Liquid-gas transition in nuclear matter: analytical formulas for the Virial coefficients*

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Abstract

In the framework of a study of the liquid-gas transition in nuclear matter, which main purpose was to investigate the impact of different Skyrme interactions on density, temperature and pressure at the critical point, we were faced with the calculation of the Virial coefficients. In this report, we provide relations, sum rules, analytical formulas and numerical values for such coefficients.

Keywords: liquid-gas transition; Skyrme interaction; Virial coefficients; Fermi ideal gas; critical point.

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1 Introduction

Using the finite-temperature Hartree-Fock theory, as presented by Fetter and Walecka [1], it is possible to derive an equation of state for a Fermi gas of nucleons interacting through the Skyrme [2] force. Details of the calculation are provided in an appendix of Ref. [3], but the resulting equation is quite simple:

$$P = -a_0\rho^2 + a_3(1+\sigma)\rho^{2+\sigma} + \left(1 - \frac{3}{2}\frac{\rho}{m^*}\frac{dm^*}{d\rho}\right) P_{\text{id}}(m^*), \tag{1}$$

where $P_{\text{id}}(m^*)$ is the pressure of a Fermi ideal gas made of particles with mass m^* at the temperature T. It can be obtained *via* the Virial expansion:

$$P_{\text{id}} = k_B T \sum_{n=1}^{\infty} B_n \rho^n, \tag{2}$$

where B_n are the so-called Virial coefficients. One has

$$\frac{P_{\text{id}}}{k_B T} = \frac{g}{\lambda^3} f_{5/2}(z), \tag{3}$$

g being the spin-isospin degeneracy factor and

$$\lambda = \left(\frac{2\pi\hbar^2}{m^* k_B T}\right)^{1/2} \tag{4}$$

the thermal de Broglie wavelength. The $f_{5/2}(z)$ Fermi function reads

$$f_{5/2}(z) = \frac{4}{\sqrt{\pi}} \int_0^\infty x^2 \ln\left(1 + z e^{-x^2}\right) dx \tag{5}$$

and can be expanded as

$$f_{5/2}(z) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{z^n}{n^{5/2}}. \tag{6}$$

The density of the Fermi ideal gas reads

$$\rho = \frac{g}{\lambda^3} f_{3/2}(z) \tag{7}$$

with

$$f_{3/2}(z) = z \frac{\partial}{\partial z} f_{5/2}(z) \tag{8}$$

satisfying the expansion

$$f_{3/2}(z) = \sum_{n=1}^{\infty} (-1)^{n+1} \frac{z^n}{n^{3/2}}. \tag{9}$$

Combining Egs. (2) and (3), one gets

$$\frac{g}{\lambda^3} \sum_{n=1}^{\infty} (-1)^{n+1} \frac{z^n}{n^{5/2}} = \sum_{n=1}^{\infty} B_n \left(\sum_{k=1}^{\infty} (-1)^{k+1} \frac{z^k}{k^{3/2}} \right)^n \tag{10}$$

2 Direct "brute force" calculation

Equation (10) is equivalent to

$$\begin{aligned}\frac{g}{\lambda^3}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{z^n}{n^{5/2}} &= B_1\frac{g}{\lambda^3}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{z^n}{n^{3/2}} \\ &+B_2\frac{g^2}{\lambda^6}\left(\sum_{n=1}^{\infty}(-1)^{n+1}\frac{z^n}{n^{3/2}}\right)^2 \\ &+\cdots \end{aligned} \tag{11}$$

and thus

$$\begin{aligned}\sum_{n=1}^{\infty}(-1)^{n+1}\frac{z^n}{n^{5/2}} &= B_1\sum_{m=1}^{\infty}(-1)^{m+1}\ \frac{z^m}{m^{3/2}} \\ &+B_2\frac{g}{\lambda^3}\sum_{m,n\geq 1}^{\infty}(-1)^{m+n+2}\ \frac{z^{m+n}}{(mn)^{3/2}} \\ &+B_3\frac{g^2}{\lambda^6}\sum_{m,n,p\geq 1}^{\infty}(-1)^{m+n+p+3}\ \frac{z^{m+n+p}}{(mnp)^{3/2}} \\ &+B_4\frac{g^3}{\lambda^9}\sum_{m,n,p,q\geq 1}^{\infty}(-1)^{m+n+p+q+4}\ \frac{z^{m+n+p+q}}{(mnpq)^{3/2}} \\ &+B_5\frac{g^4}{\lambda^{12}}\sum_{m,n,p,q,r\geq 1}^{\infty}(-1)^{m+n+p+q+r+5}\ \frac{z^{m+n+p+q+r}}{(mnpqr)^{3/2}} \\ &+B_6\frac{g^5}{\lambda^{15}}\sum_{m,n,p,q\geq 1}^{\infty}(-1)^{m+n+p+q+r+s+6}\ \frac{z^{m+n+p+q+r+s}}{(mnpqrs)^{3/2}} \\ &+B_7\frac{g^6}{\lambda^{18}}\sum_{m,n,p,q,r,s,t\geq 1}^{\infty}(-1)^{m+n+p+q+r+s+t+7}\ \frac{z^{m+n+p+q+r+s+t}}{(mnpqrst)^{3/2}} \\ &+\cdots\,. \end{aligned} \tag{12}$$

Identification of the powers of z yields the Virial B_n coefficients.

For $n = 1$:

$$\frac{1}{1^{5/2}} = B_1\frac{1}{1^{3/2}} \Rightarrow B_1 = 1. \tag{13}$$

For $n = 2$:

$$-\frac{1}{2^{5/2}} = -\frac{B_1}{2^{3/2}} + B_2\frac{g}{\lambda^3}.\frac{1}{1^{3/2}} \Rightarrow B_2 = \frac{1}{2^{5/2}}\left(\frac{\lambda^3}{g}\right). \tag{14}$$

For $n = 3$:

$$\frac{1}{3^{5/2}} = \frac{B_1}{3^{3/2}} + B_2\frac{g}{\lambda^3}\left(-\frac{2}{2^{3/2}}\right) + B_3\frac{g^2}{\lambda^6}\frac{1}{1^{3/2}} \Rightarrow B_3 = \left(\frac{1}{8} - \frac{2}{9\sqrt{3}}\right)\left(\frac{\lambda^3}{g}\right)^2. \tag{15}$$

For $n = 4$:

$$B_4 = \left(\frac{3\sqrt{6} + 5\sqrt{3} - 16}{32\sqrt{6}} \right) \left(\frac{\lambda^3}{g} \right)^3 . \tag{16}$$

For $n = 5$:

$$\begin{aligned} B_5 &= \left(\frac{5400\sqrt{30} + 7925\sqrt{15} - 25200\sqrt{5} - 6912\sqrt{3}}{43200\sqrt{15}} \right) \left(\frac{\lambda^3}{g^2} \right)^4 \\ &= \left(\frac{317}{1728} + \frac{\sqrt{2}}{8} - \frac{7\sqrt{3}}{36} - \frac{4\sqrt{5}}{125} \right) \left(\frac{\lambda^3}{g} \right)^4 \end{aligned} \tag{17}$$

For $n = 6$:

$$B_6 = \left(\frac{23}{128} + \frac{2081\sqrt{2}}{6912} - \frac{\sqrt{3}}{72} - \frac{91\sqrt{6}}{432} - \frac{\sqrt{10}}{20} \right) \left(\frac{\lambda^3}{g} \right)^5 . \tag{18}$$

For $n = 7$:

$$B_7 = \left(\frac{5957}{6912} + \frac{9\sqrt{2}}{64} - \frac{1721\sqrt{3}}{3888} - \frac{4\sqrt{5}}{25} - \frac{\sqrt{6}}{12} - \frac{6\sqrt{7}}{343} \right) \left(\frac{\lambda^3}{g} \right)^6 . \tag{19}$$

Order n	Virial coefficient $B_n \left(\frac{g}{\lambda^3}\right)^{n-1}$	Numerical value
1	1	1
2	$\frac{1}{2^{5/2}}$	0.176777
3	$\frac{1}{8} - \frac{2}{9\sqrt{3}}$	-0.00330006
4	$\frac{3\sqrt{6} + 5\sqrt{3} - 16}{32\sqrt{6}}$	0.000111289
5	$\frac{317}{1728} + \frac{\sqrt{2}}{8} - \frac{7\sqrt{3}}{36} - \frac{4\sqrt{5}}{125}$	-0.0481161
6	$\frac{23}{128} + \frac{2081\sqrt{2}}{6912} - \frac{\sqrt{3}}{72} - \frac{91\sqrt{6}}{432} - \frac{\sqrt{10}}{20}$	-0.092685
7	$\frac{5957}{6912} + \frac{9\sqrt{2}}{64} - \frac{1721\sqrt{3}}{3888} - \frac{4\sqrt{5}}{25} - \frac{\sqrt{6}}{12} - \frac{6\sqrt{7}}{343}$	-0.31415

3 Analytical formula

Setting, keeping Kilpatrick's notation

$$p_j = \frac{g}{\lambda^3}\frac{(-1)^{j+1}}{j^{3/2}}, \tag{20}$$

we have the relation

$$\sum_{j=1}^{\infty}\frac{p_j}{j}z^j = \sum_{k=1}^{\infty}B_k\left(\sum_{j=1}^{\infty}p_j z^j\right)^k \tag{21}$$

and therefore

$$p_n = \frac{n}{2\pi i}\oint \frac{1}{z^{n+1}}\sum_{k=1}^{\infty}B_k\left[\sum_{j=1}^{\infty}p_j z^j\right]^k dz \tag{22}$$

yielding

$$p_n = n\sum_{i=1}^{n} i!B_i \sum_{\{r_s\}}\prod_{s=1}^{n}\frac{p_s^{r_s}}{r_s!} \tag{23}$$

with

$$\sum_{s=1}^{n} r_s = i \tag{24}$$

and

$$\sum_{s=1}^{n} s r_s = n. \tag{25}$$

For instance, in the case $n = 3$, one has

$$\begin{cases} p_1 = p_1 B_1 \\ \frac{1}{2}p_2 = p_2 B_1 + p_1^2 B_2 \\ \frac{1}{3}p_3 = p_3 B_1 + 2p_2 p_1 B_2 + p_1^3 B_3. \end{cases} \tag{26}$$

In order to express the B_k coefficients in terms of the p_j, let us write

$$\sum_{j=1}^{\infty}\frac{p_j}{j}z^j = \sum_{k=1}^{\infty}B_k\rho^k \tag{27}$$

Integrating over ρ after multiplication by ρ^{-n+1} yields

$$B_n = \frac{1}{2\pi i}\oint \sum_{j=1}^{\infty}\frac{p_j}{j}z^j \times \frac{1}{\rho^{n-1}}d\rho. \tag{28}$$

Using

$$\rho = \sum_{j=1}^{\infty}p_j z^j, \tag{29}$$

one gets

$$B_n = \frac{1}{2\pi i}\oint \left(\sum_{j=1}^{\infty}\frac{p_j}{j}z^j\right)\left(\sum_{k=1}^{\infty}p_k z^k\right)^{-n-1}\left(\sum_{l=1}^{\infty}l p_l z^{l-1}\right)dz. \tag{30}$$

Thus, B_n is the coefficient of z^n in the expansion of

$$B_n = \frac{1}{2\pi i}\oint (p_1 z)^{-n-1}\left(1+\sum_{k=2}^{\infty}\frac{p_k}{p_1}z^{k-1}\right)^{-n-1}\left(\sum_{j=1}^{\infty}\frac{p_j}{j}z^j\right)\left(\sum_{l=1}^{\infty}l p_l z^{l-1}\right)dz. \tag{31}$$

and B_n is the coefficient of z^n in the expansion of

$$p_1^{-n-1}\left(1+\sum_{k=2}^{\infty}\frac{p_k}{p_1}z^{k-1}\right)^{-n-1}\left(\sum_{j=1}^{\infty}\frac{p_j}{j}z^j\right)\left(\sum_{l=1}^{\infty}l p_l z^{l-1}\right) \tag{32}$$

Expanding the different terms, one gets

$$B_n = \sum_{i=0}\sum_{j=1}\sum_{k=1}\frac{(-1)^i(n+i)!}{n!p_1^{n+1+i}}\frac{kp_jp_k}{j}\sum_{\{r_s\}}\prod_{s=2}^{n}\frac{p_s^{r_s}}{r_s!} \tag{33}$$

with

$$\sum_{s=2}^{n} r_s = i \tag{34}$$

and

$$\sum_{s=2}^{n} s r_s = n+i+1-j-k. \tag{35}$$

As shown by Kilpatrick [4, 5], one can set $k'_s = r_s$ for $s \geq 2$, $k''_s = \delta_{sj}$, $k'''_s = \delta_{sk}$ and $k_s = k'_s + k''_s + k'''_s$. One has subsequently

$$\sum_{s=2}^{n} k_s = i+2-k''_1-k'''_1 \tag{36}$$

and

$$\sum_{s=2}^{n} s k_s = n+i+1-k''_1-k'''_1. \tag{37}$$

Concerning the factor in p_1, the largest possible value of i is $n-1$, since no larger integer can divide $n-1+i$ into i parts, each one having size larger or equal than 2. For that reason, Kilpatrick suggested to write p_1^{2n-2} in the denominator and the remaining term in the form $p_1^{k_1}$. This defines k_1, and therefore k'_1. One gets

$$-n-1-i+k''_1+k'''_1 = k_1-(2n-2) \tag{38}$$

i. e. $i = n-3-k'_1$. The two constraints on the summation thus read

$$\boxed{\sum_{s=1} k_s = n-1}$$

and

$$\boxed{\sum_{s=1} sk_s = 2n-2}$$

and

$$\boxed{B_n = \sum_{\{k_s\}} \frac{(-1)^{n-1-k_1}(n-1)(2n-k_1-3)!}{n!p_1^{2n-2}} p_1^{k_1} \prod_{s=2}^{n} \frac{p_s^{k_s}}{k_s!}.}$$

Kilpatrick pointed out at the end of its paper that B_n is in fact the coefficient of z^{2n} in the expansion of

$$\frac{1}{n}\sum_{j=1}^{\infty}\left(p_j z^j\right)^{-n+1}. \tag{39}$$

Such a property can probably be useful in order to find the expression of B_n, using Faà di Bruno and multinomial coefficients. Replacing p_j by its value (20) in our specific case, one gets

$$\boxed{B_n = \left(\frac{\lambda^3}{g}\right)^{n-1} \frac{n-1}{n!} \sum_{\{k_s\}} (2n-k_1-3)! \frac{(-1)^{k_1}}{\prod_{s=2}^{n} k_s! s^{3k_s/2}}.}$$

For instance, the first five coefficients are

$$\left\{\begin{array}{l} B_1 = 1 \\ B_2 = -\frac{p_2}{p_1^2} \\ B_3 = \frac{1}{p_1^4}\left(-\frac{2}{3}p_3p_1 + p_2^2\right) \\ B_4 = \frac{1}{p_1^6}\left(-\frac{3}{4}p_4p_1^2 + 3p_3p_2p_1 - \frac{5}{2}p_1^3\right) \\ B_5 = \frac{1}{p_1^8}\left(-\frac{4}{5}p_5p_1^3 + 4p_4p_2p_1^2 + 2p_3^2p_1^2 - 12p_3p_2^2p_1 + 7p_2^4\right) \end{array}\right. . \tag{40}$$

Note that

$$\prod_{s=2}^{n} k_s! \tag{41}$$

is $G(n+2)$ where $G(z)$ represents the Barnes G function

$$G(n) = \prod_{k=1}^{n} \Gamma(k). \tag{42}$$

4 Sum rules

Equation (23) becomes

$$\sum_{i=1}^{n}(-1)^{i-1} i! \left(\frac{g}{\lambda^3}\right)^{i-1} B_i \sum_{\{r_s\}} \frac{1}{\prod_{s=1}^{n}\left[r_s! \times s^{3r_s/2}\right]} = \frac{1}{n^{5/2}} \tag{43}$$

with

$$\sum_{s=1}^{n} r_s = i \quad \text{and} \quad \sum_{s=1}^{n} sr_s = n. \tag{44}$$

Equation (43) constitutes a sum rule which can be useful to check numerical calculations of the B_n coefficients. It can also be used to express B_n in terms of the B_i, $i \leq n-1$ as:

$$B_n = \frac{(-1)^{n-1}}{n!}\left(\frac{\lambda^3}{g}\right)^{n-1} \times \left(\sum_{\{q_s^{(n)}\}} \frac{1}{\prod_{s=1}^{n}\left[q_s^{(n)} \times s^{3q_s^{(n)}/2}\right]}\right)^{-1} \times \left[\frac{1}{n^{5/2}} - \sum_{i=1}^{n-1}(-1)^{i-1} i! \left(\frac{g}{\lambda^3}\right)^{i-1} B_i \sum_{\{q_s^{(i)}\}} \frac{1}{\prod_{s=1}^{n}\left[q_s^{(i)} \times s^{3q_s^{(i)}/2}\right]}\right], \tag{45}$$

where

$$\sum_{s=1}^{n} q_s^{(i)} = i \tag{46}$$

and

$$\sum_{s=1}^{n} s q_s^{(i)} = n. \tag{47}$$

5 Conclusion

In this document, we proposed a discussion about the coefficients of the Virial expansion. We followed the general derivation of Kilpatrick to obtain analytical expressions for the Fermi ideal gas. It is worth mentioning that Wilson and Rogers presented relations in the cluster expansion theory of non-ideal gases using the formalism of umbral calculus [6].

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