2(r)$. Consequently for a given $(l, k)$ pair, the number of mixed chains with not too strongly connected bubble is comparable with $(b+1)!/(b+1-c)!c!$, so that their more rapid decrease makes them negligible with respect to equation (4). These results enable us to extend to all orders the representation of $w_2(r)$, obtained by del Rio and De Witt (1969), through an iteration to infinity of the second-order graphs. We generalize thus the pattern of the longest convolution chains built from $(n-1)$ 2-bubbles and replace one of these bubbles with a bridge graph of order $n$. When the latter is 12-reducible, its first non-nodal contribution with no Debye legs is subtracted out to ensure the $k$-summability in the infinite range. The required resummation is realized by the geometric series (Mitchell and Ninham 1968) running from $n = 3$ to $n = \infty$. Of course, the replacement of two and more simple 2-bubbles is feasible, leading to the general expression (Deutsch *et al* 1975a, b)

$$\begin{aligned} w_2(r) = {} & -\frac{\mathrm{e}^{-r}}{r} + \frac{1}{r}\int_0^\infty \mathrm{d}k\, k \sin kr \left\{ \frac{k^2}{k^2+1} \frac{1}{1+1/k^2 - G(k)/\Lambda} \left[ G(k) + \sum_{n=3}^{\infty} \Lambda^n B_n(k) \right.\right. \\ & \left. + \sum_{p=2}^{\infty} \Lambda^{\sum_{i=1}^{p} n_i - 1 + p} \left( \frac{k^2}{k^2+1} \right)^{p-1} \sum_{n_1, \ldots, n_p = 3}^{\infty} B_{n_1}(k), \ldots, B_{n_p}(k) \right] \\ & \left. - G(k) - \sum_{n=4}^{\infty} \Lambda^n B'_n(k) \right\} \end{aligned} \tag{5}$$

where

$$G(k) = \frac{1}{k}\int_0^\infty \mathrm{d}r\, r \sin kr \sum_{n=2}^{\infty} \frac{(-\Lambda)^n}{n!} \mathrm{e}^{-nr} \overset{|k|^2 \leqslant 1}{\simeq} A(\Lambda) - B(\Lambda)k^2, \qquad \text{for all } \Lambda. \tag{6}$$

In equation (5) are removed all the bridge graphs with multiple bonds through a short-range resummation to all orders of the graphs with a given topology, ie from the replacement of the Debye bond $(k^2+1)^{-1}$ by the sum $G(k)$ of $n$-bubbles (Iwata 1960). We emphasize that the resulting graph decreases faster at infinity than the generic one with single bonds only. This remarkable result derives from the asymptotic behaviour displayed in equation (6).

$B_n(k)$ is then reduced to the sum, at each order, of the nodal 12-irreducible topology with single bonds only, topology appearing for the first time at order $n$. On the other hand, $B'_n(k)$ represents the corresponding sum for the 12-reducible graphs (Mitchell and Ninham 1968). Next, the neglected chains $(l < 2(n-1))$ with a more involved structure which decrease asymptotically much faster than the longest chains considered so far come into play, when in the denominator of the right-hand side of equation (5) we replace with $G(k)/\Lambda$ the customary 2-bubble term used by del Rio and De Witt (1969).

As a result, the $n$-bubbles sum $G(k)$ appears through the long-range resummation, in contradistinction to their attempts at introducing it from the beginning 'with the hands'. The subtracted terms do not include the 12-irreducible bridge graphs. The above calculations give rise to the first corrections to the standard second-order expression ($B_n(k) = B'_n(k) = 0$) in the form

$$\begin{aligned} B_3(k) &= -(0{\cdot}34907 - 0{\cdot}10343k^2) \\ B_4(k) &= -(0{\cdot}14912 - 0{\cdot}040197k^2) \\ B'_4(k) &= 2(0{\cdot}13594 - 0{\cdot}0089544k^2). \end{aligned} \tag{7}$$

A detailed analysis (Deutsch *et al* 1975, Furutani and Deutsch 1975) with $2 \leqslant p \leqslant 4$ shows that the integrand in equation (5) may be written as

$$\frac{k^2}{k^2+1} G_1(k) \left(1 + \frac{1}{k^2} - \frac{G(k)}{\Lambda}\right)^{-1} - G_2(k), \qquad G_1 \simeq G_2 \simeq G, \qquad \Lambda > 1. \tag{8}$$

This expression explains quite well the success of the usual HNC techniques using $G_1 = G_2 = G = G_0$. Here $G_0$ is the numerical result reached at the end of the iteration process. Our more flexible expression (8) paves the way to a systematic improvement of the HNC approach. Finally, a critical value $\Lambda_c$ giving the onset of short-range order could be obtained by solving $1 + 1/k^2 - G(k)/\Lambda = 0$ with $G(k)$ of equation (6). Further discussion about this point will be given in great detail in a separate paper.

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