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LETTER TO THE EDITOR

The Gaussian model of a fluid in dimensions $D=0, -2$: an exact solution

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Abstract. The exact equation of state of the continuum Gaussian model is obtained for spatial dimensionalities $D=0$ and -2. We conjecture that the pressure and density are polynomials in z of degree $-D$ for all negative even D.

The fundamental problem of calculating the equation of state of an imperfect gas was solved in principle by Mayer [1], in the sense that every cluster coefficient in the fugacity series is expressible as a multiple integral. In practice the evaluation of the integrals is notoriously complicated and the exact equation of state has been obtained for only one continuum model, the system of hard lines in one dimension [2, 3]. Even the task of ascertaining the asymptotic behaviour of the cluster coefficients has proved to be extremely difficult. Information concerning these coefficients could provide useful insights concerning the gas-liquid phase transition and the separate phases. In the hope of clarifying aspects of the fugacity and virial expansion, Uhlenbeck and Ford [4, 5] introduced the continuum Gaussian model, whereby $f(r)=-\exp(-\alpha r^2)$ is adopted for the Mayer function. The quantity $V=-k_B T \ln(1+f)$ is a short-ranged, positive, two-body effective potential, diverging logarithmically for $r\to 0$, but it has the unphysical property of being temperature dependent. The important features of the Gaussian model are: firstly, the model can be treated for any spatial dimensionality D; secondly, the multiple integrals can be evaluated and thirdly, all of the cluster and virial coefficients are known through seventh order.

In this letter we present the exact equation of state for the continuum Gaussian model for the dimensions $D=0$ and -2. Although the notion of $D\leqslant 0$ is purely formal, obtained by analytic continuation of results derived for $D>0$, it is nevertheless of interest to examine the properties of the Gaussian model as a function of a parameter of such central significance as dimensionality. In particular, the properties of the model for negative even values of D are intimately associated with the value of the moments of a function of fundamental importance in linear graph theory. The exact equations of state for $D=0$ and -2 are given below in (7) and (8). For $D=0$ the pressure diverges logarithmically as the number density ρ approaches unity. In the case $D=-2$ the fugacity series $p(z)$ for the pressure is a polynomial of degree 2. The pressure increases monotonically with the density and reaches a finite maximum as ρ is increased to a critical value ρ_c, corresponding to $\rho(z)$ achieving a finite maximum.

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Just below ρ_c the quantity $dp/d\rho$ diverges as $(\rho_c - \rho)^{-1/2}$. We also present numerical evidence when $D = -4, -6$ for the pressure and density being polynomials in z of degree $-D$, with the density function possessing a finite maximum value for a positive value of z. We are thus led to conjecture that the Gaussian model exhibits the same qualitative properties for all negative even values of D. A polynomial form for the fugacity series cannot be ruled out by appealing to Groeneveld's theorem [6] since, as is discussed at the end of this letter, the theorem fails to apply for $D < 0$.

The cluster coefficient for the Gaussian model in D dimensions is expressible in terms of quantities of linear graph theory as $b_1(D) = 1$, $b_2(D) = -B_2(D)$,

$$b_m(D) = \frac{(2B_2)^{m-1}}{m!} \sum_{k=m-1}^{m(m-1)/2} (-1)^k \sum_{\lambda} \lambda^{-D/2} n(m, k, \lambda) \tag{1}$$

where B_2 denotes the second virial coefficient. For $D > 0$ the standard expression for B_2 is readily evaluated as $B_2(D) = -(1/2) \int f = (1/2)(\pi/\alpha)^{D/2}$ upon recalling that $\int H(r) = (2\pi^{D/2}/\Gamma(d/2)) \int_0^\infty dr r^{D-1} H(r)$ for a spherically symmetric integrand. Analytic continuation gives this same form as the definition of B_2 for $D < 0$. The quantity $n(m, k, \lambda)$ is the number of graphs with m labelled points, k lines and complexity λ, with the last being equal [4] to the number of distinct Cayley trees spanning all m points that can be formed from the k lines in the graph. Explicit expressions for $n(m, k, \lambda)$ are known only for a few special values of k. As a result the asymptotic behaviour of $b_m(D)$ for large m is unknown for general D, including the most important values $D = 1, 2, 3$. The choices $D = 0, -2$ are, however, exceptional since the zeroth and first moments of n are known [4, 5]. The latter are given by

$$\sum_{\lambda} n(m, k, \lambda) = c(m, k) \tag{2}$$

where $c(m, k)$ is the number of connected graphs with m labelled points and k lines, and

$$\sum_{\lambda} \lambda n(m, k, \lambda) = m^{m-2} \binom{(m-1)(m-2)/2}{k-m+1}. \tag{3}$$

Of particular relevance for (1), one can easily show that

$$\sum_{k=m-1}^{m(m-1)/2} (-1)^k c(m, k) = (-1)^{m-1}(m-1)!. \tag{4}$$

One thus obtains

$$b_m(0) = (-1)^{m-1}/m \qquad (m = 1, 2, \ldots) \tag{5}$$

$$b_n(-2) = 0 \qquad (m = 3, 4, \ldots) \tag{6}$$

upon noting that $2B_2(0) = 1$.

The resulting equation of state for the choice $D = 0$ is immediately found to be

$$p = k_B T \ln(1 + z) = -k_B T \ln(1 - \rho) \tag{7}$$

upon eliminating z using the first equality and $k_B T \rho = z\, \partial p/\partial z$. The system for $D = 0$ may thus be described as existing in a single phase, with the pressure increasing monotonically and diverging for $\rho \to 1-$. The critical exponent, γ, characterising the strength of the divergence is given by $\gamma = 0$, in contrast to $\gamma = 1$ for the system of hard lines [2, 3]. The same result, (7), is obtained for any model at $D=0$ featuring a two-body potential which diverges to $+\infty$ for $r\to 0$ [7].

For $D=-2$ the expression $p/k_BT=z-B_2z^2$, which follows from (6), gives rise to the equation of state

$$p(\sigma)=k_BT[1+4B_2\rho-(1-8B_2\rho)^{1/2}]/(8B_2). \tag{8}$$

The isotherm terminates at $\rho_c=(8B_2)^{-1}$ with a finite maximum value of p whereas $dp/d\rho$ diverges proportional to $(\rho_c-\rho)^{-1/2}$. The endpoint of the isotherm corresponds to $z_c=(4B_2)^{-1}$ where $d\rho/dz$ vanishes. This system also exists solely as a single phase.

The second and higher moments of the graph function $n(m, k, \lambda)$ are not known for general values of m and k. However, the values of n are available for all connected graphs up to and including $m=7$. Using the tabulated values [4] we calculated $b_m(-4)$ and $b_m(-6)$ for $m\leqslant 7$ and found that $b_m(-4)=0$ for $m=5, 6, 7$ whereas $b_7(-6)=0$. (The interested reader should use the corrected values $n(7, 8, 15)=8820$ and $n(7, 12, 300)=1890$.) These results lead us to conjecture that $b_m(-D)=0$ for $m>-D$ and thus that $p(z)$ are polynomials of degree $-D$ in z for all negative even D. If this conjecture is correct the fugacity series for the special cases $D=-4, -6$ are given by

$$p(z)/k_BT=z-B_2z^2-4B_2^2z^3+4B_2^3z^4 \qquad (D=-4) \tag{9}$$

$$p(z)/k_BT=z-B_2z^2-16B_2^2z^3+508B_2^3z^4+6560B_2^4z^5-2944B_2^5z^6 \qquad (D=-6). \tag{10}$$

For both of these dimensionalities the isotherm possesses the same qualitative properties as for the case $D=-2$. In particular the pressure terminates at a finite value with $dp/d\rho$ diverging as $(\rho_c-\rho)^{-1/2}$ as the density approaches the critical value ρ_c defined by the condition that $\rho(z)$ has a maximum ρ_c for z_c. The values of B_2z_c are given by 0.1312 and 1.5949 for $D=-4$ and -6, respectively.

The cluster coefficients in (9) and (10) do not alternate in sign. This feature, as well as the polynomial form of the fugacity series for negative even D, is at variance with the provisions of Groeneveld's theorem referred to at the outset. The theorem states, firstly, that the sign of the cluster coefficient b_m is positive (negative) if m is odd (even) and $m|b_m|\geqslant(2B_2)^{m-1}$ for any positive two-body central potential giving rise to a finite B_2. Secondly, the fugacity series has a finite radius of convergence R determined by a singularity at a point $z=-R$ on the negative real z axis, where R satisfies the inequality $(2e|B_2|)^{-1}<R<(2|B_2|)^{-1}$. The key point here is that Groeneveld's theorem no longer applies for $D<0$. (For $D=0$ the theorem still applies and, in fact, the cluster coefficients satisfy the *equality* $mb_m=(-1)^{m-1}$.) Put in the simplest terms, the proof of the theorem utilises the property that if $f(r)>g(r)>0$ for all r then the volume integrals of these functions necessarily satisfy the inequality $\int f>\int g$. This inequality does not necessarily apply if $D<0$. Finally, it should be recalled that n-component classical spin systems (or an equivalent lattice field theory) have been considered for negative even integer values of n and arbitrary spatial dimensionality [8, 9].

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