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On the Chemical Potential of Ideal Fermi and Bose Gases

Brian Cowan¹

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Abstract

Knowledge of the chemical potential is essential in application of the Fermi–Dirac and the Bose–Einstein distribution functions for the calculation of properties of quantum gases. We give expressions for the chemical potential of ideal Fermi and Bose gases in 1, 2 and 3 dimensions in terms of inverse polylogarithm functions. We provide *Mathematica* functions for these chemical potentials together with low- and high-temperature series expansions. In the 3d Bose case we give also expansions about T_B . The *Mathematica* routines for the series allow calculation to arbitrary order.

Keywords Quantum gases · Chemical potential · Mathematica

1 Introduction

The properties of ideal Fermi and Bose gases are the starting points for the understanding of the low-temperature behaviour of a broad range of physical systems, including electrons in metals [1,2], the helium liquids [3,4] and systems of trapped gases [5]. Associated with these is interest in systems of lower dimensionality including graphene [6], helium films [7] and ultra-cold atoms in quasi-1d and quasi-2d traps [8].

The properties of ideal quantum gases are expressed, conveniently and succinctly in terms of the so-called Fermi–Dirac and Bose–Einstein functions. And essential to this is knowledge of the chemical potential [9].

Traditionally Fermi–Dirac and Bose–Einstein functions have been found from tables and power series expansions. The 1938 paper by McDougall and Stoner [10] gave extensive tables for fermions and there was a discussion of the corresponding functions for bosons by London [11], with series expansions given by Robinson [12] and generalized by Clunie [13]. A consolidated treatment of these functions is found in Pathria [14].

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The problem with the McDougal–Stoner tables and the above treatments was that the functions were given for different values of μ/kT which made for difficulties finding the chemical potential μ . In 1974 Betts [15] published tables of (reduced) chemical potential as a function of (reduced) temperature for 3d fermions and bosons; at that time, it was a heroic achievement of minicomputer programming. Ebner and Fu [16] gave useful series expressions for 3d fermions and analytic expressions for 2d fermions. Also they produced extensive tables [17], sadly now unavailable.

A further provision of series expansions for fermions was by Hore and Frankel [18] who gave expressions for the *intermediate* quantum region. These series were expanded about $z = 1$ where z is the fugacity. Expansions in the intermediate region for both bosons and fermions have been given by Sotnikov et al. [19].

The advent of symbolic mathematics software such as *Mathematica* has revolutionized the way Fermi–Dirac and Bose–Einstein calculations may be carried out. Such software can perform series expansions, reversion of series, symbolic integration, numerical integration to arbitrary precision and general symbolic manipulation. Moreover *Mathematica* “knows of” a large number of the “special functions” and their properties. Also it has inverse function support.

The Fermi–Dirac and the Bose–Einstein integrals may both be expressed in terms of the polylogarithm functions, once the chemical potential is known. In this paper we provide *Mathematica* functions to obtain the chemical potential. From these it is then straightforward to evaluate properties of Bose and Fermi gases. For reference we include the classical (Maxwell) gas. Of course at low temperatures such a gas is un-physical; it violates the third law of thermodynamics. But at high temperatures the way that the Bose and Fermi gases deviate from the classical is instructive.

2 General Methodology

2.1 The Polylogarithm Functions

The expectation value of an extensive function of energy $Q(\varepsilon)$ is given by

$$\bar{Q} = \alpha \sum_i Q(\varepsilon_i) n(\varepsilon_i), \quad (1)$$

where the sum is taken over the single particle energy states and α is the factor which accounts for the degeneracy of the particles’ spin states. This is 2 for electrons (spin $S = \frac{1}{2}$); more generally, it will be $2S + 1$. Here $n(\varepsilon)$ is the Fermi–Dirac or the Bose–Einstein distribution function

$$n(\varepsilon) = \frac{1}{e^{(\varepsilon-\mu)/kT} + a}, \quad (2)$$

where a is understood to be +1 for fermions and –1 for bosons. Classical particles also can be accommodated by taking $a = 0$. We may refer to such particles as “maxwellons”.

The distribution function involves the chemical potential μ , and so, this must be known before any later calculations. A key result of this paper is the provision of *Mathematica* functions for evaluation of the chemical potential for free fermion and boson gases in one, two and three dimensions.

In the thermodynamic limit Eq. (1) usually may be converted to an integral

$$\bar{Q} = \alpha \int_0^{\infty} Q(\varepsilon) g(\varepsilon) n(\varepsilon) d\varepsilon, \quad (3)$$

where $g(\varepsilon)$ is the energy density of states. Since $Q(\varepsilon)$ and $g(\varepsilon)$ are often proportional to powers of ε we require to evaluate thermodynamic integrals of the form

$$\int_0^{\infty} \varepsilon^n n(\varepsilon) d\varepsilon = \int_0^{\infty} \frac{\varepsilon^n d\varepsilon}{e^{(\varepsilon-\mu)/kT} + a} = (kT)^{n+1} \int_0^{\infty} \frac{x^n dx}{e^x z^{-1} + a}, \quad (4)$$

where $z = e^{\mu/kT}$ is the fugacity. These integrals are related to the polylogarithm functions $\text{Li}_s(z)$ [20,21]:

$$\begin{aligned} \int_0^{\infty} \frac{x^{s-1}}{e^x z^{-1} + 1} dx &= -\Gamma(s) \text{Li}_s(-z) \\ \int_0^{\infty} \frac{x^{s-1}}{e^x z^{-1} - 1} dx &= \Gamma(s) \text{Li}_s(z) \\ \int_0^{\infty} \frac{x^{s-1}}{e^x z^{-1}} dx &= \Gamma(s) z. \end{aligned} \quad (5)$$

The Maxwell case has been added for completeness.

We see that the thermodynamic integrals in the Bose and the Fermi case are thus given in terms of the polylogarithm functions:

$$\begin{aligned} \int_0^{\infty} \frac{\varepsilon^n d\varepsilon}{e^{(\varepsilon-\mu)/kT} + 1} &= -(kT)^{n+1} \Gamma(n+1) \text{Li}_{n+1}(-e^{\mu/kT}) \\ \int_0^{\infty} \frac{\varepsilon^n d\varepsilon}{e^{(\varepsilon-\mu)/kT} - 1} &= +(kT)^{n+1} \Gamma(n+1) \text{Li}_{n+1}(+e^{\mu/kT}) \\ \int_0^{\infty} \frac{\varepsilon^n d\varepsilon}{e^{(\varepsilon-\mu)/kT}} &= +(kT)^{n+1} \Gamma(n+1) e^{\mu/kT}. \end{aligned} \quad (6)$$

It then follows that the calculation of thermodynamic functions of ideal Fermi and Bose gases boils down to the evaluation of polylogarithm functions—once the chemical potential is known.

2.2 Common Energy Scale

When discussing fermions it is customary to use the Fermi energy as a convenient energy scale. This is the energy of the highest filled state at $T = 0$. Such a definition is clearly not applicable to maxwellions and to bosons. But it would be convenient to have a common energy scale applicable to particles whatever their statistics. In 3d the Fermi energy ε_F and the Fermi wave vector $k_F = (2m\varepsilon_F)^{1/2}/\hbar$ are given by

$$\varepsilon_F = \frac{\hbar^2}{2m} \left(\frac{6\pi^2 N}{\alpha V} \right)^{2/3}, \quad k_F = \left(\frac{6\pi^2 N}{\alpha V} \right)^{1/3}. \quad (7)$$

The Fermi wave vector is a measure of the inverse particle spacing. And this measure is appropriate in the discussion of maxwellions and bosons. In this spirit we shall introduce a characteristic wave vector, which we call the *quantum* wave vector k_q , and relate this to a *quantum* energy $\varepsilon_q = \hbar^2 k_q^2 / 2m$. This would be the Fermi energy in the case of fermions. In 1, 2 and 3d this is

$$\begin{aligned} \varepsilon_q &= \frac{\hbar^2}{2m} \left(\frac{\pi N}{\alpha L} \right)^2 & 1d \\ &= \frac{2\pi \hbar^2 N}{\alpha m A} & 2d \\ &= \frac{\hbar^2}{2m} \left(\frac{6\pi^2 N}{\alpha V} \right)^{2/3} & 3d. \end{aligned} \quad (8)$$

We note that Betts [15] uses different definitions for Bose and Fermi characteristic energies; this can be confusing.

2.3 Density of States

The (energy) density of states for free particles in one, two and three dimensions is [22]

$$\begin{aligned} g(\varepsilon) &= \frac{L}{\pi \hbar} \left(\frac{m}{2} \right)^{1/2} \varepsilon^{-1/2} & 1d \\ &= \frac{Am}{2\pi \hbar^2} & 2d \\ &= \frac{V}{4\pi^2 \hbar^3} (2m)^{3/2} \varepsilon^{1/2} & 3d. \end{aligned} \quad (9)$$

In terms of the quantum characteristic energy these may be expressed

$$\begin{aligned}
 g(\varepsilon) &= \frac{1}{2} \frac{N}{\alpha} \frac{1}{(\varepsilon \varepsilon_q)^{1/2}} & 1d \\
 &= \frac{N}{\alpha} \frac{1}{\varepsilon_q} & 2d \\
 &= \frac{3}{2} \frac{N}{\alpha} \frac{\varepsilon^{1/2}}{\varepsilon_q^{3/2}} & 3d
 \end{aligned} \tag{10}$$

or, generally, in d dimensions

$$g(\varepsilon) = \frac{d}{2} \frac{N}{\alpha} \varepsilon^{(d-2)/2} / \varepsilon_q^{d/2}. \tag{11}$$

We note that for atoms trapped in a harmonic trap the density of states is proportional to ε^{d-2} ; then, polylogarithm functions of different orders (usually integer) will be needed in the thermodynamic limit.

3 Chemical Potential and Fugacity

The number of particles in the system is given by

$$N = \alpha \int_0^{\infty} g(\varepsilon) n(\varepsilon) d\varepsilon. \tag{12}$$

However, the density of states $g(\varepsilon)$ is proportional to N so that N cancels and Eq. (12) leads to an expression for the quantum energy

$$\varepsilon_q^{d/2} = \frac{d}{2} \int_0^{\infty} \varepsilon^{(d-2)/2} n(\varepsilon) d\varepsilon. \tag{13}$$

This gives the quantum energy in terms of the chemical potential and the temperature. By inverting this relation we may find the chemical potential as a function of the quantum energy and the temperature.

For the Maxwell, Fermi and Bose cases Eq. (13) gives

$$\begin{aligned}
 \varepsilon_q^{d/2} &= (kT)^{d/2} \Gamma(1 + d/2) e^{\mu/kT} & \text{Maxwell} \\
 &= -(kT)^{d/2} \Gamma(1 + d/2) \text{Li}_{d/2}(-e^{\mu/kT}) & \text{Fermi} \\
 &= (kT)^{d/2} \Gamma(1 + d/2) \text{Li}_{d/2}(e^{\mu/kT}) & \text{Bose.}
 \end{aligned} \tag{14}$$

In terms of the quantum energy we shall introduce the reduced chemical potential μ^* , defined as

$$\mu^* = \mu/\varepsilon_q; \quad (15)$$

and this will be expressed as a function of τ , the reduced temperature¹

$$\tau = kT/\varepsilon_q. \quad (16)$$

The fugacity is expressed in terms of τ as $z(\tau) = e^{\mu^*(\tau)/\tau}$. Using our reduced variables, Eq. (14) become

$$\begin{aligned} \tau^{-d/2} &= \Gamma(1 + d/2)z(\tau) && \text{Maxwell} \\ &= -\Gamma(1 + d/2)\text{Li}_{d/2}(-z(\tau)) && \text{Fermi} \\ &= \Gamma(1 + d/2)\text{Li}_{d/2}(z(\tau)) && \text{Bose.} \end{aligned} \quad (17)$$

Then, from inversion of these equations, $z(\tau)$ is given by

$$z(\tau) = \frac{1}{\Gamma(1 + d/2)}\tau^{-d/2} \quad \text{Maxwell} \quad (18)$$

$$= -\text{Li}_{d/2}^{-1}\left[\frac{-1}{\Gamma(1 + d/2)}\tau^{-d/2}\right] \quad \text{Fermi} \quad (19)$$

$$= +\text{Li}_{d/2}^{-1}\left[\frac{1}{\Gamma(1 + d/2)}\tau^{-d/2}\right] \quad \text{Bose} \quad (20)$$

and then $\mu^*(\tau)$ by

$$\mu^*(\tau) = \tau \ln \left\{ \frac{1}{\Gamma(1 + d/2)}\tau^{-d/2} \right\} \quad \text{Maxwell} \quad (21)$$

$$= \tau \ln \left\{ -\text{Li}_{d/2}^{-1}\left[\frac{-1}{\Gamma(1 + d/2)}\tau^{-d/2}\right] \right\} \quad \text{Fermi} \quad (22)$$

$$= \tau \ln \left\{ +\text{Li}_{d/2}^{-1}\left[\frac{1}{\Gamma(1 + d/2)}\tau^{-d/2}\right] \right\} \quad \text{Bose.} \quad (23)$$

Mathematica routines for these functions (Fermi and Bose) are given in Appendix A.

4 Functions and Their Series Expressions

Details of the calculation of the low-temperature and high-temperature series are given in the appendices. Associated *Mathematica* Notebooks are included in Supplementary Information, allowing evaluation of these series to arbitrary order.

A key point about the *Mathematica* calculations is that while *Mathematica* provides the `InverseFunction` command used in the chemical potential and fugacity

¹ We note that our $\mu^*(\tau)$ is equivalent, in the Fermi case, to Ebner and Fu's [16] $\zeta(t)$.

expressions, the `InverseFunction` provision does not extend to symbolic series calculations. For this reason we have to perform the series expansion first and then obtain the inverse by reversing the power series.

In this section below we summarize the results of these calculations. We shall use the *Mathematica* functions of Appendix A to create plots of the chemical potential and the series approximations given. A *Mathematica* notebook creating the plots below is given in Supplementary Information MOESM1_ESM.nb.

4.1 Maxwellons in 1d

In Eqs. (21) and (18) we put $d = 1$ giving

$$\mu_{M1}^*(\tau) = \tau \log \left(\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right), \quad (24)$$

$$z_{M1}(\tau) = \frac{2}{\sqrt{\pi}} \tau^{-1/2}. \quad (25)$$

4.2 Fermions in 1d

In Eqs. (22) and (19) we put $d = 1$ giving

$$\mu_{F1}^*(\tau) = \tau \ln \left\{ -\text{Li}_{1/2}^{-1} \left[-\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right] \right\}, \quad (26)$$

$$z_{F1}(\tau) = -\text{Li}_{1/2}^{-1} \left[-\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right]. \quad (27)$$

Chemical potential—low-temperature series

$$\mu_{F1}^*(\tau) = 1 + \frac{\pi^2}{12} \tau^2 + \frac{\pi^4}{36} \tau^4 + \frac{7\pi^6}{144} \tau^6 + \dots \quad (28)$$

Chemical potential—high-temperature series

$$\begin{aligned} \mu_{F1}^*(\tau) = & \tau \log \left(\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right) + \sqrt{\frac{2}{\pi}} \tau^{1/2} + \frac{(9 - 4\sqrt{3})}{3\pi} + \\ & + \frac{4(5\sqrt{2} - 4\sqrt{6} + 3)}{3\pi^{3/2}} \frac{1}{\tau^{1/2}} - \frac{(12\sqrt{2} - 48\sqrt{3} + 71)}{3\pi^2} \frac{1}{\tau} + \dots \end{aligned} \quad (29)$$

The first term is the Maxwell chemical potential.

The 1d Fermi chemical potential, together with low- T and high- T approximations, is shown in Fig. 1.

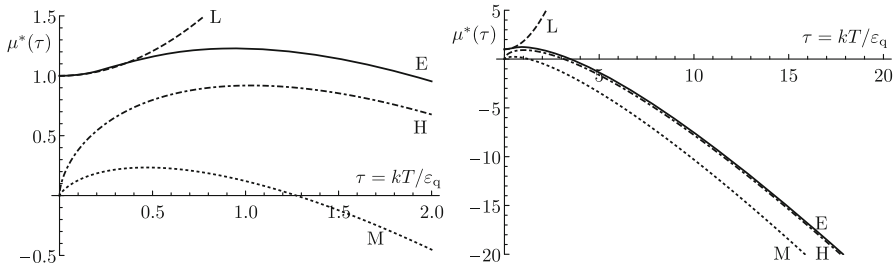


Fig. 1 Fermi chemical potential in 1d. E is the exact result Eq. (26), L is the low-temperature approximation: the first two terms of Eq. (28), M is the Maxwell expression Eq. (24), H is the high-temperature approximation: the first two terms of Eq. (29)

Fugacity—low-temperature series. Since $z_{F1}(\tau)$ diverges as $\tau \rightarrow 0$ there is no simple low-temperature power series. But the low-temperature behaviour can be expressed as

$$z_{F1}(\tau) = e^{1/\tau} \left\{ 1 + \frac{\pi^2}{12} \tau + \frac{\pi^4}{288} \tau^2 + \frac{(288\pi^4 + \pi^6)}{10368} \tau^3 + \dots \right\} \tag{30}$$

with the limiting low-temperature behaviour

$$z_{F1}(\tau) \sim e^{1/\tau}. \tag{31}$$

Fugacity—high-temperature series

$$z_{F1}(\tau) = \frac{2}{\sqrt{\pi}} \frac{1}{\tau^{1/2}} + \frac{2\sqrt{2}}{\pi} \frac{1}{\tau} + \frac{8(3 - \sqrt{3})}{3\pi^{3/2}} \frac{1}{\tau^{3/2}} + \frac{4(15\sqrt{2} - 10\sqrt{6} + 6)}{3\pi^2} \frac{1}{\tau^2} + \dots \tag{32}$$

The first term is the Maxwell fugacity.

4.3 Bosons in 1d

In Eqs. (23) and (20) we put $d = 1$ giving

$$\mu_{B1}^*(\tau) = \tau \ln \left\{ \text{Li}_{1/2}^{-1} \left[\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right] \right\}, \tag{33}$$

$$z_{B1}(\tau) = \text{Li}_{1/2}^{-1} \left[\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right]. \tag{34}$$

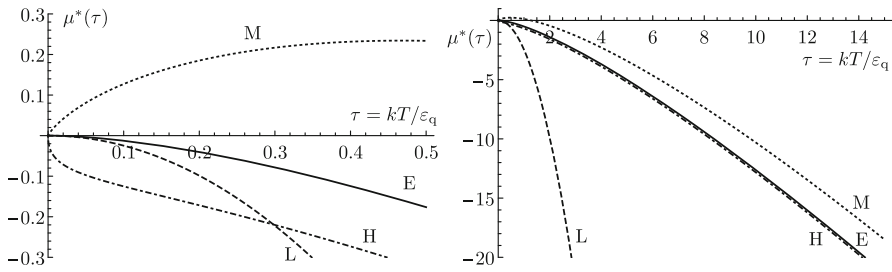


Fig. 2 Bose chemical potential in 1d. E is the exact result Eq. (33), L is the low-temperature approximation: the first term of Eq. (35), M is the Maxwell expression Eq. (24), H is the high-temperature approximation: the first two terms of Eq. (36)

Chemical potential—low-temperature series

$$\begin{aligned} \mu_{B1}^*(\tau) = & -\frac{1}{4}\pi^2\tau^2 - \frac{1}{4}\pi^{5/2}\zeta\left(\frac{1}{2}\right)\tau^{5/2} - \frac{3}{16}\zeta\left(\frac{1}{2}\right)^2\pi^3\tau^3 \\ & + \frac{1}{16}\pi^{7/2}\left(\pi\zeta\left(-\frac{1}{2}\right) - 2\zeta\left(\frac{1}{2}\right)^3\right)\tau^{7/2} + \dots \end{aligned} \tag{35}$$

where $\zeta()$ is the Reimann zeta function.

Chemical potential—high-temperature series

$$\begin{aligned} \mu_{B1}^*(\tau) = & \tau \log\left(\frac{2}{\sqrt{\pi}}\tau^{-1/2}\right) - \sqrt{\frac{2}{\pi}}\tau^{1/2} + \frac{(9 - 4\sqrt{3})}{3\pi} \\ & - \frac{4(5\sqrt{2} - 4\sqrt{6} + 3)}{3\pi^{3/2}}\frac{1}{\tau^{1/2}} - \frac{(12\sqrt{2} - 48\sqrt{3} + 71)}{3\pi^2}\frac{1}{\tau} + \dots \end{aligned} \tag{36}$$

The first term is the Maxwell chemical potential.

The 1d Bose chemical potential, together with low- T and high- T approximations, is shown in Fig. 2.

Fugacity—low-temperature series

$$z_{B1}(\tau) = 1 - \frac{\pi^2}{4}\tau - \frac{\pi^{5/2}}{4}\zeta\left(\frac{1}{2}\right)\tau^{3/2} - \frac{1}{32}\left(6\pi^3\zeta\left(\frac{1}{2}\right)^2 - 4\pi^4\right)\tau^2 + \dots \tag{37}$$

Fugacity—high-temperature series

$$\begin{aligned} z_{B1}(\tau) = & \frac{2}{\sqrt{\pi}}\frac{1}{\tau^{1/2}} - \frac{2\sqrt{2}}{\pi}\frac{1}{\tau} + \frac{8(3 - \sqrt{3})}{3\pi^{3/2}}\frac{1}{\tau^{3/2}} \\ & - \frac{4(15\sqrt{2} - 10\sqrt{6} + 6)}{3\pi^2}\frac{1}{\tau^2} + \dots \end{aligned} \tag{38}$$

The first term is the Maxwell fugacity.

4.4 Maxwellons in 2d

In Eqs. (21) and (18) we put $d = 2$ giving

$$\mu_{M2}^*(\tau) = -\tau \ln(\tau), \quad (39)$$

$$z_{M2}(\tau) = \frac{1}{\tau}. \quad (40)$$

4.5 Fermions in 2d

In Eqs. (22) and (19) we put $d = 2$ giving

$$\mu_{F2}^*(\tau) = \tau \ln \left\{ -\text{Li}_1^{-1} \left(-\frac{1}{\tau} \right) \right\}, \quad (41)$$

$$z_{F2}(\tau) = -\text{Li}_1^{-1} \left(-\frac{1}{\tau} \right). \quad (42)$$

But since $\text{Li}_1(-z) = -\ln(1+z)$, it follows that in 2d explicit expressions may be obtained. Thus:

$$\mu_{F2}^*(\tau) = \tau \ln(e^{1/\tau} - 1), \quad (43)$$

$$z_{F2}(\tau) = e^{1/\tau} - 1. \quad (44)$$

Our Eq. (43) corresponds to Eq. (1) of Ebner and Fu.

Chemical potential—low-temperature series There is no series in ascending powers of τ , but the following series of exponentials follows from Eq. (43) at low temperatures.

$$\mu_{F2}^*(\tau) = 1 - \tau \left\{ e^{-1/\tau} + \frac{1}{2}e^{-2/\tau} + \frac{1}{3}e^{-3/\tau} + \dots \right\}. \quad (45)$$

Chemical potential—high-temperature series

$$\mu_{F2}^*(\tau) = -\tau \log(\tau) + \frac{1}{2} + \frac{1}{24} \frac{1}{\tau} - \frac{1}{2880} \frac{1}{\tau^3} + \dots, \quad (46)$$

corresponding to Eq. (2) of Ebner and Fu. The first term of Eq. (46) is the Maxwell chemical potential.

The 2d Fermi chemical potential, together with low- T and high- T approximations, is shown in Fig. 3.

Fugacity—low temperatures. Since $z_{F2}(\tau)$ diverges as $\tau \rightarrow 0$ there is no simple low-temperature power series. But in the spirit of Eq. (45) and writing $z_{F2}(\tau)$ as

$$z_{F2}(\tau) = e^{1/\tau} (1 - e^{-1/\tau}) \quad (47)$$

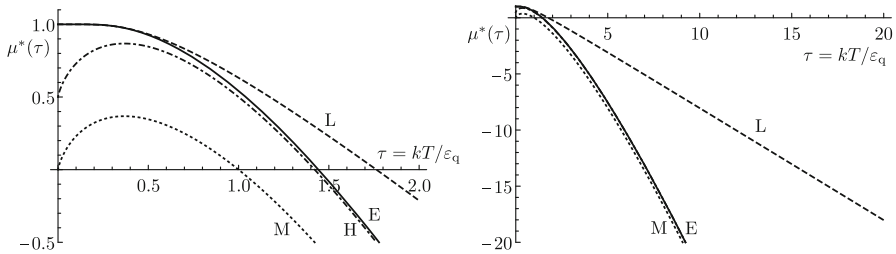


Fig. 3 Fermi gas in 2d. E is the exact result Eq. (43), L is the low-temperature approximation: the first two terms of Eq. (45), M is the Maxwell expression Eq. (39), H is the high-temperature approximation: the first two terms of Eq. (46)

we may regard the two terms in the brackets as a terminating low-temperature expansion, with the divergent

$$z_{F2}(\tau) \sim e^{1/\tau} \tag{48}$$

giving the limiting low-temperature behaviour.

Fugacity—high-temperature series

$$z_{F2}(\tau) = \frac{1}{\tau} + \frac{1}{2} \frac{1}{\tau^2} + \frac{1}{6} \frac{1}{\tau^3} + \frac{1}{24} \frac{1}{\tau^4} + \frac{1}{120} \frac{1}{\tau^5} + \dots \tag{49}$$

The first term is the Maxwell fugacity.

4.6 Bosons in 2d

In Eqs. (23) and (20) we put $d = 2$ giving

$$\mu_{B2}^*(\tau) = \tau \ln \left\{ \text{Li}_1^{-1} \left(\frac{1}{\tau} \right) \right\}, \tag{50}$$

$$z_{B2}(\tau) = \text{Li}_1^{-1} \left(\frac{1}{\tau} \right). \tag{51}$$

But since $\text{Li}_1(z) = -\ln(1 - z)$, it follows that in 2d explicit expressions may be obtained. Thus:

$$\mu_{B2}^*(\tau) = \tau \ln(1 - e^{-1/\tau}), \tag{52}$$

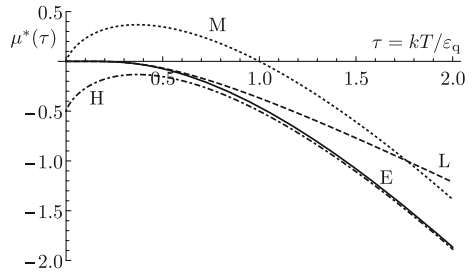
$$z_{B2}(\tau) = 1 - e^{-1/\tau}. \tag{53}$$

In 2d we have the special results

$$\mu_{B2}^*(\tau) = \mu_{F2}^*(\tau) - 1 \tag{54}$$

$$z_{B2}(\tau) = z_{F2}(\tau)/(1 + z_{F2}(\tau)), \tag{55}$$

Fig. 4 Bose gas in 2d. E is the exact result Eq. (52), L is the low-temperature approximation: the first term of Eq. (56), M is the Maxwell expression Eq. (39), H is the high-temperature approximation: the first two terms of Eq. (57)



manifestations of May’s theorem on Fermi–Bose correspondence in 2d [23]. We note that May’s theorem holds only in the thermodynamic limit; it breaks down for finite systems [24].

Chemical potential—low-temperature series There is no series in ascending powers of τ , but the following series of exponentials follows from Eq. (52) at low temperatures.

$$\mu_{B2}^*(\tau) = -\tau \left\{ e^{-1/\tau} + \frac{1}{2}e^{-2/\tau} + \frac{1}{3}e^{-3/\tau} + \dots \right\}. \tag{56}$$

Chemical potential—high-temperature series

$$\mu_{B2}^*(\tau) = -\tau \log(\tau) - \frac{1}{2} + \frac{1}{24\tau} - \frac{1}{2880\tau^3} + \dots \tag{57}$$

The first term is the Maxwell chemical potential.

The 2d Bose chemical potential, together with low- T and high- T approximations, is shown in Fig. 4.

Fugacity—low temperatures There is no low-temperature series for the fugacity, but we may regard the expression for $z_{B2}(\tau)$, Eq. (53), as a terminating low-temperature expansion:

$$z_{B2}(\tau) = 1 - e^{-1/\tau} + \text{no higher terms}, \tag{58}$$

with low-temperature limit $z_{B2}(0) = 1$.

Fugacity—high-temperature series

$$z_{B2}(\tau) = \frac{1}{\tau} - \frac{1}{2} \frac{1}{\tau^2} + \frac{1}{6} \frac{1}{\tau^3} - \frac{1}{24} \frac{1}{\tau^4} + \frac{1}{120} \frac{1}{\tau^5} + \dots \tag{59}$$

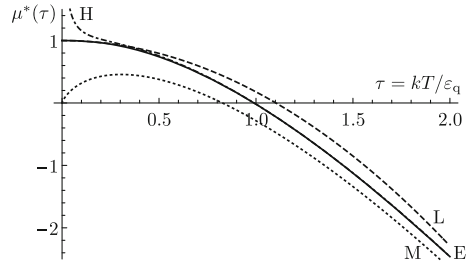
The first term is the Maxwell fugacity.

4.7 Maxwellons in 3d

In Eqs. (21) and (18) we put $d = 3$ giving

$$\mu_{M3}^*(\tau) = \tau \ln \left(\frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} \right), \tag{60}$$

Fig. 5 Fermi gas in 3d. E is the exact result Eq. (62), L is the low-temperature approximation: the first two terms of Eq. (64), M is the Maxwell expression Eq. (60), H is the high-temperature approximation: the first two terms of Eq. (65)



$$z_{M3}(\tau) = \frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}}. \tag{61}$$

4.8 Fermions in 3d

In Eqs. (22) and (19) we put $d = 3$ giving

$$\mu_{F3}^*(\tau) = \tau \ln \left\{ -\text{Li}_{3/2}^{-1} \left[-\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] \right\}, \tag{62}$$

$$z_{F3}(\tau) = -\text{Li}_{3/2}^{-1} \left[-\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right]. \tag{63}$$

Chemical potential—low-temperature series

$$\mu_{F3}^*(\tau) = 1 - \frac{\pi^2}{12} \tau^2 - \frac{\pi^4}{80} \tau^4 - \frac{247\pi^6}{25920} \tau^6 - \frac{16291\pi^8}{777600} \tau^8 + \dots \tag{64}$$

Chemical potential—high-temperature series

$$\begin{aligned} \mu_{F3}^*(\tau) = & \tau \ln \left(\frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} \right) + \frac{1}{3} \sqrt{\frac{2}{\pi}} \frac{1}{\tau^{1/2}} - \frac{16\sqrt{3} - 27}{81\pi} \frac{1}{\tau^2} + \\ & + \frac{4(15\sqrt{2} - 16\sqrt{6} + 18)}{243\pi^{3/2}} \frac{1}{\tau^{7/2}} + \dots \end{aligned} \tag{65}$$

This equation corresponds to that given by Ebner and Fu after their Eq. (3). But their equation has a typo. The first term of Eq. (65) is the Maxwell chemical potential.

The 3d Fermi chemical potential, together with low- T and high- T approximations, is shown in Fig. 5.

Fugacity—low-temperature series Since z_{F3} diverges as $\tau \rightarrow 0$ there is no simple low-temperature power series. But the low-temperature behaviour can be expressed as

$$z_{F3}(\tau) = e^{1/\tau} \left\{ 1 - \frac{\pi^2}{12} \tau + \frac{\pi^4}{288} \tau^2 - \frac{1}{3} \left(\frac{3\pi^4}{80} + \frac{\pi^6}{3456} \right) \tau^3 + \dots \right\} \tag{66}$$

with the limiting low-temperature behaviour

$$z_{F3}(\tau) \sim e^{1/\tau}. \tag{67}$$

Fugacity—high-temperature series

$$\begin{aligned} z_{F3}(\tau) = & \frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} + \frac{4\sqrt{2}}{9\pi} \frac{1}{\tau^3} + \frac{16(9 - 4\sqrt{3})}{243\pi^{3/2}} \frac{1}{\tau^{9/2}} + \\ & + \frac{8(45\sqrt{2} - 40\sqrt{6} + 36)}{729\pi^2 t^6} \frac{1}{\tau^6} + \dots \end{aligned} \tag{68}$$

The first term is the Maxwell fugacity.

4.9 Bosons in 3d

In three dimensions bosons can undergo Bose–Einstein condensation. When this happens the chemical potential will be zero and the fugacity will be unity. We denote the reduced Bose temperature by τ_B .

In Eqs. (23) and (20) we put $d = 3$ to give μ^* and z when $\tau > \tau_B$. Then the reduced chemical potential and the fugacity are given by

$$\begin{aligned} \mu_{B3}^*(\tau) = 0 & & \tau < \tau_B \\ = \tau \ln \left\{ \text{Li}_{3/2}^{-1} \left[\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] \right\} & & \tau > \tau_B \end{aligned} \tag{69}$$

$$\begin{aligned} z_{B3}(\tau) = 1 & & \tau < \tau_B \\ = \text{Li}_{3/2}^{-1} \left[\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] & & \tau > \tau_B. \end{aligned} \tag{70}$$

The Bose temperature τ_B is the zero of $\mu^*(\tau)$ of Eq. (69), that is,

$$\tau_B = \left(\frac{3\sqrt{\pi}}{4} \zeta\left(\frac{3}{2}\right) \right)^{-2/3} \approx 0.436\dots \tag{71}$$

Chemical potential—low-temperature series

$$\begin{aligned} \mu_{B3}^*(\tau) = 0 & & \tau < \tau_B \\ = -\frac{9\zeta\left(\frac{3}{2}\right)^2}{16\pi} \frac{(\tau - \tau_B)^2}{\tau_B} + & & \\ + \frac{27\zeta\left(\frac{3}{2}\right)^2 \left(\zeta\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) + 2\pi \right)}{64\pi^2} \frac{(\tau - \tau_B)^3}{\tau_B^2} + \dots & & \tau > \tau_B. \end{aligned} \tag{72}$$

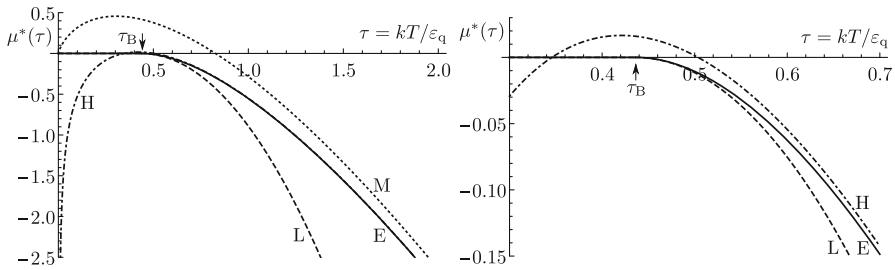


Fig. 6 Bose gas in 3d. E is the exact result Eq. (69), L is the low-temperature approximation: the first term of Eq. (72), M is the Maxwell expression Eq. (60), H is the high-temperature approximation: the first two terms of Eq. (73)

An expression equivalent to the first term of the series is given by London [11]; the author thanks Bill Mullin for drawing his attention to this.

Chemical potential—high-temperature series

$$\begin{aligned} \mu_{B3}^*(\tau) = & \tau \ln \left(\frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} \right) - \frac{1}{3} \sqrt{\frac{2}{\pi}} \frac{1}{\tau^{1/2}} - \frac{16\sqrt{3} - 27}{81\pi} \frac{1}{\tau^2} \\ & - \frac{4(15\sqrt{2} - 16\sqrt{6} + 18)}{243\pi^{3/2}} \frac{1}{\tau^{7/2}} + \dots \end{aligned} \tag{73}$$

The first term is the Maxwell chemical potential.

The 3d Bose chemical potential, together with low-*T* and high-*T* approximations, is shown in Fig. 6.

Fugacity—low-temperature series

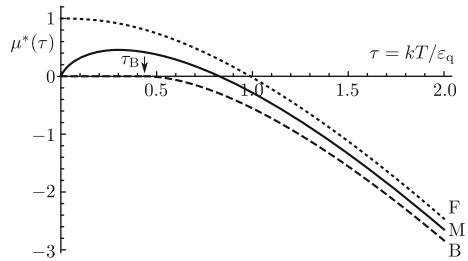
$$\begin{aligned} z_{B3}(\tau) = & 1 \qquad \qquad \qquad \tau < \tau_B \\ = & 1 - \frac{9\zeta\left(\frac{3}{2}\right)^2}{16\pi} \left(\frac{\tau - \tau_B}{\tau_B} \right)^2 + \\ & + \frac{9\zeta\left(\frac{3}{2}\right)^2 \left(3\zeta\left(\frac{1}{2}\right)\zeta\left(\frac{3}{2}\right) + 10\pi \right)}{64\pi^2} \left(\frac{\tau - \tau_B}{\tau_B} \right)^3 + \dots \quad \tau < \tau_B \end{aligned} \tag{74}$$

Fugacity—high-temperature series

$$\begin{aligned} z_{B3}(\tau) = & \frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} - \frac{4\sqrt{2}}{9\pi} \frac{1}{\tau^3} + \frac{16(9 - 4\sqrt{3})}{243\pi^{3/2}} \frac{1}{\tau^{9/2}} \\ & - \frac{8(45\sqrt{2} - 40\sqrt{6} + 36)}{729\pi^2 t^6} \frac{1}{\tau^6} + \dots \end{aligned} \tag{75}$$

The first term is the Maxwell fugacity.

Fig. 7 Chemical potential in three dimensions—Fermi, Bose and Maxwell cases



5 Chemical Potential Plots in 1, 2 and 3d

We now use the *Mathematica* functions to create plots of the chemical potential in one-, two- and three dimensions. These will contrast the differences and similarities of the Fermi, Bose and Maxwell cases.

5.1 Three Dimensions

The temperature dependence of the 3d chemical potential is shown in Fig. 7. At high temperatures the Fermi and Bose chemical potentials tend towards the classical Maxwell behaviour, Eq. (91/92),

$$\begin{aligned} \mu^*(\tau) &= \tau \ln \left(\frac{4}{3\sqrt{\pi}} \frac{1}{\tau^{3/2}} \right) + a \frac{1}{3} \sqrt{\frac{2}{\pi}} \frac{1}{\tau^{1/2}} + \dots \\ &= \mu_M^*(\tau) + a \frac{1}{3} \sqrt{\frac{2}{\pi}} \frac{1}{\tau^{1/2}} + \dots \end{aligned} \tag{76}$$

becoming equal as $\tau \rightarrow \infty$. (Recall $a = +1$ for fermions, -1 for bosons and 0 for maxwellons.)

At low temperatures the fermion $\mu^*(\tau) \rightarrow 1$ as $\tau \rightarrow 0$ ($\mu(T) \rightarrow \epsilon_F$ as $T \rightarrow 0$).

Upon cooling, bosons in 3d undergo BEC at the Bose temperature τ_B where the chemical potential goes to zero. Just above the Bose temperature $\mu^*(\tau)$ increases quadratically in $(\tau - \tau_B)$, while below the Bose temperature $\mu^*(\tau)$ is identically zero. There is a discontinuity in the second derivative of $\mu^*(\tau)$ at $\tau = \tau_B$. We shall in the following sections see that there is no BEC for $d < 3$; this is an example of the Mermin–Wagner theorem [25]. Then there is macroscopic occupation only at $T = 0$.

The maxwellon chemical potential increases from zero as the temperature increases from zero, with a nonzero slope; this is a violation of the third law of thermodynamics, which requires $\partial\mu/\partial T \rightarrow 0$ as $T \rightarrow 0$.

5.2 Two Dimensions

The temperature dependence of the 2d chemical potential is shown in Fig. 8.

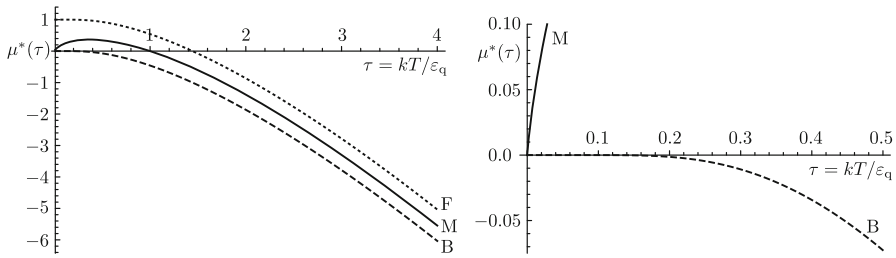


Fig. 8 Chemical potential in two dimensions—Fermi, Bose and Maxwell cases

At high temperatures the Fermi and Bose chemical potentials, Eq. (91/92), tend towards the classical Maxwell behaviour

$$\begin{aligned} \mu^*(\tau) &= -\tau \log(\tau) + a \frac{1}{2} + \dots \\ &= \mu_M^*(\tau) + a \frac{1}{2} + \dots, \end{aligned} \tag{77}$$

but they never actually get there. In 2d we have the May’s theorem result

$$\mu_{B2}^*(\tau) = \mu_{F2}^*(\tau) - 1, \tag{78}$$

and at high temperatures, the Maxwell μ is midway between those of the Fermi and the Bose cases. In other words, in the high-temperature limit the Fermi chemical potential is $\varepsilon_q/2$ higher than the Maxwell value and the Bose chemical potential is $\varepsilon_q/2$ below.

At low temperatures the Bose chemical potential goes to zero. There is no BEC, so μ is zero only at zero temperature. But the low-temperature μ is “very flat” (see Fig. 8 right plot); it is as if the 2d bosons are “trying to” condense. We shall see in Sect. 5.3 that there is certainly no BEC in 1d. But here, in 2d, we might say that BEC is “marginal”.

The low-temperature Fermi chemical potential is similar to the Bose case, just shifted up by ε_q .

The Maxwell chemical potential increases from zero as the temperature increases from zero with nonzero slope, in violation of the third law of thermodynamics.

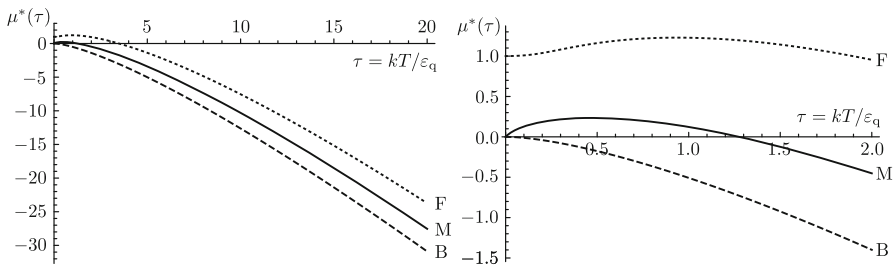


Fig. 9 Chemical potential in one dimension—Fermi, Bose and Maxwell cases

5.3 One Dimension

The temperature dependence of the 1d chemical potential is shown in Fig. 9.

At high temperatures the Fermi and Bose chemical potentials, Eq. (91/92), are going in the same direction as the Maxwell case: the Fermi above and the Bose below

$$\begin{aligned}\mu^*(\tau) &= \tau \log\left(\frac{2}{\sqrt{\pi}}\tau^{-1/2}\right) + a\sqrt{\frac{2}{\pi}}\tau^{1/2} + \dots \\ &= \mu_M^*(\tau) + a\sqrt{\frac{2}{\pi}}\tau^{1/2} + \dots,\end{aligned}\quad (79)$$

but as the temperature increases the Fermi and Bose curves move further away from the Maxwell. The *fractional* deviation $(\mu_{F,B}^*(\tau) - \mu_M^*(\tau))/\mu_M^*(\tau)$ does go to zero as $\tau \rightarrow \infty$.

The low-temperature Bose chemical potential goes to zero as τ^2 . There is not even a hint of BEC; the macroscopic occupation of the ground state occurs only at $T = 0$.

The low-temperature Fermi chemical potential has an interesting form. As the temperature increases from zero μ increases a little before turning over and decreasing. This is not a violation of the third law since $\partial\mu/\partial T \rightarrow 0$ as $T \rightarrow 0$.

The Maxwell chemical potential increases from zero with nonzero slope as the temperature increases from zero, in violation of the third law of thermodynamics.

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A Mathematica Functions for Chemical Potential and Fugacity

A.1 Mathematica Functions

The Maxwell chemical potential and fugacity expressions in 1, 2 and 3d: Eqs. (24), (25), (39), (40), (60), (61) are straightforward; they do not require special *Mathematica* functions. The 2d Fermi and Bose chemical potential and fugacity expressions also are straightforward; although they do not require special *Mathematica* functions, these are given below for completeness.

A.1.1 Fermi Chemical Potential in 1d

This is given by Eq. (26):

$$\mu_{F1}^*(\tau) = \tau \ln \left\{ -\text{Li}_{1/2}^{-1} \left[-\frac{2}{\sqrt{\pi}}\tau^{-1/2} \right] \right\}$$

with *Mathematica* implementation

```
muF1d[tau_] := tau InverseFunction[Function[z,
  -(Sqrt[Pi]/2 PolyLog[1/2, -Exp[z]])]][tau^(-1/2)]
```

A.1.2 Fermi Fugacity in 1d

This is given by Eq. (27):

$$z_{F1}(\tau) = -\text{Li}_{1/2}^{-1} \left[-\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right]$$

with *Mathematica* implementation

```
zF1d[tau_] := InverseFunction[Function[z,
  -(Sqrt[Pi]/2 PolyLog[1/2, -z])]][tau^(-1/2)]
```

A.1.3 Bose Chemical Potential in 1d

This is given by Eq. (33):

$$\mu_{B1}^*(\tau) = \tau \ln \left\{ \text{Li}_{1/2}^{-1} \left[\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right] \right\}$$

with *Mathematica* implementation

```
muB1d[tau_] := tau InverseFunction[Function[z,
  (Sqrt[Pi]/2 PolyLog[1/2, Exp[z]])]][tau^(-1/2)]
```

A.1.4 Bose Fugacity in 1d

This is given by Eq. (34):

$$z_{B1}(\tau) = \text{Li}_{1/2}^{-1} \left[\frac{2}{\sqrt{\pi}} \tau^{-1/2} \right]$$

with *Mathematica* implementation

```
zB1d[tau_] := InverseFunction[Function[z,
  (Sqrt[Pi]/2 PolyLog[1/2, z])]][tau^(-1/2)]
```

A.1.5 Fermi Chemical Potential in 2d

This is given by Eq. (43):

$$\mu_{F2}^*(\tau) = \tau \ln(e^{1/\tau} - 1)$$

with *Mathematica* implementation

```
muF2d[tau_] := tau Log[Exp[1/tau]-1]
```

A.1.6 Fermi Fugacity in 2d

This is given by Eq. (44):

$$z_{F2}(\tau) = e^{1/\tau} - 1$$

with *Mathematica* implementation

$$zF2d[\tau_] := \text{Exp}[1/\tau] - 1$$

A.1.7 Bose Chemical Potential in 2d

This is given by Eq. (52):

$$\mu_{B2}^*(\tau) = \tau \ln(1 - e^{-1/\tau})$$

with *Mathematica* implementation

$$\text{muB2d}[\tau_] := \tau \text{Log}[1 - \text{Exp}[-1/\tau]]$$

A.1.8 Bose Fugacity in 2d

This is given by Eq. (53):

$$z_{B2}(\tau) = 1 - e^{-1/\tau}$$

with *Mathematica* implementation

$$zB2d[\tau_] := 1 - \text{Exp}[-1/\tau]$$

A.1.9 Fermi Chemical Potential in 3d

This is given by Eq. (62):

$$\mu_{F3}^*(\tau) = \tau \ln \left\{ -\text{Li}_{3/2}^{-1} \left[-\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] \right\}$$

with *Mathematica* implementation

$$\text{muF3d}[\tau_] := \tau \text{InverseFunction}[\text{Function}[z, \\ -(3 \text{Sqrt}[\text{Pi}]/4 \text{PolyLog}[3/2, -\text{Exp}[z]])]] \\ [\tau^{\wedge}(-3/2)]$$

A.1.10 Fermi Fugacity in 3d

This is given by Eq. (63):

$$z_{F3}(\tau) = -\text{Li}_{3/2}^{-1} \left[-\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right]$$

with *Mathematica* implementation

$$zF3d[\tau_] := \text{InverseFunction}[\text{Function}[z, \\ -(3 \text{Sqrt}[\text{Pi}]/4 \text{PolyLog}[3/2, -z]])]] [\tau^{\wedge}(-3/2)]$$

A.1.11 Bose Chemical Potential in 3d

This is given by Eq. (69):

$$\begin{aligned}\mu_{B3}^*(\tau) &= 0 & \tau < \tau_B \\ &= \tau \ln \left\{ \text{Li}_{3/2}^{-1} \left[\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] \right\} & \tau > \tau_B,\end{aligned}$$

where

$$\tau_B = \left(\frac{3\sqrt{\pi}}{4} \zeta\left(\frac{3}{2}\right) \right)^{-2/3}$$

with *Mathematica* implementation

```
muB3d[tau_] := If[tau > (3 Sqrt[Pi]/4 PolyLog[3/2, 1])^(-2/3),
  tau InverseFunction
  [Function [zz, (3 Sqrt[Pi]/4 PolyLog[3/2, Exp[zz]])]
  [tau^(-3/2)], 0]
```

A.1.12 Bose Fugacity in 3d

This is given by Eq. (70):

$$\begin{aligned}z_{B3}(\tau) &= 1 & \tau < \tau_B \\ &= \text{Li}_{3/2}^{-1} \left[\frac{4}{3\sqrt{\pi}} \tau^{-3/2} \right] & \tau > \tau_B\end{aligned}$$

with *Mathematica* implementation

```
zB3d[tau_] := If[tau > (3 Sqrt[Pi]/4 PolyLog[3/2, 1])^(-2/3),
  InverseFunction[Function[z, (3 Sqrt[Pi]/4 PolyLog[3/2, z])]
  [tau^(-3/2)], 1]
```

A.2 Implementation Notes

The calculations for $d = 1$ and $d = 3$ can be relatively time-consuming as these involve the evaluation of inverse functions. However, in the $d = 2$ case the evaluations will be much quicker. In order to make comparisons I timed the evaluation and plotting of each function over the range $0 \leq \tau \leq 2$. The timings, in seconds, are given in the table below.

d	μ_F^*	z_F	μ_B^*	z_B
1	5.13	42.9	21.2 (4.28)	3.59
2	0.0145	0.0427	0.0918	0.0323
3	2.34	23.13	2.64	1.31

Clearly these depend on the computer and software (I used a MacBook Pro (Retina, Mid 2012) with 16 GB of RAM, under macOS High Sierra version 10.13.6, running *Mathematica* 11.3.0.0). The relative timings are significant.

For fermions in 1 and 3d we see it is approximately ten times faster to evaluate the chemical potential than the fugacity. In these cases, if the fugacity is required, it is better to evaluate the chemical potential and obtain the fugacity from $z = e^{-\mu^*/\tau}$.

For bosons in 1 and 3d it is faster to evaluate the fugacity. Indeed numerical evaluation of $\mu_B^*(\tau)$ can give (erroneous) small imaginary contributions because of the accumulation of round-off errors. The number in the brackets for the timing of the 1d Bose chemical potential corresponds to the time for evaluating and plotting the “real” part of μ^* .

B High-Temperature Expansions

The high-temperature expansions are able to accommodate the Fermi, Bose and Maxwell cases together, indicating how they tend to the same value in the $T \rightarrow \infty$ limit. Moreover, in what follows we shall treat the dimensionality d as a variable. It is instructive to keep d general at this stage and then specify it at the end. Alternatively d could be set now, whereupon the following expressions are much simplified.

B.1 Quantum Energy

We start from Eq. (13) for the quantum energy:

$$\begin{aligned}\varepsilon_q^{d/2} &= \frac{d}{2} \int_0^\infty \varepsilon^{(d-2)/2} n(\varepsilon) \, d\varepsilon \\ &= \frac{d}{2} \int_0^\infty \frac{\varepsilon^{(d-2)/2} \, d\varepsilon}{e^{\varepsilon/kT} z^{-1} + a};\end{aligned}$$

in the high-temperature case, it is preferable to work, initially, in terms of the fugacity z .

Upon changing the variable of integration to the dimensionless $x = \varepsilon/kT$ we have

$$\varepsilon_q^{d/2} = (kT)^{d/2} \frac{d}{2} \int_0^\infty \frac{x^{(d-2)/2} \, dx}{e^x z^{-1} + a} \quad (80)$$

or

$$\frac{1}{\tau^{d/2}} = \frac{d}{2} \int_0^\infty x^{(d-2)/2} (e^x z^{-1} + a)^{-1} \, dx. \quad (81)$$

Here τ is the reduced temperature. This is the starting point for the *Mathematica* series calculation.

B.2 Series Expansion

At high temperatures $n(\varepsilon)$ is small, and so, z is small. We expand the bracket factor in powers of z

$$(e^x z^{-1} + a)^{-1} = e^{-x} z - a e^{-2x} z^2 + a^2 e^{-3x} z^3 - a^3 e^{-4x} z^4 + \dots \tag{82}$$

in terms which Eq. (81) becomes the series

$$\begin{aligned} \frac{1}{\tau^{d/2}} = \frac{d}{2} \left\{ z \int_0^\infty e^{-x} x^{(d-2)/2} dx - a z^2 \int_0^\infty e^{-2x} x^{(d-2)/2} dx + \right. \\ \left. + a^2 z^3 \int_0^\infty e^{-3x} x^{(d-2)/2} dx - a^3 z^4 \int_0^\infty e^{-4x} x^{(d-2)/2} dx + \dots \right\}. \end{aligned} \tag{83}$$

The integrals are straightforward

$$\int_0^\infty e^{-mx} x^{(d-2)/2} dx = \frac{1}{m^{d/2}} \Gamma(d/2) \tag{84}$$

so that

$$\frac{1}{\tau^{d/2}} = \frac{d}{2} \Gamma(d/2) \left\{ z - a z^2 \frac{1}{2^{d/2}} + a^2 z^3 \frac{1}{3^{d/2}} - a^3 z^4 \frac{1}{4^{d/2}} + \dots \right\}. \tag{85}$$

B.3 Fugacity

Equation (85) is a series for $1/\tau^{d/2}$ in powers of z . We invert this to give a series for z in powers of $1/\tau^{d/2}$:

$$\begin{aligned} z(\tau) = \frac{1}{\Gamma(1+d/2)} \frac{1}{\tau^{d/2}} + a \frac{2^{-d/2}}{\Gamma(1+d/2)^2} \frac{1}{\tau^d} + a^2 \frac{(2^{1-d} - 3^{-d/2})}{\Gamma(1+d/2)^3} \frac{1}{\tau^{3d/2}} + \\ + a^3 \frac{2^{-3d/2} 3^{-d/2} (-5 \times 2^d + 5 \times 3^{d/2} + 6^{d/2})}{\Gamma(1+d/2)^4} \frac{1}{\tau^{2d}} + \dots \end{aligned} \tag{86}$$

In the Maxwell case ($a = 0$) we find

$$z_M(\tau) = \frac{1}{\Gamma(1+d/2)} \frac{1}{\tau^{d/2}} \tag{87}$$

corresponding to Eq. (18), with $d = 1$, $d = 2$ and $d = 3$ cases corresponding to Eqs. (25), (40) and (61).

The $d = 1$, $d = 2$ and $d = 3$ cases of Eq. (86), for $a = 1$ and $a = -1$ (Fermi and Bose) correspond to the high-temperature series, Eqs. (32), (38), (49), (59), (68), (75).

B.4 Chemical Potential

The Maxwell (reduced) chemical potential $\mu_M^*(\tau) = \tau \ln z_M(\tau)$ is

$$\mu_M^*(\tau) = \tau \ln \left\{ \frac{1}{\Gamma(1 + d/2)} \frac{1}{\tau^{d/2}} \right\} \tag{88}$$

corresponding to Eq. (21). In expressing the high-temperature power series for Fermi and Bose gases it is convenient to write the chemical potential as the Maxwell chemical potential plus the Fermi/Bose correction.

Thus we shall examine the high-temperature expansion of $\mu^*(\tau) - \mu_M^*(\tau)$. Now

$$\mu^*(\tau) - \mu_M^*(\tau) = \tau \ln (z(\tau)/z_M(\tau)). \tag{89}$$

The ratio $z(\tau)/z_M(\tau)$ is

$$\begin{aligned} z(\tau)/z_M(\tau) = & 1 + a \frac{2^{-d/2}}{\Gamma(1 + d/2)} \frac{1}{\tau^{d/2}} + a^2 \frac{(2^{1-d} - 3^{-d/2})}{\Gamma(1 + d/2)^2} \frac{1}{\tau^d} + \\ & + a^3 \frac{2^{-3d/2} 3^{-d/2} (-5 \times 2^d + 5 \times 3^{d/2} + 6^{d/2})}{\Gamma(1 + d/2)^3} \frac{1}{\tau^{3d/2}} + \dots \end{aligned} \tag{90}$$

The logarithm of this series multiplied by τ then gives the μ series

$$\begin{aligned} \mu^*(\tau) = & \mu_M^*(\tau) + a \frac{2^{-d/2}}{\Gamma(1 + d/2)} \tau^{1-d/2} + a^2 \frac{(3 \times 2^{-d} - 2 \times 3^{-d/2})}{2\Gamma(1 + d/2)^2} \tau^{1-d} \\ & - a^3 \frac{2^{-3d/2} 3^{-(1+d/2)} (3 \times 2^{d+2} - 3^{d/2} (3 \times 2^{d/2} + 10))}{\Gamma(1 + d/2)^3} \tau^{1-3d/2} + \dots \end{aligned} \tag{91}$$

or, writing $\mu_M^*(\tau)$ explicitly

$$\begin{aligned} \mu^*(\tau) = & \tau \ln \left(\frac{1}{\Gamma(1 + d/2)} \frac{1}{\tau^{d/2}} \right) + a \frac{2^{-d/2}}{\Gamma(1 + d/2)} \tau^{1-d/2} \\ & + a^2 \frac{(3 \times 2^{-d} - 2 \times 3^{-d/2})}{2\Gamma(1 + d/2)^2} \tau^{1-d} \\ & - a^3 \frac{2^{-3d/2} 3^{-(1+d/2)} (3 \times 2^{d+2} - 3^{d/2} (3 \times 2^{d/2} + 10))}{\Gamma(1 + d/2)^3} \tau^{1-3d/2} + \dots \end{aligned} \tag{92}$$

The $d = 1$, $d = 2$ and $d = 3$ cases of this equation, for $a = 1$ and $a = -1$ (Fermi and Bose) correspond to the high-temperature chemical potential series, Eqs. (29), (36), (46), (57), (65), (73).

B.5 Mathematica Calculation

This *Mathematica* calculation is given in the Notebook MOESM2_ESM.nb in Supplementary Information. These are the steps.

To perform the *Mathematica* calculation of the high-temperature expansions we start from inverse temperature integral, Eq. (81):

$$\frac{1}{\tau^{d/2}} = \frac{d}{2} \int_0^\infty \frac{x^{(d-2)/2} dx}{e^x z^{-1} + a}. \quad (93)$$

1. Expand the denominator in the integrand in powers of the small z .
2. The integration is then done term by term on the expansion.
3. This gives $\tau^{-d/2}$ as a power series in z .
4. This series is “reversed” to give z as a series in (decreasing) powers of $\tau^{d/2}$.

C Fermi Low-Temperature (Sommerfeld) Expansions

The low-temperature Fermi expansions procedure was pioneered by Sommerfeld [26]. We shall follow the intuitive treatment of Reif [27], based on the observation that the derivative of the Fermi–Dirac distribution is sharply peaked at low temperatures.

As in the high-temperature case we shall keep d general at this stage and then specify it at the end. Alternatively d could be set now, whereupon the following expressions are much simplified.

C.1 Fermi Energy

We start from Eq. (13) for the quantum energy:

$$\varepsilon_q^{d/2} = \frac{d}{2} \int_0^\infty \varepsilon^{(d-2)/2} n(\varepsilon) d\varepsilon.$$

Since here we are restricted to fermions only we shall revert to the terminology ε_F . We integrate by parts:

$$\varepsilon_F^{d/2} = \varepsilon^{d/2} n'(\varepsilon) \Big|_0^\infty - \int_0^\infty \varepsilon^{d/2} n'(\varepsilon) d\varepsilon. \quad (94)$$

Here $n'(\varepsilon)$ is the derivative of the Fermi–Dirac distribution function with respect to energy and we note that the first term vanishes so long as $d > 0$.

Now $n'(\varepsilon)$ is sharply peaked about $\varepsilon = \mu$. We transform the variable of integration to $x = (\varepsilon - \mu)/kT$:

$$\varepsilon_F^{d/2} = \int_{-\mu/kT}^{\infty} \frac{e^x}{(e^x + 1)^2} (\mu + kTx)^{d/2} dx, \tag{95}$$

and then, only small values of x will contribute to the integral. This means that “negligible error” will be introduced by extending the lower limit of the integral to $-\infty$. Thus we are making an approximation for the Fermi energy integral:

$$\varepsilon_F^{d/2} = \mu^{d/2} \int_{-\infty}^{\infty} \frac{e^x}{(e^x + 1)^2} (1 + kTx/\mu)^{d/2} dx. \tag{96}$$

We call this a Sommerfeld integral.

Upon dividing both sides of this equation by $(kT)^{d/2}$ we have an equation in reduced variables

$$\tau^{-d/2} = \left(\frac{\tau}{\mu^*}\right)^{-d/2} \int_{-\infty}^{\infty} \frac{e^x}{(e^x + 1)^2} \left(1 + \frac{\tau}{\mu^*}x\right)^{d/2} dx. \tag{97}$$

This is an expression for τ in terms of τ/μ^* . We shall invert this to obtain τ/μ^* in terms of τ , and from this, obtain μ^* in terms of τ .

Equation (97) is the starting point for the *Mathematica* series calculation.

C.2 Sommerfeld Expansion

The Sommerfeld expansion then follows by expanding the rightmost bracket of Eq. (97) in powers of x and integrating term by term.

$$\begin{aligned} \tau^{-d/2} = & \left(\frac{\tau}{\mu^*}\right)^{-d/2} \left\{ \int_{-\infty}^{\infty} \frac{e^x dx}{(e^x + 1)^2} + \frac{d}{2} \int_{-\infty}^{\infty} \frac{e^x x dx}{(e^x + 1)^2} \left(\frac{\tau}{\mu^*}\right) + \right. \\ & \left. + \frac{d(d-2)}{8} \int_{-\infty}^{\infty} \frac{e^x x^2 dx}{(e^x + 1)^2} \left(\frac{\tau}{\mu^*}\right)^2 + \dots \right\}. \end{aligned} \tag{98}$$

These integrals are pure numbers. Denote

$$I_n = \int_{-\infty}^{\infty} \frac{e^x x^n dx}{(e^x + 1)^2} \tag{99}$$

so that

$$\tau^{-d/2} = \left(\frac{\tau}{\mu^*}\right)^{-d/2} \left\{ I_0 + \frac{d}{2} I_1 \left(\frac{\tau}{\mu^*}\right) + \frac{d(d-2)}{8} I_2 \left(\frac{\tau}{\mu^*}\right)^2 + \dots \right\}. \quad (100)$$

The integrals I_n are given in terms of the Riemann zeta function $\zeta(n)$:

$$I_n = \begin{cases} (2 - 2^{2-n})\zeta(n)n! & n \text{ even} \\ 0 & n \text{ odd.} \end{cases} \quad (101)$$

Since only the even n terms contribute to the series I shall remove the odd terms of Eq. (100) and include a further term, giving

$$\begin{aligned} \tau^{-d/2} = \left(\frac{\tau}{\mu^*}\right)^{-d/2} \left\{ 1 + d(d-2) \frac{\pi^2}{24} \left(\frac{\tau}{\mu^*}\right)^2 + \right. \\ \left. + d(d-2)(d-4)(d-6) \frac{7\pi^4}{5760} \left(\frac{\tau}{\mu^*}\right)^4 + \dots \right\}. \end{aligned} \quad (102)$$

Then we take the $-2/d$ power of this, so that

$$\tau = \left(\frac{\tau}{\mu^*}\right) \left\{ 1 - (d-2) \frac{\pi^2}{12} \left(\frac{\tau}{\mu^*}\right)^2 - (d-2)(d^2 - 35d + 94) \frac{\pi^4}{1440} \left(\frac{\tau}{\mu^*}\right)^4 + \dots \right\} \quad (103)$$

or

$$\tau = \left(\frac{\tau}{\mu^*}\right) - (d-2) \frac{\pi^2}{12} \left(\frac{\tau}{\mu^*}\right)^3 - (d-2)(d^2 - 35d + 94) \frac{\pi^4}{1440} \left(\frac{\tau}{\mu^*}\right)^5 + \dots \quad (104)$$

C.3 Chemical Potential

Equation (104) is series expression for τ in powers of τ/μ^* . We reverse this to give the series for τ/μ^* in powers of τ :

$$\frac{\tau}{\mu^*} = \tau + (d-2) \frac{\pi^2}{12} \tau^3 + (d-2)(d^2 - 5d + 34) \frac{\pi^4}{1440} \tau^5 + \dots, \quad (105)$$

so $1/\mu^*$ is

$$\frac{1}{\mu^*} = 1 + (d-2) \frac{\pi^2}{12} \tau^2 + (d-2)(d^2 - 5d + 34) \frac{\pi^4}{1440} \tau^4 + \dots \quad (106)$$

We take the reciprocal of this series, to give

$$\mu^*(\tau) = 1 - (d-2) \frac{\pi^2}{12} \tau^2 - (d-2)(d-6)(d-9) \frac{\pi^4}{1440} \tau^4 + \dots \quad (107)$$

The $d = 1$ and $d = 3$ cases of this correspond to Eqs. (28) and (64). We note immediately a problem for $d = 2$; in this case, there is no power series in τ (see Sect. C.5).

C.4 Fugacity

The fugacity may be expressed as $z(\tau) = e^{\mu^*(\tau)/\tau}$. From Eq. (107) we see that $\mu^*/\tau \rightarrow \infty$ as $\tau \rightarrow 0$ so z will diverge and there is no low-temperature power series expansion. But $(\mu^* - 1)/\tau$ remains finite as $\tau \rightarrow 0$ and so $e^{(\mu^* - 1)/\tau} = e^{\mu^*/\tau} e^{-1/\tau} = z e^{-1/\tau}$ will have a low-temperature power series expansion. This gives

$$z(\tau) = e^{-1/\tau} \left\{ 1 - (d - 2) \frac{\pi^2}{12} \tau + (d - 2)^2 \frac{\pi^4}{288} \tau^2 + \dots \right\}. \tag{108}$$

The $d = 1$ and $d = 3$ cases of this correspond to Eqs. (30) and (66).

Again there is a problem for $d = 2$; right from Eq. (102), there appear $(d - 2)$ factors in the expansion coefficients (see Sect. C.5).

C.5 Errors in the Sommerfeld Expansion

Landau and Lifshitz [28], in treating the 3d Fermi gas, note that the error introduced in the Sommerfeld procedure, whereby the lower limit of the integral is extended to $-\infty$ involves neglecting “exponentially small” terms. These terms are negligibly small so long as the Sommerfeld series does not terminate. However, for even d the series does terminate, and then, these exponential terms can dominate. Indeed when $d = 2$ we have the Sommerfeld approximation $\mu^* = 1$; there are *no* powers of τ . Fortunately in 2d we have the exact result, expressed as the series of Eq. (45). This shows the “neglected” exponential terms. There is a further discussion of the errors in Sachs [2], p. 165.

C.6 Mathematica Calculation

This *Mathematica* calculation is given in the Notebook MOESM3_ESM.nb in Supplementary Information. These are the steps.

To perform the *Mathematica* calculation of the low-temperature expansions we start from the Sommerfeld expression for $\tau^{-d/2}$, Eq. (97):

$$\tau^{-d/2} = \left(\frac{\tau}{\mu^*} \right)^{-d/2} \int_{-\infty}^{\infty} \frac{e^x}{(e^x + 1)^2} \left(1 + \frac{\tau}{\mu^*} x \right)^{d/2} dx.$$

1. Expand the rightmost bracket in powers of the small $\tau x/\mu^*$.
2. The integration is then done term by term with the expansion, giving a series in τ/μ^* .

3. The integral series is raised to the power $-2/d$ and multiplied by τ/μ^* to give τ as a series in τ/μ^* .
4. This series is “reversed” to give a τ/μ^* as a series in τ .
5. Finally this series is divided by τ and we then take the reciprocal; this gives the series for μ^* in powers of τ .

Note: *Mathematica* looks after the I_n integrals automatically. Actually it cannot do the general (symbolic) n case, but for each numerical integer value it is happy.

D Bose Low-Temperature Expansions: One Dimension

The starting point for this calculation is the $d = 1$ case of Eq. (17c), that is,

$$\frac{1}{\tau^{1/2}} = \Gamma(3/2) \text{Li}_{1/2}(z), \tag{109}$$

from which it follows that τ is

$$\tau = \frac{4}{\pi} (\text{Li}_{1/2}(z))^{-2}. \tag{110}$$

D.1 Series Expansion

We are interested in the behaviour at small τ . At $\tau = 0$ we have $z = 1$ (all particles in the ground state) and then as τ increases from zero, z decreases from 1 towards zero. So at low temperatures $z - 1$ is a small quantity so we shall (or at least *Mathematica* will) expand τ in powers of this:

$$\begin{aligned} \tau = & \frac{4}{\pi^2}(z - 1) - \frac{8\zeta\left(\frac{1}{2}\right)}{\pi^{5/2}}(z - 1)^{3/2} + \frac{2\left(6\zeta\left(\frac{1}{2}\right)^2 + \pi\right)}{\pi^3}(z - 1)^2 + \\ & + \frac{2\left(-8\zeta\left(\frac{1}{2}\right)^3 - 3\pi\zeta\left(\frac{1}{2}\right) + 4\pi\zeta\left(-\frac{1}{2}\right)\right)}{\pi^{7/2}}(z - 1)^{5/2} + \dots, \end{aligned} \tag{111}$$

where $\zeta()$ are Riemann zeta functions.

D.2 Fugacity and Chemical Potential

This expansion is reversed, to give z as a power series in τ :

$$\begin{aligned} z(\tau) = & 1 - \frac{1}{4}\pi^2\tau - \frac{1}{4}\pi^{5/2}\zeta\left(\frac{1}{2}\right)\tau^{3/2} + \frac{1}{32}\pi^3\left(\pi - 6\zeta\left(\frac{1}{2}\right)^2\right)\tau^2 + \\ & + \frac{1}{16}\pi^{7/2}\left(\pi\left(\zeta\left(\frac{1}{2}\right) + \zeta\left(-\frac{1}{2}\right)\right) - 2\zeta\left(\frac{1}{2}\right)^3\right)\tau^{5/2} + \dots \end{aligned} \tag{112}$$

corresponding to Eq. (37), and then, the chemical potential $\mu^*(\tau) = \tau \ln z(\tau)$ is

$$\begin{aligned} \mu^*(\tau) = & -\frac{1}{4}\pi^2\tau^2 - \frac{1}{4}\pi^{5/2}\zeta\left(\frac{1}{2}\right)\tau^{5/2} - \frac{3}{16}\pi^3\zeta\left(\frac{1}{2}\right)^2\tau^3 + \\ & + \frac{1}{16}\pi^{7/2}\left(\pi\zeta\left(-\frac{1}{2}\right) - 2\zeta\left(\frac{1}{2}\right)^3\right)\tau^{7/2} + \dots \end{aligned} \quad (113)$$

corresponding to Eq. (35).

The *Mathematica* calculation of these results is given in the Notebook MOESM4_ESM.nb in Supplementary Information. It follows the steps outlined above.

E Bose Low-Temperature Expansions: Three Dimensions

The starting point for this calculation is the $d = 3$ case of Eq. (17c), that is,

$$\frac{1}{\tau^{3/2}} = \Gamma(5/2) \text{Li}_{3/2}(z), \quad (114)$$

from which it follows that τ is

$$\tau = \frac{2}{3^{2/3}} \left(\frac{2}{\pi}\right)^{1/3} (\text{Li}_{1/2}(z))^{-2/3}. \quad (115)$$

The (reduced) Bose temperature τ_B is the $z = 1$ value of this expression

$$\tau_B = \left(\frac{3\sqrt{\pi}}{4}\zeta\left(\frac{3}{2}\right)\right)^{-2/3}. \quad (116)$$

We note that for all $0 < z < 1$ (the allowed range for z), Eq. (115) will give values of τ only greater or equal to τ_B . In other words the inversion of this equation will apply only when $\tau \geq \tau_B$.

E.1 Series Expansion

We are interested in the behaviour at small τ . For $\tau < \tau_B$ we have $z = 1$ (macroscopic number of particles in the ground state) and then as τ increases τ_B , z decreases from 1 towards zero. So at low temperatures $1 - z$ is a small quantity so we shall (or at least

Mathematica will) expand τ in powers of this:

$$\begin{aligned} \tau = & \left(\frac{3\sqrt{\pi}}{4} \zeta\left(\frac{3}{2}\right) \right)^{-2/3} + \frac{8 \times 2^{1/3} \pi^{1/6}}{3 \times 3^{2/3} \zeta\left(\frac{3}{2}\right)^{5/3}} (1-z)^{1/2} + \\ & + \frac{4\left(\frac{2}{\pi}\right)^{1/3} \left(3\zeta\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) + 10\pi\right)}{9 \times 3^{2/3} \zeta\left(\frac{3}{2}\right)^{8/3}} (1-z) + \\ & + \frac{2 \times 2^{1/3} \pi^{1/6} \left(9\zeta\left(\frac{3}{2}\right) \left(20\zeta\left(\frac{1}{2}\right) + 3\zeta\left(\frac{3}{2}\right)\right) + 320\pi\right)}{81 \times 3^{2/3} \zeta\left(\frac{3}{2}\right)^{11/3}} (1-z)^{3/2} + \dots \end{aligned} \tag{117}$$

Observe that the first term is the Bose temperature τ_B .

E.2 Fugacity

We want to find z as a power series in $\tau - \tau_B$ or, equivalently, as a power series in $(\tau - \tau_B)/\tau_B$. From Eq. (117) we have

$$\begin{aligned} \frac{\tau - \tau_B}{\tau_B} = & \frac{4\pi^{1/2}}{3\zeta\left(\frac{3}{2}\right)} (1-z)^{1/2} + \frac{\left(6\zeta\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) + 20\pi\right)}{9\zeta\left(\frac{3}{2}\right)^2} (1-z) + \\ & + \frac{\pi^{1/2} \left(9\zeta\left(\frac{3}{2}\right) \left(20\zeta\left(\frac{1}{2}\right) + 3\zeta\left(\frac{3}{2}\right)\right) + 320\pi\right)}{81\zeta\left(\frac{3}{2}\right)^3} (1-z)^{3/2} + \dots \end{aligned} \tag{118}$$

This is a series for $(\tau - \tau_B)/\tau_B$ in powers of $1 - z$. We reverse this to get $1 - z$ as a series in $(\tau - \tau_B)/\tau_B$. And then subtracting this from 1 we have the series for $z(\tau)$:

$$z(\tau) = 1 - \frac{9\zeta\left(\frac{3}{2}\right)^2}{16\pi} \left(\frac{\tau - \tau_B}{\tau_B}\right)^2 + \frac{9\zeta\left(\frac{3}{2}\right)^2 \left(3\zeta\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) + 10\pi\right)}{64\pi^2} \left(\frac{\tau - \tau_B}{\tau_B}\right)^3 + \dots \tag{119}$$

corresponding to Eq. (74).

E.3 Chemical Potential

The reduced chemical potential is $\mu^* = \tau \ln z$. But here we need to be careful with the powers of $\tau - \tau_B$. So let us write

$$\mu^* = (\tau - \tau_B) \ln z + \tau_B \ln z. \tag{120}$$

The series for $\ln z$ from Eq. (119) is

$$\ln z(\tau) = -\frac{9\zeta\left(\frac{3}{2}\right)^2}{16\pi} \left(\frac{\tau - \tau_B}{\tau_B}\right)^2 + \frac{9\zeta\left(\frac{3}{2}\right)^2 \left(3\zeta\left(\frac{1}{2}\right) \zeta\left(\frac{3}{2}\right) + 10\pi\right)}{64\pi^2} \left(\frac{\tau - \tau_B}{\tau_B}\right)^3 + \dots; \tag{121}$$

then, doing the multiplications by $\tau - \tau_B$ and by τ_B , adding and collecting the $\tau - \tau_B$ powers give

$$\mu^*(\tau) = -\frac{9\zeta\left(\frac{3}{2}\right)^2}{16\pi} \tau_B \left(\frac{\tau - \tau_B}{\tau_B}\right)^2 + \frac{27\zeta\left(\frac{3}{2}\right)^2 \left(\zeta\left(\frac{1}{2}\right)\zeta\left(\frac{3}{2}\right) + 2\pi\right)}{64\pi^2} \tau_B \left(\frac{\tau - \tau_B}{\tau_B}\right)^3 + \dots \quad (122)$$

corresponding to Eq. (72).

The *Mathematica* calculation of these results is given in the Notebook MOESM5_ESM.nb in Supplementary Information. It follows the steps outlined above.

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