The Bose gas beyond mean field

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Abstract
We study a homogeneous Bose gas with purely repulsive forces. Using the Kac scaling of the binary potential we derive analytically the form of the thermodynamic functions of the gas for small but finite values of the scaling parameter in the low density regime. In this way we determine dominant corrections to the mean-field theory. It turns out that repulsive forces increase the pressure at fixed density and decrease the density at given chemical potential (the temperature is kept constant). They also flatten the Bose momentum distribution. However, the present analysis cannot be extended to the region where the mean-field theory predicts the appearence of condensate.

1 Introduction
Whereas the mean-field theory of an interacting Bose gas is now well understood, going beyond the mean-field description in a systematic way presents still an open problem (see [1] and references given therein). A natural tool for such a study is provided by the Kac scaling of the binary potential $V(r)$. The scaled potential

$$V_\gamma(r) = \gamma^3 V(\gamma r)$$

(1)
becomes weak and long-range when the dimensionless parameter $\gamma$ approaches zero. However, the integrated potential energy

$$a = \int dr V(r) = \int dr V_\gamma(r) < \infty$$

is $\gamma$-independent, and thus remains constant. The so-called van der Waals limit (i.e. the thermodynamic limit followed by $\gamma \to 0$) permits then to derive the mean-field effects corresponding to the potential $V(r)$. They depend on the mean potential energy $a\rho$, where $\rho$ is the number density of particles. For example, it has been shown that in the case of repulsive forces the van der Waals limit of the free energy density $f$ yields the mean-field formula

$$f_{mf} = f_0 + \frac{a}{2} \rho^2$$

where $f_0$ refers to the reference system without interaction $V(r)$. The formula holds both for classical and for quantum gases. In the theory of classical fluids one could go even further: the corrections to the zero order mean-field results have been derived, exhibiting the role of fluctuations for small but finite values of $\gamma$.

In the present paper we perform an analogous analysis for a homogeneous Bose gas, continuing our previous study. Our object is thus to determine and to investigate the leading corrections to the mean-field theory predictions for equilibrium properties of a gas composed of identical bosons interacting via purely repulsive forces. The rigorous part of our analysis will be restricted the region of thermodynamic parameters in which quantum Mayer series (virial expansions) converge uniformly with respect to the small parameter $\gamma$. In fact, under the assumption that both the potential and its Fourier transform are non-negative

$$V(r) \geq 0, \quad \hat{V}(k) = \int dr \exp(-ik \cdot r)V(r) \geq 0,$$

we can directly apply here the main results of. In the Bose gas is represented as a classical-like system of random polymers by using the Feynman-Kac path integral formulation of the Gibbs weight together with a cycle decomposition of the permutation group. Applying standard Mayer graph summation technique it has been shown therein that the density $\rho$ and the chemical potential $\mu$ of the Bose gas were related by a self-consistent relation

$$\rho(\mu) = F(\mu - a\rho(\mu))$$

The function $F$ is defined by a convergent series of multiconnected graphs whenever the chemical potential is sufficiently negative, and the convergence
is uniform with respect to the scaling parameter $\gamma$. In this regime, and for $\gamma \ll 1$ the function $F$ for a scaled potential takes the asymptotic form

$$F^\gamma(\nu) = F^\gamma_{\text{tree}}(\nu) + \gamma^3 F^{(1)}(\nu) + o(\gamma^3)$$  \hspace{1cm} (6)

Here $F^\gamma_{\text{tree}}(\nu)$ represents the sum of zero order contributions from the tree diagrams. It turns out that

$$F^\gamma_{\text{tree}}(\nu) = \rho_0(\nu)$$  \hspace{1cm} (7)

where $\rho_0$ denotes the perfect gas density. The limit $\gamma \to 0$ yields thus the self-consistent mean field equation

$$\rho_{m\!f}(\mu) = \rho_0(\mu - a\rho_{m\!f}(\mu))$$  \hspace{1cm} (8)

Equation (6) implies that the dominant corrections to equation (8) are of the order $\gamma^3$. The correcting term

$$F^{(1)}(\nu) = F^{(1)}_{\text{tree}}(\nu) + F^{(1)}_{\text{ring}}(\nu)$$  \hspace{1cm} (9)

results from the summation of the tree diagrams and from the summation of the ring diagrams. In Section 2 the form of the functions $F^{(1)}_{\text{tree}}(\nu)$ and $F^{(1)}_{\text{ring}}(\nu)$ is derived. The corresponding equation of state of the Bose gas is presented and analyzed in Section 3. It is remarkable that the dominant correction to the pressure has the same structure as that found by Hemmer for a classical fluid [4]. Under the additional assumption that the formula remains valid up to a neighborhood of the critical free density, we observe that the mean-field theory always underestimates the pressure in this region. We study then the one-particle reduced density operator displaying the nature of the momentum distribution (Section 4). Concluding remarks are presented in Section 5.

## 2 Self-consistent equation beyond mean-field

The function

$$F^\gamma_{\text{tree}}(\nu) = \frac{1}{(2\pi \lambda^2)^{3/2}} \sum_{q=1}^{\infty} \frac{\exp(\beta \nu q)}{q^{3/2}} \kappa^\gamma(q)$$  \hspace{1cm} (10)

when used in the self-consistent equation (3) yields the term corresponding to the summation of the tree diagrams (section V.A in [II]). Here

$$\kappa^\gamma(q) = \langle \exp(-\beta U_\gamma) \rangle_q$$  \hspace{1cm} (11)
is the partition function of a single closed \( q \)-polymer, \( \beta = 1/k_B T \), \( T \) is the temperature, \( k_B \) the Boltzmann constant, \( q \) the number of particles in the polymer and

\[
\lambda = \hbar \sqrt{\frac{\beta}{m}} \tag{12}
\]

is the de Broglie thermal wave length. The asymptotic \( \gamma \)-expansion of the scaled self-energy \( U_\gamma \) of the polymer follows from the definition given in [1]

\[
U_\gamma = \gamma^3 \frac{q(q-1)}{2} V(0) + o(\gamma^3), \quad \gamma \to 0 \tag{13}
\]

so that

\[
\kappa_\gamma(q) = 1 - \gamma^2 \frac{q(q-1)}{2} \beta V(0) + o(\gamma^3) \tag{14}
\]

Inserting (14) into (10) we get

\[
F_{\gamma \text{tree}}(\nu) = \rho_0(\nu) + \gamma^3 F^{(1)}_{\gamma \text{tree}}(\nu) + o(\gamma^3) \tag{15}
\]

where

\[
F^{(1)}_{\gamma \text{tree}}(\nu) = \frac{\beta V(0)}{2} \left( f^{(1)}(\nu) - f^{(2)}(\nu) \right) \tag{16}
\]

We have adopted the notation \(^1\)

\[
f^{(k)}(\nu) = \frac{1}{\beta^k} \frac{\partial^k}{\partial \nu^k} \rho_0(\nu) = \frac{1}{(2\pi \lambda^2)^{3/2}} \sum_{q=1}^{\infty} \frac{q^k}{q^{3/2}} \exp(\beta q \nu) \tag{17}
\]

The dominant contribution from resummation of the ring diagrams \( \gamma^3 F^{(1)}_{\gamma \text{ring}}(\nu) \) has been also calculated in [1] (see eq. (70); it is derived here in the appendix for the sake of convenience, see eq.(84)). It reads

\[
F^{(1)}_{\gamma \text{ring}}(\nu) = \frac{1}{2} f^{(2)}(\nu) \int \frac{dk}{(2\pi)^3} \frac{[\beta \hat{V}(k)]^2 f^{(1)}(\nu)}{1 + \beta \hat{V}(k)f^{(1)}(\nu)} \tag{18}
\]

Using the definition (17) and denoting respectively by \( \rho'_0 \) and by \( \rho''_0 \) the first- and the second-order derivative of the perfect gas density with respect to the chemical potential, we rewrite equations (10), (18) in the form

\[
F^{(1)}_{\gamma \text{tree}}(\nu) = \frac{V(0)}{2} \rho'_0(\nu) - \frac{V(0)}{2\beta} \rho''_0(\nu) \tag{19}
\]

\(^1\)In [1] \( f^{(k)}(\nu) \) designates the \( \gamma \)-dependent function, including the vertex contribution \( \kappa_\gamma(q) \). Here we have set \( \gamma = 0 \), and \( \kappa_\gamma(q) = 1 \), which yields the definition (17).
The dominant correction to the mean field form $\rho_0$ of the function $F$ is represented in equation (9) by a term of the order $\gamma^3$ involving the sum of the tree and of the ring contributions. Adding up (19) and (20) we eventually find that the function $F^{(1)}(\nu)$ takes the form of the derivative

$$F^{(1)}(\nu) = F^{(1)}_{\text{tree}}(\nu) + F^{(1)}_{\text{ring}}(\nu) = \frac{\partial g(\nu)}{\partial \nu}$$

where

$$g(\nu) = \frac{V(0)}{2} \rho_0(\nu) - \frac{1}{2\beta} \int \frac{dk}{(2\pi)^3} \log[1 + \hat{V}(k) \rho_0(\nu)]$$

Having derived the form of $F^{(1)}(\nu)$ we can analyze now the thermodynamic properties of the Bose gas including the corrections of the order $\gamma^3$.

3 Equation of state beyond mean-field

3.1 Pressure at order $\gamma^3$

The grand canonical pressure $P(\mu)$ satisfies the thermodynamic relation

$$\frac{\partial P(\mu)}{\partial \mu} = \rho(\mu)$$

Considering the chemical potential $\mu$ as a function of density $\mu = \mu(\rho)$ we get from (23) the formula

$$P(\rho) = \int_0^\rho d\sigma \sigma \frac{\partial \mu(\sigma)}{\partial \sigma}$$

The $\gamma$-expansion of the chemical potential reads

$$\mu(\rho) = \mu_{mf}(\rho) + \gamma^3 \mu^{(1)}(\rho) + o(\gamma^3)$$

where

$$\mu_{mf}(\rho) = \mu_0(\rho) + a\rho$$

and $\mu_0(\rho) = \partial f_0(\rho)/\partial \rho$ is the chemical potential of the perfect gas (compare with equation (3)). Up to the terms of order $\gamma^3$ the pressure is thus given by

$$P(\rho) = P_0(\rho) + \frac{a}{2} \rho^2 + \gamma^3 P^{(1)}(\rho) + o(\gamma^3)$$
where
\[ P^{(1)}(\rho) = \int_0^{\rho} d\sigma \sigma \frac{\partial \mu^{(1)}(\sigma)}{\partial \sigma} \] (27)

The correction \( \mu^{(1)}(\rho) \) can be readily determined from the self-consistent equation (5). Indeed, up to terms of order \( \gamma^3 \)
\[ \rho = \rho_0[\mu_{mf}(\rho) - a\rho + \gamma^3 \mu^{(1)}(\rho)] + \gamma^3 F^{(1)}(\mu_{mf}(\rho) - a\rho) \] (28)

As \( \mu_{mf}(\rho) - a\rho = \mu_0(\rho) \), upon further expanding of the first term on the right-hand side of (28) one finds
\[ \rho = \rho_0[\mu_0(\rho)] + \gamma^3[\rho_0'(\mu_0(\rho)) \mu^{(1)}(\rho) + F^1(\mu_0(\rho))] \] (29)

The identity \( \rho_0(\mu_0(\rho)) = \rho \) implies thus the relation
\[ \mu^{(1)}(\rho) = -\frac{F^{(1)}(\mu_0(\rho))}{\rho_0'(\mu_0(\rho))} \] (30)

Moreover, since \( F^{(1)}(\mu) \) is the derivative of the function \( g(\mu) \) defined in (22), we have
\[ \mu^{(1)}(\rho) = -\frac{\partial \mu_0(\rho)}{\partial \rho} \left[ \frac{\partial g(\mu)}{\partial \mu} \right]_{\mu=\mu_0(\rho)} = -\frac{\partial g(\mu_0(\rho))}{\partial \rho} \] (31)

Upon inserting (31) into (27) we get the formula
\[ P^{(1)}(\rho) = -\int_0^{\rho} d\sigma \sigma \frac{\partial^2 g(\mu_0(\sigma))}{\partial \sigma^2} = \left( -\rho \frac{\partial}{\partial \rho} + 1 \right) g(\mu_0(\rho)) \] (32)

where the second equality follows from integration by parts and the fact that \( g(\mu_0(\rho)) \big|_{\rho=0} = g(\mu) \big|_{\mu=-\infty} = 0 \). Using the explicit form (22) of \( g(\mu) \) we arrive at the final formula
\[ P^{(1)}(\rho) = \frac{1}{2\beta} \left( \rho \frac{\partial}{\partial \rho} - 1 \right) \int \frac{dk}{(2\pi)^3} \log[1 + \hat{V}(k)\chi_0(\rho)] \] (33)

where
\[ \chi_0(\rho) = \rho_0'(\mu_0(\rho)) = \rho \left( \frac{\partial P_0}{\partial \rho} \right)^{-1} \]
denotes the compressibility of the perfect Bose gas.

Equation (33) involves not only the thermodynamic functions characterizing the perfect gas but also the shape of the binary potential. It permits thus to write down the equation of state (26) of the interacting Bose gas beyond the mean-field theory. Remarkably enough, the additional pressure term \( P^{(1)}(\rho) \) representing the effect of fluctuations around the mean field has exactly the same structure as the analogous term derived by Hemmer for classical fluids (see [4] eq. (55)).
3.2 Low density behaviour

It is interesting to analyze in more detail the formula (33) in the low density limit, where the compressibility \(\chi_0(\rho)\) approaches zero

\[
\chi_0(\rho) = \beta \rho + \frac{\beta}{2}(\pi \lambda^2)^{3/2} \rho^2 + ..., \quad \rho \to 0
\]  

(34)

The expansion of the logarithm in (33) yields

\[
P^{(1)}(\rho) = \frac{1}{2\beta} \left( \rho \frac{\partial}{\partial \rho} - 1 \right) \left[ V(0)\chi_0(\rho) - \frac{1}{2} \int \frac{d\mathbf{k}}{(2\pi)^3} [\hat{V}(k)\chi_0(\rho)]^2 + ... \right]
\]  

(35)

Inserting here (34) we find

\[
P^{(1)}(\rho) = \frac{\rho^2}{4} \left[ V(0)\pi^{3/2} \lambda^3 - \beta \int \frac{d\mathbf{k}}{(2\pi)^3} [\hat{V}(k)]^2 \right]
\]  

(36)

The term proportional to \(\lambda^3 \sim T^{-3/2}\) reflects the effect of quantum statistics whereas the term proportional to \(\beta = 1/k_B T\) is of classical type, not involving the Planck constant. The repulsive potential \(V(0) > 0\) tends to increase the pressure, but the negative classical term acts in the opposite direction. Clearly, the lower the temperature the more important is the Bose statistics.

Notice that the low density equation of state maintains the mean-field form

\[
P(\rho) = P_0(\rho) + \frac{1}{2} a_\gamma \rho^2
\]  

(37)

but now with a \(\gamma\)-dependent constant

\[
a_\gamma = a + \gamma^3 \frac{1}{2} \left[ V(0)\pi^{3/2} \lambda^3 - \beta \int \frac{d\mathbf{k}}{(2\pi)^3} [\hat{V}(k)]^2 \right]
\]

Finally, equation (37) should be supplemented with the low density expansion of the perfect gas pressure

\[
P_0(\rho) = \frac{1}{\beta} \left[ \rho - \frac{\rho^2}{2} \pi^{3/2} \lambda^3 + ... \right]
\]  

(38)

Then equation (37) yields the second virial coefficient at the order \(\gamma^3\).
3.3 Critical region

At this point we make the working hypothesis that the validity of the formula \( P^{(1)}(\rho) \) extends from low density up to the critical density \( \rho_{0,c} \) of the free gas provided that \( \gamma \) is small enough when \( \rho \) is close to \( \rho_{0,c} \). This is a plausible assumption if in the range \( 0 \leq \rho < \rho_{0,c} \), at fixed temperature \( T \), the system does not undergo other phase transitions (solidification, liquefaction).

At \( \rho_{0,c} \), the compressibility of the free gas is known to diverge as

\[
\chi_0(\rho) \sim \frac{c}{\rho_{0,c} - \rho}
\]

where \( c = 1.086 \beta \rho_{0,c}^2 \). For \( \rho \) close to \( \rho_{0,c} \) we can write

\[
P^{(1)}(\rho) \sim \frac{1}{2\beta} \left( \rho \frac{\partial}{\partial \rho} - 1 \right) \int \frac{dk}{(2\pi)^3} \log \left[ 1 + \frac{\hat{V}(k)}{\rho_{0,c} - \rho} \right]
\]

\[
\sim \frac{\rho_{0,c}}{2\beta(\rho_{0,c} - \rho)} \int \frac{dk}{(2\pi)^3} \frac{c\hat{V}(k)}{\rho_{0,c} - \rho + c\hat{V}(k)}
\]

\[
- \frac{1}{2\beta} \int \frac{dk}{(2\pi)^3} \log \left[ 1 + \frac{c\hat{V}(k)}{\rho_{0,c} - \rho} \right].
\]

One sees that \( P^{(1)}(\rho) \to \infty \) as \( \rho \to \rho_{0,c} \), the positive term \( \text{(40)} \) being the most divergent one. Thus, choosing \( \rho \) close to \( \rho_{0,c} \) and \( \gamma^3 \) sufficiently small, the pressure correction \( \gamma^3 P^{(1)}(\rho) \) to the mean field can be made positive. We conclude that fluctuations beyond mean field always tend to increase the pressure in the vicinity of \( \rho_{0,c} \).

The nature of the divergence depends on the behaviour of \( \hat{V}(k) \) as \( k \to \infty \). As an example we consider a power-like decay \( \hat{V}(k) \sim bk^{-\eta}, k \to \infty, \eta > 3 \). Then the strongest divergence comes from the large values of \( k \) in the integral \( \text{(40)} \). Choosing \( k_0 \) sufficiently large we find

\[
\rho_{0,c} \int_{k_0}^{\infty} \frac{dk}{2\pi^2} \frac{b\hat{V}(k)}{k^\eta(\rho_{0,c} - \rho) + b\hat{V}(k)}
\]

\[
\sim \left( \frac{1}{(\rho_{0,c} - \rho)^{1+3/\eta}} \right) \frac{\rho_{0,c}}{8\beta\pi^2} \int_{0}^{\infty} du \frac{b\hat{V}(u)}{u^\eta + b\hat{V}(u)}. \quad \text{(42)}
\]

Since the second integral \( \text{(41)} \) behaves as \( (\rho_{0,c} - \rho)^{-3/\eta} \), we see that the pressure correction diverges as \( (\rho_{0,c} - \rho)^{-1+3/\eta} \), \( \rho \to \rho_{0,c} \). An illustration corresponding to the choice

\[
V(r) = \frac{a}{8\pi r_0^3} \exp(-r/r_0), \quad \hat{V}(k) = \frac{a}{(1 + k^2 r_0^2)^2}
\]

\[
\gamma^3 \pi (\lambda/r_0)^3 = 1, \quad a\beta/(2\pi\lambda^{3/2}) = 0.1
\]

is presented in Fig.1.
Figure 1: Dimensionless pressure $p = P(2\pi\lambda^2)^{3/2}/\beta$ as function of density $n = \rho(2\pi\lambda^2)^{3/2}$ for the binary interaction $\rho$. The pressure correction diverges at $n = n_{0,c} = 2.612$. The dashed line represents the mean-field prediction which underestimates the pressure.

4 One-body density matrix at order $\gamma^3$

The grand canonical one-body density matrix $R$ for a Bose gas in volume $\Lambda$ is defined by its configurational matrix elements

$$\langle r| R(\mu)| r' \rangle = \frac{1}{\Xi_{\Lambda}} \sum_{N=1}^{\infty} \frac{e^{\beta \mu N}}{(N-1)!} \int_{\Lambda} dr_2 \cdots \int_{\Lambda} dr_N \langle r, r_2, \ldots, r_N| e^{-\beta H_{N,\Lambda}}| r', r_2, \ldots, r_N \rangle_{\text{sym}}$$

with $H_{N,\Lambda}$ the $N$-particle Hamiltonian and the matrix elements taken in the space of symmetrized wave functions. In the low density regime it admits the classical-like representation (equations (68) and (71) of the Appendix) in terms of an open polymer immersed in a gas of closed polymers. In the thermodynamic limit Mayer graphs resummations enable to determine $\langle r| R(\mu)| r' \rangle$ from the formula (see Appendix, eq. (73))

$$\langle r| R(\mu)| r' \rangle = F_{r,r'}(\mu - a\rho(\mu))$$

where, as in (5), $F_{r,r'}(\nu)$ is the sum of multiply connected graphs with a root point labelled by an open polymer. It reduces to $F(\nu)$ as $r = r'$, so the diagonal part $\langle r| R(\mu)| r \rangle = \rho(\mu)$ satisfies the self-consistent equation (5).
Because of the invariance under translations and under rotations $F_{r,r'}(\nu) = F(|r - r'|, \nu)$, so that $\langle r | R(\mu) | r' \rangle = R(|r - r'|, \mu)$ depend only on the distance $|r - r'|$. Hence we can set $r' = 0$ without loss of generality. The Fourier transform
\[ \hat{R}(p, \mu) = \int dr e^{ip \cdot r} R(r, \mu), \quad p = |p| \]
gives the distribution of momentum $\hbar p$ of an interacting Bose particle. It is determined by equation (45) in the Fourier representation
\[ \hat{R}(p, \mu) = \hat{F}(p, \mu - a\rho(\mu)) \]

4.1 Grand-canonical density

We first consider the diagonal part of the density matrix (i.e. the particle density) up to terms of order $\gamma^3$
\[ \rho(\mu) = \rho_{mf}(\mu) + \gamma^3 \rho^{(1)}(\mu) \]
where $\rho_{mf}$ is the solution of equation (8). Using (5) and the $\gamma$-expansion (6) of function $F\gamma$ we thus find
\[ \rho_{mf}(\mu) + \gamma^3 \rho^{(1)}(\mu) = \rho_0[\mu - a\rho_{mf}(\mu)] + \gamma^3 F^{(1)}[\mu - a\rho_{mf}(\mu)] \]
\[ = \rho_0[\mu - a\rho_{mf}(\mu)] - \gamma^3 a\rho^{(1)}(\mu)\rho'_0[\mu - a\rho_{mf}(\mu)] + \gamma^3 F^{(1)}[\mu - a\rho_{mf}(\mu)] \]
Owing to equation (8) the above relation yields the formula
\[ \rho^{(1)}(\mu) = \frac{F^{(1)}[\mu - a\rho_{mf}(\mu)]}{1 + a\rho'_0[\mu - a\rho_{mf}(\mu)]} \]
where $F^{(1)}$ is given by (21).

The density correction $\rho^{(1)}(\mu)$ involves functions of the argument
\[ \nu(\mu) = \mu - a\rho_{mf}(\mu) \]
Notice that on one hand
\[ \frac{\partial \nu}{\partial \mu} = 1 - a\rho'_{mf}(\mu), \]
and on the other hand the mean field equation (8) implies
\[ \frac{\partial \nu}{\partial \mu} = \frac{\rho'_{mf}(\mu)}{\rho'_0(\nu)} \]
so that
\[ \frac{\partial \nu}{\partial \mu} = \frac{1}{1 + a\rho_0(\nu)} \] (52)
The density correction (50) can be thus rewritten in the form
\[ \rho^{(1)}(\mu) = F^{(1)}[\nu(\mu)] \frac{\partial \nu}{\partial \mu} \] (53)
which in view of the structure of equation (21) finally yields
\[ \rho^{(1)}(\mu) = \frac{\partial g(\nu(\mu))}{\partial \mu} \] (54)
where function \( g(\nu) \) has been defined in (22).

This correction to the grand-canonical density can also be studied at low density and in the critical region. If \( \nu \sim \mu \to -\infty \) (i.e. low density) one finds that \( \rho^{(1)}(\mu) \sim A(\beta)e^{2\beta\mu} \) where, as for the pressure, the sign of the coefficient \( A(\beta) \) depends if effects of Bose statistics dominate classical corrections or not. Extrapolating the formula (54) to the neighborhood of the critical mean field chemical potential \( \mu_{m.f,c} = a\rho_0,c \), one deduces first from the mean field equation that \( \nu(\mu) \sim -C(\beta)(\mu_{m.f,c} - \mu)^2, C(\beta) > 0, \) as \( \mu \to \mu_{m.f,c} (\mu < \mu_{m.f,c}) \). Then analyzing the \( k \)-integrals as in subsection 3.3 one sees that \( \rho^{(1)}(\mu) \) diverges to \(-\infty\) as \( \mu \to \mu_{m.f,c} \) (for \( \hat{V}(k) \sim bk^{-\eta}, \rho^{(1)}(\mu) \sim -(\mu_{m.f,c} - \mu)^{-1+3/2\eta} \) as for the pressure). Thus, taking \( \mu \) close to \( \mu_{m.f,c} \) and \( \gamma \) small enough, the density decreases when fluctuations are taken into account. This is illustrated in Fig.2.

### 4.2 The momentum distribution

The momentum distribution \( \hat{R}(p, \rho) \) at order \( \gamma^3 \), considered as a function of the density
\[ \hat{R}(p, \rho) = \hat{R}^{(0)}(p, \rho) + \gamma^3 \hat{R}^{(1)}(p, \rho) \] (55)
is found from the relation (17) by using the \( \gamma \)-expansion of \( \hat{F}^{\gamma} \) which follows from (55) an from the relation \( \nu(\mu_{m.f}(\rho)) = [\mu_{m.f} - a\rho(\mu)]_{\mu=\mu_{m.f}}(\rho) = \mu_0(\rho) \).

We observe that at the dominant order (see (76), (77))
\[ \hat{R}^{(0)}(p, \rho) = n_0(p, \nu)|_{\nu=\mu_0(\rho)} \] (56)
is the free Bose momentum distribution at density \( \rho \). Proceeding as in (28), (30) one finds
\[ \hat{R}^{(1)}(p, \rho) = \hat{F}^{(1)}(p, \mu_0(\rho)) - \left[ \frac{n_0^0(p, \nu) F^{(1)}(\nu)}{\rho_0(\nu)} \right]_{\nu=\mu_0(\rho)} \] (57)
Figure 2: Dimensionless density \( n = \rho(2\pi\lambda^2)^{3/2} \) as function of the chemical potential \( m = \mu\beta \) for the binary interaction \( \langle \rangle \). The dashed line represents the mean-field prediction which overestimates the density. We put here \( \alpha \equiv a\beta/(2\pi\lambda^2)^{3/2} = 1.5 \), \( \alpha(\gamma\lambda/r_0)^3 = 4\sqrt{2}/\pi \). The density correction diverges at \( m = m_{0,c} = a\rho_{0,c} = 3.93 \).

Inserting the expression \( \langle \rangle \) for \( \hat{F}(1)(p, \nu) \) and for \( F^{(1)}(\nu) = \int d\mathbf{p} \hat{F}(1)(p, \nu)/(2\pi)^3 \) one obtains the final result

\[
\hat{R}^{(1)}(p, \rho) = c(\rho, \beta) \left[ \frac{\rho'_0(\nu)}{\rho'_0(\nu)} n_0(p, \nu) - n''_0(p, \nu) \right]_{\nu=\mu_0(\rho)}
\]

where

\[
c(\rho, \beta) = \frac{1}{2\beta} \int \frac{d\mathbf{k}}{(2\pi)^3} \left( \frac{\hat{V}(k)}{1 + \hat{V}(k)\rho'_0(\mu_0(\rho))} \right)
\]

Notice that

\[
\int \frac{d\mathbf{p}}{(2\pi)^3} \hat{R}^{(1)}(p, \rho) = 0
\]

as requested by the fact that the integrals

\[
\int \frac{d\mathbf{p}}{(2\pi)^3} \hat{R}(p, \rho) = \int \frac{d\mathbf{p}}{(2\pi)^3} \hat{R}^{(0)}(p, \rho) = \rho
\]

are fixed by the total density.

Some properties of \( \hat{R}(p, \rho) \) can be derived from those of the free Bose distribution

\[
n_0(p, z) = \frac{z}{\exp(\lambda^2p^2/2) - z}
\]
where \( z = e^{\beta \nu}, 0 \leq z < 1 \), is the activity parameter. One sets
\[
\begin{align*}
n_1(p, z) &= \beta^{-1}n'_0(p, \nu) = n_0(p, z)(1 + n_0(p, z)) \\
n_2(p, z) &= \beta^{-2}n''_0(p, \nu) = n_1(p, z)(1 + 2n_0(p, z))
\end{align*}
\]

Then
\[
\dot{R}(p, z) = n_0(p, z) + \epsilon[n_1(p, z)r(z) - n_2(p, z)]
\]
with
\[
r(z) = \frac{\rho''_0(\nu)}{\beta \rho'_0(\nu)} = \int d\mathbf{p} \frac{n_2(p, z)}{n_1(p, z)}
\]
The parameter \( \epsilon = \gamma^3 c(\rho, \beta)\beta^2 \) in (62) incorporates all the \( p \)-independant factors (see eq.(58)). Since \( \epsilon \) is proportional to \( \gamma^3 \) it can be chosen as small as one wishes at any density \( \rho < \rho_{0,c} \). We observe that
\[
n_2(p, z) \leq n_1(p, z) \left(1 + \frac{2z}{1 - z}\right) = n_1(p, z) \left(\frac{1 + z}{1 - z}\right)
\]
implying
\[
r(z) \leq \frac{1 + z}{1 - z}
\]
\[
[n_1(p, z)r(z) - n_2(p, z)]_{p=0} = \frac{z}{(1 - z)^2} \left[r(z) - \frac{1 + z}{1 - z}\right] \leq 0
\]
One concludes that the distribution at \( p = 0 \) in presence of the interaction is always less than the free value \( z/(1 - z) \). Evaluating the correction as \( p \to \infty \) gives
\[
[n_1(p, z)r(z) - n_2(p, z)] \sim z \exp(-\lambda^2 p^2/2)(r(z) - 1) \geq 0
\]
since \( n_0(p, z) \sim n_1(p, z) \sim n_2(p, z) \sim z \exp(-\lambda^2 p^2/2) \), \( p \to \infty \), and for all \( p \) and \( z \), \( n_2(p, z) \geq n_1(p, z) \), implying \( r(z) \geq 1 \). Thus the momentum distribution is flattened and broadened by repulsive interactions, as illustrated in Fig.3.

5 Concluding remarks

One can make the following points:
(i) Divergences occuring at the critical values of the free gas reflect the fact that the order \( \gamma^3 \) of the correction is not adequate there. Since we know from rigorous work that the exact pressure \( P_\gamma \) converges to the mean field pressure \( P_{mf} \) for all values of the thermodynamical parameters \([6]\), one may conclude that the rate of approach to mean field at critical values of the
free gas is of the order $\gamma^\delta$ for some $0 < \delta < 3$. The determination of this exponent is an open problem which necessitates a more thorough analysis of Mayer series.

(ii) In our analysis, the critical values of density and of temperature are still those of the free gas. One could expect that for non-zero but small $\gamma$ the critical mean field chemical potential $\mu_{mf,c} = a\rho_{0,c}$ and density $\rho_{0,c}$ will be slightly displaced. Such an information cannot been obtained here, but requires, for instance, a deeper non-perturbative understanding of the behaviour of the partition of a single polymer as also discussed in Section V.A of [1].

(iii) The results of the paper enable nevertheless to explore the immediate vicinity of the critical mean field values by taking $\gamma$ sufficiently small (provided that our formulae keep their validity up to this point). Then qualitative statement could be established, as the fact that the exact pressure should be higher than that predicted in this region by the mean field. Another conclusion from our analysis is that approaching the critical mean field chemical potential $\mu_{mf,c} = a\rho_{0,c}$ along an isotherm one finds the interacting gas at a density lower than that appearing in the mean field approach.

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A Appendix

A.1 Polymer representation of the one-body reduced density matrix

The representation of the off-diagonal reduced density matrix $\langle r|R(\mu)|r'\rangle$ in the formalism of random polymers described in Section 2 of [1] requires the consideration of open Brownian paths (open polymers) in the time interval $0 \leq s \leq q$ with extremities at $r$ and $r'$. In the Brownian bridge notation they are parametrized as

$$
\left(1 - \frac{s}{q}\right) r + \frac{s}{q} r' + \lambda X(s), \quad 0 \leq s \leq q.
$$

where $X(s)$ is a closed path distributed with the Brownian bridge measure (eq. (18) in [1]); here and in the sequel we use the same notations as in [1]). The open polymer $L_{r,r'} = (r, r', q, X(s))$, $0 \leq s \leq q$ is characterized by its end points $r, r'$, the number $q$ of particles belonging to it and its random shape $X(s)$. By a slight generalisation of the analysis that led to the ”magic formula” (eq. (14) in [1]) one obtains the density for an open polymer immersed in a grand canonical ensemble of closed polymers as

$$
\rho_{\text{op}}(L_{r,r'}) = \frac{1}{\Xi} \sum_{n=1}^{\infty} \frac{1}{(n-1)!} z(L_{r,r'}) \int dL_i z(L_i) \exp(-\beta U(L_{r,r'}, L_2, \ldots, L_n)).
$$

where $\Xi$ is the partition function. If $r = r'$ this reduces to the loop density $\rho_{\text{loop}}$ studied in [1]. In view of its form (68) $\rho_{\text{op}}(L_{r,r'})$ has the Mayer expansion presented in eqs.(29)-(31) of [1] in terms of Ursell functions. The only difference is that the argument of the root point $1 = L_{r,r'}$ has to be identified with the open polymer (67). Polymer interactions, effective activities and Mayer bonds are the same as in [1] except at the root point, where the interaction between a loop $L_j = (R_j, q_j, X_j)$ with an open polymer

\[\text{2The quantity } -k_BT\log \rho_{\text{op}}(L_{r,r'}) \text{ can be interpreted as the excess grand potential when a fixed open polymer } L_{r,r'} \text{ is introduced in the system of closed polymers.}\]
\[ V(L_r, r', L_j) = \int_0^q ds \int_0^{q_j} ds_j \delta(s - s_j) V \left( \left( 1 - \frac{s}{q} \right) r + \frac{s}{q} r' + \lambda X(s) - R_j - \lambda X_j(s_j) \right) \]  
\quad (69)

and the self-energy of the open polymer is
\[ U(L_r, r') = \frac{1}{2} \int_0^q ds_1 \int_0^q ds_2 \delta(s_1 - s_2) V \left( \frac{s_1 - s_2}{q} (r - r') + \lambda (X(s_1) - X(s_2)) \right) \]  
\quad - \frac{1}{2} q V(0) \quad (70)

Finally, to obtain the one-body density matrix \( \langle r | R(\mu) | r' \rangle \), one has to integrate on the internal degrees of freedom of the open polymer
\[ \langle r | R(\mu) | r' \rangle = \sum_{q=1}^{\infty} q \int D_q(X) \exp \left( -\frac{|r - r'|^2}{2q \lambda^2} \right) \rho_{op}(L_r, r') \]  
\quad (71)

The \( q \) factor takes into account the presence of \( q \) particles in the open polymer and the additional Gaussian comes from the Brownian Wiener weight for a path starting in \( r \) at time \( s = 0 \) and ending at \( r' \) at time \( s = q \). From now on the analysis of the Mayer series can be performed exactly along the same lines as that given in \[1\] with the following results.

(i) The Mayer series representing \( \langle r | R(\mu) | r' \rangle \) converges for \( \mu \) sufficiently negative \( (\mu < -a \rho_{0,c}) \); for a scaled potential \( V_\gamma(r) \), the convergence is uniform with respect to \( \gamma \).

(ii) Let \( I(L_r, r') \) be the value of the sum of all multiply connected graphs with root point \( L_r, r' \), and define the function of the chemical potential \( \nu \)
\[ F_{r, r'}(\nu) = \sum_{q=1}^{\infty} q \int D_q(X) \exp \left( -\frac{|r - r'|^2}{2q \lambda^2} \right) I(L_r, r'). \]  
\quad (72)

Then the reduced density matrix is given by
\[ \langle r | R(\mu) | r' \rangle = F_{r, r'}(\mu - a \rho(\mu)). \]  
\quad (73)

where the density \( \rho(\mu) \) solves the self-consistent equation \[5\].

16
A.2 The $\gamma^3$ correction

For a scaled potential ($\gamma \ll 1$), the function $F^\gamma(r, \nu)$ takes the asymptotic form

$$F^\gamma(r, \nu) = F^0_{\text{tree}}(r, \nu) + \gamma^3[F^1_{\text{tree}}(r, \nu) + F^1_{\text{ring}}(r, \nu)] + o(\gamma^3)$$

(74)
as in [6] where $F^0_{\text{tree}}(r, \nu)$ represents the sum of zero order contributions coming from the tree diagrams. The sum of tree diagrams yields

$$F^\gamma_{\text{tree}}(r, \nu) = \frac{1}{(2\pi \lambda^2)^{3/2}} \sum_{q=1}^{\infty} \exp \left( \frac{\beta \nu q - \frac{r^2}{2\lambda^2 q}}{q^{3/2}} \right) \kappa^2(q), \quad \text{quadr} = |r|$$

(75)

so that

$$F^0_{\text{tree}}(r, \nu) = \lim_{\gamma \to 0} F^\gamma_{\text{tree}}(r, \nu) = \frac{1}{(2\pi \lambda^2)^{3/2}} \sum_{q=1}^{\infty} \exp \left( \frac{\beta \nu q - \frac{r^2}{2\lambda^2 q}}{q^{3/2}} \right)$$

(76)
is nothing else than the off-diagonal reduced density matrix $\rho_0(r, \nu)$ of the free gas at chemical potential $\nu$. Indeed, $F^0_{\text{tree}}(r, \nu)$ is the Fourier transform of the Bose occupation number density $n_0(k, \nu)$

$$n_0(k, \nu) = \frac{1}{\exp \left( \frac{\beta |k|^2}{2} - \beta \nu \right) - 1}.$$  

(77)

The $\gamma^3$ correction is obtained in expanding the partition function $\kappa^2(q)$ of a single polymer in $F^\gamma_{\text{tree}}(r, \nu)$ as done in eqs (11) to (16)

$$F^{(1)}_{\text{tree}}(r, \nu) = \frac{\beta V(0)}{2} \left( f^{(1)}(r, \nu) - f^{(2)}(r, \nu) \right), \quad \text{with} \quad f^{(k)}(r, \nu) = \frac{1}{\beta^k} \frac{\partial^k}{\partial \nu^k} \rho_0(r, \nu).$$

(78)

Clearly $f^{(k)}(r, \nu)|_{r=0} = f^{(k)}(\nu)$ defined in (17). We now perform the ring summation to determine $F^{(1)}_{\text{ring}}(r, \nu)$. The contribution to $I_{\text{ring}}(L_{r,r'})$ of a ring with one root point $L_{r,r'}$, $n$ integrated vertices $L_j$ and $n+1$ linearized bonds $(-\beta V)$ is

$$\frac{1}{2} z(L_{r,r'}) \int dL_1 \cdots \int dL_n (-\beta V(L_{r,r'}, L_1)) \times \left[ \prod_{j=1}^{n-1} z(L_j)(-\beta V(L_j, L_{j+1})) \right] (-\beta V(L_n, L_{r,r'}))$$

(79)
The factor $1/2$ is the symmetry factor of the graph. Introducing the scaled potential $\gamma^3 V(\gamma r)$ and changing the $n$ spatial integration variables $R_j$ to $\gamma R_j$ will produce an overall factor $\gamma^3$ in (79) since there are $n + 1$ bonds. At order $\gamma^3$, we are thus entitled to neglect the quantum fluctuation part $\gamma \lambda X(s_j)$ in the arguments of the potential (use dominated convergence and the fact that the Gaussian measures $D_q(X_j)$ are normalized). For the same reason we neglect the $\gamma$ dependence in the activities. Within this approximation we take the bonds and the vertices equal to

$$
V_\gamma(L_{r,r'}, L_j) = \gamma^3 q_j \int_0^q ds V \left( \left(1 - \frac{s}{q}\right) \gamma r + \frac{s}{q} \gamma r' - \gamma R_j \right)
$$

$$
V_\gamma(L_j, L_{j+1}) = q_j q_{j+1} \gamma^3 V(\gamma R_j - \gamma R_{j+1})
$$

$$
z(L_{r,r'}) = z(L_j) = \frac{e^{\beta V}}{q(2\pi \lambda^2 q)^{3/2}} \equiv z^{(0)}(q) \quad (80)
$$

At this point we keep the $\gamma$ parameter in combinations $\gamma r$ and $\gamma r'$ since $r$, $r'$ can be large. Hence after the change of variables $R_j \to \gamma R_j$ (79) becomes

$$
\frac{\gamma^3}{2} z^{(0)}(q) \sum_{q_1, \ldots, q_n} \int dR_1 \cdots dR_n \left[ -\beta \int_0^q ds V \left( \left(1 - \frac{s}{q}\right) \gamma r + \frac{s}{q} \gamma r' - R_1 \right) \right]
\left( \prod_{j=1}^n q_j^2 z^{(0)}(q_j) \right) \left( \prod_{j=1}^n (-\beta V(R_j - R_{j+1})) \right) \int_0^q ds' V \left( R_n - \left(1 - \frac{s'}{q}\right) \gamma r - \frac{s'}{q} \gamma r' \right)
\quad (81)
$$

Introducing the Fourier transform $\hat{V}(k)$ and using the convolution theorem yields

$$
\frac{\gamma^3}{2} z^{(0)}(q) (f^{(1)}(\nu))^n \int_0^q ds \int_0^q ds' \int \frac{dk}{(2\pi)^3} \exp \left[ i \gamma k \cdot (r - r') \left( \frac{s - s'}{q} \right) \right] (-\beta \hat{V}(k))^{n+1}
\quad (82)
$$

where $f^{(1)}(\nu) = \sum_{q=1}^\infty q^2 z^{(0)}(q)$ is the function (17). This has to be summed on $n = 1, 2, \ldots$ and integrated over the internal degrees of freedom of the root point according to (72). One finds

$$
F^{(1)}_{\text{ring}}(r - r', \nu) = \frac{1}{2} \sum_{q=1}^\infty q^2 z^{(0)}(q) \exp \left( -\frac{|r - r'|^2}{2q^2} \right)
\int \frac{dk}{(2\pi)^3} \int_0^q ds \int_0^q ds' \exp \left[ i \gamma k \cdot (r - r') \left( \frac{s - s'}{q} \right) \right] \frac{(\beta \hat{V}(k))^2 f^{(1)}(\nu)}{1 + \beta \hat{V}(k) f^{(1)}(\nu)}
\quad (83)
$$
Finally, taking (80) into account, the Fourier transform  
\[ \hat{F}^{(1)}(p, \nu) = \int d\mathbf{r} e^{i\mathbf{p} \cdot \mathbf{r}} F_{\text{ring}}^{(1)}(\mathbf{r}, \nu) \]
at wave number \( p \) is found to be

\[ \hat{F}_{\text{ring}}^{(1)}(p, \nu) = \frac{1}{2} \sum_{q=1}^{\infty} q e^{\beta \nu q} \int_0^q ds \int_0^q ds' \int \frac{dk}{(2\pi)^3} \exp \left[ -\frac{\lambda^2}{2} \left| p + \gamma k \left( \frac{s-s'}{q} \right) \right|^2 q \right] \frac{(\beta \hat{V}(k))^2 f^{(1)}(\nu)}{1 + \beta \hat{V}(k)f^{(1)}(\nu)} \]

As a consequence of the Gaussian weight occurring for off-diagonal elements \( \mathbf{r} \neq \mathbf{r}' \) the remaining \( \gamma \) dependance has been neglected in (84). \( \hat{f}^{(2)}(p, \nu) \) is the Fourier transform of the function (78). We note that

\[ \int \frac{dp}{(2\pi)^3} \hat{F}_{\text{ring}}^{(1)}(p, \nu) = F_{\text{ring}}^{(1)}(\nu) \]

reduces to the formula (18) used in Section 2.

The final result for the \( \gamma^3 \) correction is obtained by adding the tree contribution (78) to (84)

\[ \hat{F}^{(1)}(p, \nu) = \hat{F}^{(1)}_{\text{tree}}(p, \nu) + \hat{F}^{(1)}_{\text{ring}}(p, \nu) \]

\[ = \frac{V(0)}{2} n'_0(p, \nu) - \frac{1}{2\beta} n''_0(p, \nu) \int \frac{dk}{(2\pi)^3} \frac{\hat{V}(k)}{1 + \hat{V}(k)\rho_0(\nu)} \]

where we have expressed all quantities in terms of the density and the Bose momentum distribution (77) of the free gas.

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