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LETTER TO THE EDITOR

Exact calculations of Coulomb bridge graphs in one dimension

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Abstract. Bridge nodal diagrams built upon the screened Debye interaction are considered in $2+\epsilon$ dimensions for the classical one-component plasma (OCP) model. Their asymptotic behaviour is shown to be nearly ϵ-independent. They are evaluated analytically in one dimension. The corresponding asymptotic decay $\sim\exp(-K_k r)$, with K_k a positive integer ≥ 2, is thus extrapolated to any ϵ.

One of the main problems left unsatisfactorily solved (Deutsch 1978) in the nodal expansion with respect to the plasma parameter of the classical one-component plasma (OCP) model is the asymptotic behaviour of non-convolution and 1,2-irreducible (with respect to the root points 1 and 2) diagrams—the so-called bridge built on the first-order and screened Debye interaction. The asymptotic decay of these graphs is of paramount importance (Deutsch *et al* 1976) for implementing the numerical hypernetted chain (HNC) scheme (Springer *et al* 1973) for the canonical equilibrium pair distribution, and for nearly any value of the plasma parameter $\Lambda_\epsilon = e^2/k_B T\lambda_D^\epsilon$. λ_D denotes the Debye length $(k_B T/S_\nu\rho\, e^2)^{1/2}$, with $S_\nu = 2\pi^{\nu/2}/\Gamma(\nu/2)$ and $\rho = N/V$, and $\nu = 2+\epsilon$ is the real space dimension. Thanks to the Λ_ϵ expansion, this HNC scheme is the only one which permits us to reconnect the small-Λ_ϵ regime to the strongly coupled one ($\Lambda_\epsilon \geq 1$) where numerical simulations can be used.

The resummations up to infinity of the convolution chains, built from n-bubbles with single Debye lines intertwined between them, constitute the basic ingredient of the HNC scheme, provided the non-convolution diagrams vanish faster than the Coulomb tail $r^{-\epsilon}$ when $r\to\infty$. It has been demonstrated in three dimensions (Deutsch *et al* 1976) that the given bridge behaves as $\beta\, e^{-\alpha r}/r$ with $\alpha > 1$, when $r \geq \lambda_D$. These results have been subsequently confirmed by a systematic topological approach (Lavaud 1977, 1978) for the $\nu = 3$ bridge graphs having a number of Debye lines l not greater than $3k$, where k is the number of nodal points. Whenever the $\nu = 3$ bridge graphs may be given finite upper bounds, their asymptotic decay is expected to be essentially governed by an $\exp(-K_k r)$ term, with K_k the connection number, i.e. the maximum number of self-avoiding (without common lines) paths connecting the root points.

The purpose of this Letter is to present a novel method which allows the extraction of the asymptotic decay of any bridge diagram, with single- or multiple bonded, and with any values k and l, by means of well-behaved and finite analytic manipulations.

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This new approach makes use of the ϵ independence of the essential part of the asymptotic behaviour. This crucial remark permits us to circumvent the difficulty of evaluating the numerous $\nu = 3$ angular averages, by projecting out the nodal diagrams on their $\epsilon = -1$ values. These methods are based on the ϵ-unified Mayer–Salpeter expansion (Deutsch 1976).

Thus, we take the Coulomb interaction as

$$\phi^{(\nu)}(r) = \begin{cases} r^{2-\nu}/(\nu-2), & \nu \neq 2, \\ \ln |r|, & \nu = 2, \end{cases} \tag{1}$$

with its Fourier transform $S_\nu k^{-2}$. The corresponding first-order Debye line reads ($x = r/\lambda_{\mathrm{D}}$)

$$C_\nu(x) = -\frac{\Lambda_\epsilon}{2^{\epsilon/2}\Gamma(1+\epsilon/2)} \frac{\mathrm{K}_{\epsilon/2}(x)}{x^{\epsilon/2}} \tag{2}$$

$$\underset{x\to\infty}{\sim} -\Lambda_\epsilon\, \mathrm{e}^{-x}/x^{(1+\epsilon)/2},$$

with $\mathrm{K}_{\epsilon/2}(x)$ a modified Bessel function of the second kind.

According to the above conjecture, we expect the asymptotic decay of any nodal graphs built on the screened interaction (2) to be monitored by $\exp(-K_k r)$ for $\epsilon \geq -1$, the ϵ dependence being relegated within a marginal overall factor. Such a statement is in agreement with $\lim_{x\to\infty} C_\nu(x)$. This first-order behaviour transmits itself to all the chain diagrams built from n-bubbles $[C_\nu(r)]^n/n!$ and Debye lines $C_\nu(r)$, through the asymptotic decay

$$-(2/\pi x)^{\epsilon/2}\Lambda_\epsilon(1+\Lambda_\epsilon G_2(0))^{\epsilon/2}\mathrm{K}_{\epsilon/2}[(1+\Lambda_\epsilon G_2(0)x^2)^{1/2}], \tag{3}$$

where $G_2(K)$ is the Fourier transform of the two-bubble ladder. Turning now to the bridge class, the ϵ independence of the exponential decay may be easily checked out on the simplest diagram, (30) (see figure 1), which satisfies (Cauchy–Schwartz)

$$|(30)| \leq A^{(\epsilon)}(x)\, \mathrm{e}^{-2x}, \qquad \text{with } A^{(0)}(x) = \text{constant and } A^{(1)}(x) \simeq (\ln x)/x^2. \tag{4}$$

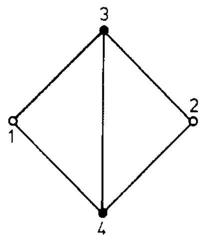

Figure 1. Simplest and third-order bridge graph denoted by (30).

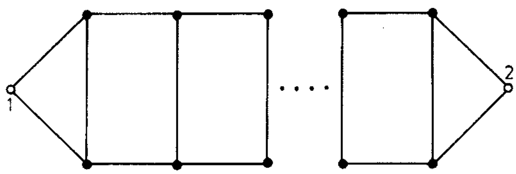

Figure 2. Horizontal 'ladder' bridge graph.

Analogous behaviour may be shown by the horizontal ladder (figure 2), the upper bound of which is the convolution product at order n of $n-1$ two-bubbles decaying as

$$e^{-2x}/x^{1+\epsilon/2}, \qquad \epsilon \leqslant 1. \tag{5}$$

These partial results lend further support to the previous conjecture. The marginal ϵ dependence left in these upper bounds suggest that, at least for $l < 3k$, the single-bonded bridges are smaller (in absolute value) than the $\nu = 1$ ones. This second and appealing conjecture may be shown to survive the short-ranged resummation ($\epsilon > 0$)

$$\exp(C_\nu(r)) - 1 - C_\nu(r) \tag{6}$$

needed for multiple-bonded graphs. A detailed study of equation (6) in k-space (Cohen and Murphy 1969, Furutani and Deutsch 1977, 1979) shows that the bridges ($\epsilon > 0$) built on the line (6) are bounded above (in absolute value) by their non-resumed $\epsilon = -1$ counterparts.

All these considerations render very attractive the computation of one-dimensional bridge diagrams. We thus first consider the bridge (30) (figure 1). Bearing in mind that $\Lambda_{-1} = \beta\, e^2 \lambda_D$ and $2\rho\, \Lambda_{-1}\lambda_D = 1$, its contribution to the potential of average force $W_2(x) = k_B T \ln g_2(x)$ reads

$$\begin{aligned} W_2^{(30)}(x) &= \rho^2(-\Lambda_1)^5 \int_{-\infty}^{\infty} dr_3 \int_{-\infty}^{\infty} dr_4 \exp - (r_{13}+r_{32}+r_{14}+r_{42}+r_{34})\lambda_D^{-1} \\ &= \tfrac{1}{12}\Lambda_{-1}^3(1 - 6x - \tfrac{8}{3}e^{-x})\, e^{-2x} \qquad (K_i = k_i\lambda_D). \end{aligned} \tag{7}$$

The result (7) produces, as expected, an upper bound to the previous $\nu = 3$ results (equations (4) and (5)) when $\nu \geqslant 1$, with the same ϵ-independent 'integer' exponential decay $\exp(-K_k r)$. Similarly, all the bridge graphs which are topologically equivalent to (30), with the transverse Debye line 3–4 replaced by the p-bubble $(-\Lambda_{-1})^p\, e^{-px}/p!$, can be handled as above. The graphs depicted in figure 3 thus provide the following contribution to the potential of average force,

$$W_2^{(p,0)}(x) = \frac{(-)^p \Lambda_{-1}^{p+2}}{4pp!}\, e^{-2x}\left(1 + 2x - \frac{4}{p(p+2)} + \frac{8\, e^{-px}}{p(p+2)^2}\right), \tag{8}$$

yielding back the result (7) for $p = 1$. This calculation demonstrates unambiguously that K_k monitors the asymptotic decay irrespective of the multiple-bondedness. The only significant effect of the 'transverse' p-bubble is to decrease the absolute value of the graph, which tends to zero when $p \to \infty$.

Any other asymmetric topology can be computed at the cost of more tedious manipulations. For instance, the graph depicted in figure 4, with a lateral p-bubble, is

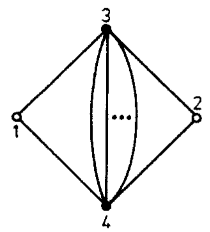

Figure 3. Simplest bridge graph $(p, 0)$ at order $n = p + 2$.

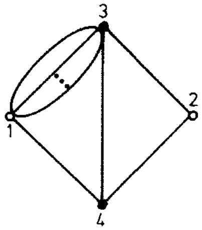

Figure 4. Asymmetric bridge graph $(p, 1)$ at order $n = p + 2$.

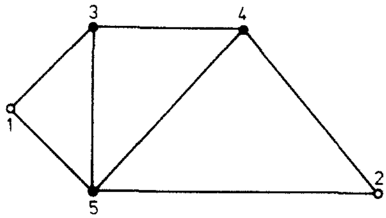

Figure 5. Simplest fourth-order bridge graph with three nodal points.

obtained through the Fourier transform

$$W_2^{(p,1)}(K) = \frac{\pi^2}{\Delta}\left(\frac{1}{3}\frac{K^4 + (p^2+33)K^2 + 24(p^2-1)}{(K^2+4)(K^2+9)} + \frac{K^4 + (3p^2+18p+13)K^2 - 2(p^2-1)(p+2)(p+3)}{p(p+2)(K^2+4)[K^2+(p+2)^2]}\right), \tag{9}$$

with $\Delta = [K^2 + (p+1)^2][K^2 + (p-1)^2]$. Again we recover equation (7) for $p = 1$. The occurrence of double poles in equation (9) leads to different results according to whether $p = 2$, 3 or 4. So we obtain the separate expressions

$$W_2^{(2,1)}(x) = \frac{61\Lambda_{-1}^4}{240} e^{-2x}\left(1 - \frac{2}{61}(27 + 10x)e^{-x} + \frac{5}{61}e^{-2x}\right), \tag{10}$$

$$W_2^{(3,1)}(x) = -\frac{\Lambda_{-1}^5 e^{-2x}}{6!18}(563 + 30x - 432 e^{-x} + 40 e^{-3x}), \tag{11}$$

$$W_2^{(4,1)}(x) = \frac{\Lambda_{-1}^6}{18} e^{-2x}\left(\frac{31}{215} - \frac{e^{-x}}{12} - \frac{e^{-3x}}{45} - \frac{e^{-4x}}{96}\right). \tag{12}$$

There are no longer double poles in equation (9) for $p \geqslant 5$, so we obtain the general quantity

$$W_2^{(p,1)}(x) = \frac{\frac{1}{3}(-)^p \Lambda_{-1}^{p+2} e^{-2x}}{p!(p+2)}\left(\frac{2p^3 + 8p^2 + 5 + 3}{p(p-1)(p+3)} - \frac{p\, e^{-x}}{p-2} - \frac{(p+8)\, e^{-(p-1)x}}{(p-2)(p+3)} + \frac{e^{-px}}{p}\right), \quad p \geqslant 5, \tag{13}$$

which behaves in a similar way to the previous $(p, 0)$. As a last example, let us consider the simplest $n=4$ bridge graph with three nodal points (figure 5). Its contribution to $W_2(x)$ reads

$$-\frac{23}{72}\Lambda_{-1}^{4}\,\mathrm{e}^{-2x}\left(1-\frac{16}{23}\mathrm{e}^{-x}+\frac{3}{23}\mathrm{e}^{-2x}\right) \tag{14}$$

These one-dimensional computations make clear that the universal exponential decay $\sim\exp(-K_k r)$ can be obtained for any bridge diagram through exact analytical manipulations. Moreover, the previous lines of reasoning demonstrate that these results may be transferred to any OCP of higher dimensionality ($\epsilon > -1$).

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