

Fluctuations in the Population of the Ground State of Bose Systems

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Formulas are given which show how the fluctuations of the ground-state occupation number in a Bose System are strongly suppressed at low temperatures.

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1. INTRODUCTION

The standard expression for the fluctuation of the occupation numbers in Bose statistics,⁽¹⁾

$$\overline{(\Delta n/\bar{n})^2} = 1 + (1/\bar{n}) \quad (1)$$

meets with difficulties when applied to the ground state at very low temperatures. As an asymptotic formula for this special case,⁽²⁾ we propose instead

$$\overline{(\Delta n_0/\bar{n}_0)^2} \rightarrow [(N/\bar{n}_0) - 1]^2 \quad (2)$$

as $T \rightarrow 0$. In contrast to formula (1), this fulfills the fundamental requirement that *the fluctuations in the population of the lowest energy level must go to zero with the temperature*—in Bose statistics, no less than in Fermi statistics.

To be sure, formula (1), which implies relative fluctuations of about 100%, is “exact” in as much as it follows without approximation from the grand canonical ensemble. This ensemble is tacitly implied in most current formulations of quantum statistics; and as a rule, there are no observable differences in the results obtained from the various ensembles. This is certainly true for Fermi statistics, and for Bose statistics the only exception is when we consider the ground state at very low temperatures.

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In this particular case, however, it must be remembered that, strictly speaking, the grand canonical ensemble describes open systems only—although incidentally it almost always gives correct formulas even for closed systems. The large fluctuations in n_0 indicated by (1) thus refer to systems which can freely exchange particles with an infinite reservoir or with another phase. But this picture is not at all appropriate to experimental situations where the system is a macroscopically conserved amount of matter: in Bose statistics, n_0 may, at sufficiently low temperature, be a *macroscopic* quantity and its relative fluctuation must certainly vanish lest the theory predict very startling phenomena.

For a proper treatment of the present problem, it is thus necessary to take conservation of the total number of particles N into account. This will be shown to require, for the ground state at low temperatures, formula (2) instead of formula (1). A more general formula comprising both (1) and (2) as special cases will be given in Section 2.

These formulas are applied in Section 3 to the ideal Bose gas. Since the result is based upon the method of steepest descent, we shall in Section 4 briefly consider a *two-level system* as a model which can be treated without recourse to this method. Auxiliary calculations and an extension to particles with a continuous energy spectrum are collected in the Appendices.

Before discussing specific examples, we shall write down a description of the canonical ensemble which is suitable for the present purpose: Let the molecular energy levels in a closed system of N noninteracting particles be ϵ_s , $s = 0, 1, 2, \dots$.

The possibility of a continuous energy-spectrum should also be taken into account, but we defer the necessary amendments to Appendix C. In Bose statistics, the number of particles n_s occupying the s th level may assume any integer value $n_s = 0, 1, 2, \dots$, but we shall now consider the total number of particles

$$\sum_s n_s = N \quad (3)$$

to be fixed in the strong sense—not merely in canonical average. Accordingly, the sum over states must be restricted:

$$Z = \sum' \prod_s e^{-\beta n_s \epsilon_s} \quad (4)$$

Here, \sum' denotes a multiple sum over only those sets of occupation numbers $\{n_s\}$ that satisfy the condition (3).

Such a condition is conveniently imposed upon the summation (4) by multiplying each term of the unrestricted sum by a discontinuous factor:

$$(1/2\pi i) \int_{-\pi i}^{\pi i} dt \exp \left\{ - \left(N - \sum_s n_s \right) t \right\} = \begin{cases} 1 & \text{when (3) is fulfilled} \\ 0 & \text{otherwise} \end{cases}$$

In this way, the sum over states can be written as an integral

$$Z = (1/2\pi i) \int dt e^{-Nt} \prod_s \left\{ \sum_{n_s} e^{n_s(t - \beta \epsilon_s)} \right\} \quad (5)$$

which can be evaluated by the Darwin-Fowler method.

Usually, the sums over the n_s are understood to be from 0 to ∞ ,

$$\sum_{n_s=0}^{\infty} = 1/(1 - e^{t-\beta\epsilon_s}) \tag{6}$$

but this is not the only possibility: we may truncate them at any number $M \geq N$, inserting, instead of the sum (6),

$$\sum_{n_s=0}^{M_s} = (1 - e^{(M_s+1)(t-\beta\epsilon_s)})/(1 - e^{t-\beta\epsilon_s}) \tag{7}$$

for the s th factor in the integrand (5). So far, the replacements of the infinite series (6) by finite sums (7) are quite arbitrary. They cannot alter the exact value of the integral (5).

In most cases however, only asymptotic approximations for large N are available, and in order to obtain them it will sometimes be a considerable advantage to take the factors of the infinite product in the form (7), which are entire functions of t , instead of (6), which are not. This will turn out to “temper” the analytical properties of the integrand, and thus to make it more amenable to a saddle-point approximation. We shall here choose all $M_s = N$, i.e., pick the smoothest form possible (*salva veritate*) for the integrand (5).

Incidentally, this choice ($M = N$) leads to the particular form of distribution law for the occupation numbers which was proposed by Gentile⁽³⁾ on somewhat different grounds. Although Gentile’s procedure (7) cannot claim to be more than a computational device, we shall see that it is useful for boson systems at very low temperatures. Actually, it extends the applicability of the method of steepest descent to a range of states where in the usual formalism this method was very problematic. For the purposes of our fluctuation problem, we shall therefore adopt his version of the sum over states,

$$Z = (1/2\pi i) \int dt e^{-Nt} \prod_s \{(1 - e^{-Dz_s})/(1 - e^{-z_s})\} \tag{8}$$

where $D = N + 1$, $z = \beta\epsilon_s - t$. By the definition (4) of our ensemble, the average occupation numbers and their fluctuations are given by

$$\bar{n} = -\partial(\ln Z)/\partial\beta\epsilon, \quad \overline{\Delta n^2} = \partial^2(\ln Z)/\partial(\beta\epsilon)^2 \tag{9}$$

respectively.

2. AVERAGE AND FLUCTUATION OF n_0 IN THE SADDLE-POINT APPROXIMATION

Using the saddle-point approximation, we get from Eq. (9)

$$\ln Z = -Nt + \sum_s \chi(\beta\epsilon_s - t) \tag{10}$$

where

$$\chi(z) = -\ln(1 - e^{-z}) + \ln(1 - e^{-Dz})$$

and terms of the order $\ln N$ have been neglected. The principal saddle point t is the real root of the equation

$$N = \sum_s \dot{\chi}_s, \quad \dot{\chi} = \partial\chi/\partial t = -\chi' \quad (11)$$

While χ is a universal function, the parameter t depends specifically upon the system through the energy spectrum ϵ_s . Inserting the approximation (10) in the general equations (9), one thus obtains

$$\bar{n}_s = \dot{\chi}_s, \quad \overline{\Delta n_s^2} = \ddot{\chi}_s [1 - (\partial t/\partial \beta \epsilon_s)] \quad (12)$$

These formulas are of a well-known type, except that Gentile's expression

$$\dot{\chi}(z) = [1/(e^z - 1)] - [D/(e^{Dz} - 1)], \quad z = \beta\epsilon - t \quad (13)$$

differs from the familiar distribution law of Bose statistics:

$$f(z) = 1/(e^z - 1) \quad (14)$$

by the extra term $-Df(Dz)$. This term, however, makes the function $\bar{n} = \dot{\chi}(z)$ always finite, positive, and monotonically decreasing:

$$\dot{\chi}(-\infty) = N, \quad \dot{\chi}(0) = N/2, \quad \dot{\chi}(\infty) = 0 \quad (15)$$

with a steep drop at $z = 0$ (Appendix A).

By the usual thermodynamic identification, t is related to the chemical potential ($t = \beta\mu$). At ordinary temperatures, the chemical potential is negative whether we define it by the conventional means or by Gentile's formula. Then, $z = \beta\epsilon - t$ is positive for all quantum states and the term $-Df(Dz)$ is completely negligible, as of course it must be in this case. In the usual formalism, which employs the distribution law (14), z must in fact always be positive, that is, t can never exceed $\beta\epsilon_0$.

Gentile's function $\bar{n} = \dot{\chi}(z)$, on the other hand, is always finite and z may well assume negative values, as indeed it does for the lowest quantum state at sufficiently low temperatures. Thus, t may exceed $\beta\epsilon_0$ although it must always remain below $\beta\epsilon_1$ [$t > \beta\epsilon_1 > \beta\epsilon_0$ violates Eq. (11); cf. Eqs. (15)]. The thermodynamic states in which we are here primarily interested are just those belonging to positive values of t : $0 \leq t < \beta\epsilon_1$. When $t = \beta\epsilon_0$, we have $\bar{n}_0 = \dot{\chi}(0) = N/2$: one half of the particles are in the ground state. At absolute zero, $\beta = \infty$, we shall have $t = +\infty$, and in Eq. (14), $\bar{n}_0 = N$, as must be the case.

Our main concern, however, is the fluctuations. These depend upon the function $\ddot{\chi}_0$ entering in the formula

$$\overline{\Delta n_0^2} = \ddot{\chi}_0 [1 - (\partial t/\partial \beta \epsilon_0)] \quad (16)$$

which, as we shall see, embodies both (1) and (2)—the former at ordinary temperatures and the latter in the limit $T \rightarrow 0$.

In order to make this plausible, we use the identity [see Appendix A, Eq. (44)]

$$\ddot{\chi}_0 = D\bar{n}_0 - \bar{n}_0^2 + (2n_0 - N)f(z_0) \tag{17}$$

At ordinary temperatures, when the term $Df(Dz)$ in Eq. (13) can be neglected, we have clearly $f(z_0) = \bar{n}_0$, and accordingly,

$$\ddot{\chi}_0 = (\bar{n}_0)^2 + \bar{n}_0$$

which leads to formula (1). At sufficiently low temperatures, however, z will be negative and we may have, by Eqs. (12) and (13), $f(z_0) = \bar{n}_0 - N + o(N)$, while $\bar{n}_0 = o(N)$, that is,

$$\ddot{\chi}_0 = (N - \bar{n}_0)^2 + o(N)$$

and this gives formula (2).

So far, we have disregarded the factor $1 - (\partial t/\partial\beta\epsilon)$ in Eq. (12). By variation of the saddle-point equation (11) with respect to the spectrum, one finds

$$(\partial t/\partial\beta\epsilon)_N = \ddot{\chi}_0/\sum \ddot{\chi}_s < 1 \tag{18}$$

Whatever the magnitude of $\partial t/\partial\beta\epsilon$, this term can therefore only decrease the fluctuation. At ordinary temperatures, it is obviously negligible, and as we shall see, also at sufficiently low temperatures.

However, as was pointed out by Hiis Hauge, the factor $1 - (\partial t/\partial\beta\epsilon_0)$ may be extremely important: as he showed⁽⁴⁾ in the case of the ideal Bose gas, this factor will effectively suppress the fluctuation to zero at all temperatures below the Einstein transition point although $\ddot{\chi}_0$ is of the order N^2 in most of this range. But in any case, $\partial t/\partial\beta\epsilon$ will depend upon the spectrum and, as will be shown both for the ideal gas and the two-level systems treated in Sections 3 and 4, the fluctuation formula (2) subsists in the limit $T \rightarrow 0$.

With suitable adjustments, the preceding formula (16) may be extended to systems with continuous or (piecewise continuous) energies. The average number of particles with energy below ϵ is then given by (Appendix C)

$$\overline{N(\epsilon)} = \int_0^{\beta\epsilon} g(x) dx \dot{\chi}(x - t) \tag{19}$$

and its fluctuation by

$$\overline{\Delta N(\epsilon)^2} = \left(\int_0^{\beta\epsilon} \ddot{\chi}g dx \right) \left[1 - \left(\int_0^{\beta\epsilon} \ddot{\chi}g dx / \int_0^\infty \ddot{\chi}g dx \right) \right]$$

3. THE IDEAL BOSE GAS

According to Eq. (11) the saddle point t will be determined by

$$N = \sum_\epsilon \{ [1/(e^{\beta\epsilon-t} - 1)] - [D/(e^{D(\beta\epsilon-t)} - 1)] \} \tag{20}$$

Now, for macroscopic volumes V , the energy levels of an ideal gas are so densely spaced that, even at the lowest attainable temperatures, they cannot be resolved in thermal experiments. One is therefore inclined to replace sum by integral [cf. Eq. (67)]:

$$\sum_{\epsilon} \rightarrow [\beta^{3/2}/\Gamma(3/2)](V/\lambda^3) \int \epsilon^{1/2} d\epsilon \quad (21)$$

where $\lambda = (h^2\beta/2\pi m)^{1/2}$ is the thermal de Broglie wavelength. In the usual formulation of Bose statistics, this causes a well-known difficulty because the function

$$I(t) = [1/\Gamma(3/2)] \int_0^{\infty} [x^{1/2} dx / (e^{x-t} - 1)] \quad (22)$$

has an essential singularity at $t = 0$. In Gentile's formulation, however, this is exactly compensated by the second sum in the curly bracket and thus the integral

$$N = (V/\lambda^3)[1/\Gamma(3/2)] \int_0^{\infty} x^{1/2} dx \chi(x - t) \quad (23)$$

is regular along the entire real t axis. We may therefore with some confidence use Eq. (23) to determine the saddle point. At temperatures above the Einstein transition, t will be negative. This is the domain of validity of formula (1), which does not interest us here. Upon cooling of the system, the saddle point will (*ceteris paribus*) move to the right along the real axis, reaching $t = 0$ at the temperature

$$T_E = [N\lambda^3 T^{3/2} / \zeta(3/2) V]^{2/3} \quad (24)$$

At temperatures $T < T_E$, the saddle point appears on the *positive* real axis and its location is roughly given by (Appendix B)

$$t \sim [1 - (T/T_E)^{3/2}] \lambda^2 / V^{2/3} \quad (25)$$

which is of the order $N^{-2/3}$ for moderately low temperatures $T \lesssim T_E$. To obtain a more accurate value, one must solve for $t = \beta\epsilon_0 - z$ the equation [Appendix B, Eq. (58)]

$$N = \chi(z) + (V/\lambda^3) \zeta(3/2) + o(N) \quad (26)$$

Since $\chi_0 = \bar{n}_0$ and $V\zeta(3/2)/\lambda^3 = (T/T_E)^{3/2}$, this is the same as London's equation⁽⁵⁾

$$\bar{n}_0 = [1 - (T/T_E)^{3/2}] N \quad (27)$$

which is thus true in a quotient asymptotic sense.

It is not difficult to map the whole range of temperatures $(0, T_E)$ upon the range $(\infty, 0)$ of t , but such detail is not necessary for our discussion of the relative fluctuation:

$$\overline{(\Delta n_0 / \bar{n}_0)^2} = (\ddot{\chi}_0 / \bar{n}_0^2) [1 - (\partial t / \partial \beta \epsilon_0)] \quad (28)$$

All we need is a survey of \bar{n}_0 , $\ddot{\chi}_0$, and $\partial t / \partial \beta \epsilon_0$ in their dependence upon the state.

For the ideal gas, one finds [Appendix D, Eq. (83)]

$$\partial t / \partial \beta \epsilon_0 \sim \ddot{\chi}_0 / [\ddot{\chi}_0 + N(V/\lambda^3)^{2/3}] \tag{29}$$

At the transition point $T = T_E$ [Appendix D, Eq. (86)],

$$\ddot{\chi}_0 \sim N^{4/3}, \quad \bar{n}_0 \sim N^{2/3}, \quad V/\lambda^3 \sim N \tag{30}$$

The relative fluctuation will therefore be of order 1, or more precisely, it is just given by the standard formula (1).

In the middle of the range, $T \lesssim T_E$ [$\ell(z) \sim N^{-1}$], we have [Eqs. (27) and (46)]

$$\ddot{\chi}_0 \sim N^2, \quad \bar{n}_0 \sim N, \quad V/\lambda^3 \sim N \tag{31}$$

so that $\ddot{\chi}_0/(\bar{n}_0)^2$ is still of order 1. Here, however, $\partial t / \partial \beta \epsilon_0$ is indeed close to 1, as observed by Hiis Hauge.⁽⁴⁾ From the relations (29) and (31), we have

$$1 - (\partial t / \partial \beta \epsilon_0) \sim N^{5/3} / (N^2 + N^{5/3}) \sim N^{-1/3} \tag{32}$$

hence the relative fluctuation vanishes to this order. At still lower temperatures, z is negative and ultimately of larger order than N^{-1} . In this case, the order of $\ddot{\chi}_0$ is given by Eq. (84) and (85) of Appendix D:

$$\ddot{\chi}_0 \sim (N - n_0)^2 \sim (V/\lambda^3)^2 \tag{33}$$

The magnitude of $\partial t / \partial \beta \epsilon_0$ then depends upon the ratio

$$(V/\lambda^3)^2 / N(V/\lambda^3)^{2/3} \sim N^{1/3}(T/T_E)^2 \tag{34}$$

That is, for temperatures $T \lesssim T_E N^{-1/6}$, the factor, $1 - (\partial t / \partial \beta \epsilon_0)$ is of order 1 and the fluctuation approaches

$$\overline{(\Delta n_0 / \bar{n}_0)^2} \sim [(N/\bar{n}_0) - 1]^2 \tag{35}$$

in agreement with formula (2). These are certainly very low temperatures, but it is noteworthy that they vastly exceed the range of temperatures $T < T_E N^{-2/3}$ envisaged in Planck's formulation of the third law.³

4. TWO-LEVEL SYSTEMS

This model may be even more nonphysical than the ideal gas, but it will allow us to dispense with the saddle point approximation. It is now convenient to write the sum over states

$$Z = (1/2\pi i) \oint (dt/t^{N+1}) \prod_s \{1 - te^{-\beta \epsilon_s}\}^{-1} \tag{36}$$

³ For a related discussion of the third law, see Casimir ⁽⁶⁾ and ter Haar and Wergeland.⁽⁷⁾

There is no need to “tame” the integrand by truncating the sums at $n_s = N$ since we can now evaluate it exactly. For any system of noninteracting bosons, the occupation number of the lowest energy level will thus be given by

$$Z\bar{n}_0 = \frac{1}{2\pi i} \oint \frac{dt}{t^{N+1}} \cdot \frac{te^{-\beta\epsilon_0}}{(1 - te^{-\beta\epsilon_0})^2} \cdot \frac{1}{1 - te^{-\beta\epsilon_1}} \cdots \quad (37)$$

and at low temperatures only the few lowest levels will give factors appreciably different from 1 in the product. Therefore, in the extreme case $kT < \epsilon_1 - \epsilon_0$, even a model with these two levels only must suffice to describe the population of the lowest level.

For the two-level model, one can of course write down exact expressions, e.g.,

$$\begin{aligned} \frac{1}{1 - te^{-\beta\epsilon_0}} \frac{1}{1 - te^{-\beta\epsilon_1}} &= \sum_{N=0}^{\infty} a_N t^N \\ \frac{te^{-\beta\epsilon_0}}{(1 - te^{-\beta\epsilon_0})^2} \frac{1}{1 - te^{-\beta\epsilon_1}} &= \sum b_N t^N \\ a_N &= e^{-N\beta\epsilon_1} (1 - e^{-Dz}) / (1 - e^{-z}) \\ b_N &= a_N \{ [1/(e^z - 1)] - [D/(e^{Dz} - 1)] \} \end{aligned} \quad (38)$$

where $z = \beta(\epsilon_0 - \epsilon_1)$.

Since $Z = a_N$, we have therefore, by Eq. (37), for the occupation number of the ground state

$$\bar{n}_0 = b_N/a_N \quad (39)$$

which is precisely Gentile's formula (13) with $t = \beta\epsilon_1$.

Now, this is partly fortuitous, since models with three levels and so forth give rise to more complicated formulas. However, the result (39) may serve to show that Gentile's device gives suitable interpolation formulas for the ground state at very low temperatures. In particular, the fluctuation of n_0 will for the two-level system always be given by Eq. (17), $\overline{\Delta n_0^2} = \ddot{\chi}_0$, which at sufficiently low temperatures leads to formula (2).

APPENDIX A. PROPERTIES OF GENTILE'S FUNCTION $\bar{n} = \dot{\chi}(z)$

The function

$$\dot{\chi}(z) = [1/(e^z - 1)] - [D/(e^{Dz} - 1)], \quad D = N - 1 \quad (40)$$

is (i) positive and (ii) monotonically decreasing from $\dot{\chi}(-\infty) = N$ through $\dot{\chi}(0) = N/2$ to $\dot{\chi}(\infty) = 0$.

Proof. It is true for an infinite set of integers $D = 2^n$. Writing

$$\dot{\chi} = [1/(x - 1)] - [2^n/(x^{2^n} - 1)], \quad x = e^z$$

and noting that

$$x^{2^n} - 1 = (x - 1) \prod_{k=0}^{n-1} (1 + x^{2^k})$$

we have

$$\dot{\chi} = [1/(x - 1)] \left\{ 1 - \left[2^n / \prod_{k=0}^{n-1} (1 + x^{2^k}) \right] \right\} \quad (41)$$

and

$$-d\dot{\chi}/dz = [1/(x - 1)]^2 \left\{ 1 - \left[(2^{2n} x^{2^{2n}-1}) / \prod_{k=0}^{n-1} (1 + x^{2^k})^2 \right] \right\} \quad (42)$$

The right hand side of Eq. (41) is clearly positive whether we have $x > 1$ or $x < 1$, which proves that $\dot{\chi}(z)$ is always positive. In order to see that $\dot{\chi}(z)$ is monotonically decreasing, one may rewrite the curly bracket in (42) as

$$1 - \prod_{t=0}^{n-1} [2/(x^{2^{k-1}} + x^{-2^{k-1}})]^2$$

This is always positive, which proves the second part of our proposition.

It is further useful to note that $\ddot{\chi} = -d\dot{\chi}/dz$ is an even function of $z = \beta\epsilon - t$ and has a sharp maximum $\approx N^2/12$ with a width $\Delta z \sim 1/N$ at $z = 0$. Since we must always have

$$\int_a^\infty \ddot{\chi} dz = \begin{cases} N & \text{for } a = -\infty \\ N/2 & \text{for } a = 0 \end{cases}$$

we shall in the limit $N \rightarrow \infty$ have

$$\dot{\chi}/N \rightarrow \text{unit step function, } 1 - \Theta(z)$$

$$\ddot{\chi}/N \rightarrow \delta(z)$$

The special values $\dot{\chi}(0) = N/2$ and $\ddot{\chi}(0) = (D^2 - 1)/12$ follow directly from the Bernoulli expansion

$$f(z) = 1/(e^z - 1) = (1/z) - (1/2) + (z/12) - (z^3/720) + \dots$$

It is convenient to rewrite the quantity $\ddot{\chi}_0$ entering the fluctuation formula (16) as

$$\ddot{\chi} = D\dot{\chi} - \dot{\chi}^2 + (2\dot{\chi} - N)f(z) \quad (43)$$

which follows by differentiation of (40). We can thus relate $\ddot{\chi}_0$ to $\bar{n}_0 = \dot{\chi}_0$ and $f(z_0)$. In order to survey $\ddot{\chi}$ as a function of z , we note, that for $\vartheta(z) > N^{-1}$,

$$f(z) \sim \begin{cases} \dot{\chi}(z), & z > 0 \\ \dot{\chi}(z) - D, & z < 0 \end{cases} \quad (44)$$

Inserting $\dot{\chi}_0 = \bar{n}_0$, we obtain then from Eqs. (43) and (45)

$$\ddot{\chi}_0 \sim \begin{cases} (\bar{n}_0)^2 + \bar{n}_0, & z > 0 \\ (N - \bar{n}_0)^2 + (N - n_0), & z < 0 \end{cases} \quad (45)$$

If, on the other hand, $\mathcal{O}(z) \leq N^{-1}$, then

$$\begin{aligned} f &\sim N^2/6(N - 2\bar{n}_0) \\ \ddot{\chi} &\sim [\bar{n}_0 - (N/2)]^2 + (N^2/12) \end{aligned} \quad (46)$$

follows from the Bernoulli expansion of (40). Since the radius of convergence is $|z| = 2\pi$, the solution $z \approx (6/D)(N - 2\bar{n}_0)$ is not accurate at its extreme values ± 6 .

APPENDIX B. LOCATION OF THE SADDLE POINT

In first approximation, we replace the sum (20) by an integral

$$N = \int_0^\infty g(x) dx \chi(x - t) \quad (47)$$

where

$$\begin{aligned} g &= (V/\lambda^3) x^{1/2}/\Gamma(3/2) \\ \dot{\chi} &= [1/(e^{x-t} - 1)] - [D/(e^{D(x-t)} - 1)] \end{aligned} \quad (48)$$

Here, $\dot{\chi}$ is perfectly regular on the path of integration, but since it is a difference of two terms which we shall sometimes need to consider separately, a convention must be made about how to bypass the point $x = t$. Any convention will do if applied identically to both terms. We shall choose to consider both as Cauchy principal values:

$$I_D = [D/\Gamma(3/2)] P \int_0^\infty [x^{1/2} dx/(e^{D(x-t)} - 1)] \quad (49)$$

and correspondingly for I_1 . For the small positive values of t in which we are mainly interested, the principal value of I_1 can most conveniently be displayed by the contour integral

$$I_1 = [(-1/2)/\Gamma(3/2)] \int_C [z^{1/2}/(e^{z-t} - 1)] dz \quad (50)$$

where C is a lace around a branch-cut along the positive real axis. Noting that $z^{1/2}$ changes sign across the cut, one sees that the contributions from small indentations above and below $z = t$ cancel, so that the contour integral (50) indeed represents the principal value desired. Expanding

$$\begin{aligned} \int_C &= \int_C \{(t + \bar{z})^{1/2} d\bar{z}/[\exp \bar{z} - 1]\} \\ &= \sum_0^\infty \binom{1/2}{n} t^n \int \{\bar{z}^{(1/2)-n} dz'/[\exp \bar{z} - 1]\} \end{aligned}$$

where $|\bar{z}| > t$ on \bar{C} , and using one of the defining integrals of Riemann's ζ -function⁽⁸⁾

$$\zeta(s) = [1/(e^{2\pi is} - 1)][1/\Gamma(s)] \int_{-\infty}^{(0^+)} [z^{s-1} dz/(e^z - 1)]$$

one obtains the power series

$$I_1 = \sum_{n=0}^{\infty} [\zeta(\frac{3}{2} - n)/n!] t^n, \quad |t| < 2\pi \tag{51}$$

Due to the small radius of convergence ($|t| = 2\pi/D$), the corresponding series is useless for the representation of I_D , but here one can proceed directly from the definition:

$$P \int_0^{\infty} x^{1/2} dx f(D[x - t]) = \lim_{\epsilon \rightarrow 0} \left(\int_{-t}^{\epsilon} + \int_{\epsilon}^{\infty} \right) (z + t)^{1/2} f(Dz) dz \tag{52}$$

Rewriting the first part

$$\int_{-t}^{-\epsilon} = \int_{\epsilon}^t (t - z)^{1/2} f(-Dz) dz$$

and using the identity

$$f(-Dz) = -1 - f(Dz)$$

we have

$$\begin{aligned} P \int_0^{\infty} &= - \int_0^t (t - z)^{1/2} dz + \int_0^t \frac{(t + z)^{1/2} - (t - z)^{1/2}}{e^{Dz} - 1} dz + \int_t^{\infty} \frac{(t + z)^{1/2}}{e^{Dz} - 1} dz \\ &= t^{3/2}(-\frac{2}{3} + J_1 + J_2) \end{aligned}$$

Here, the two latter integrals can be neglected.

$$J_1 = \int_0^1 \{[(1 + x)^{1/2} - (1 - x)^{1/2}]/(e^{Dtx} - 1)\} dx:$$

in the interval $0 < x < 1$, we have, for instance,

$$\begin{aligned} (1 + x)^{1/2} - (1 - x)^{1/2} &< \frac{3}{2}x < \frac{3}{2}x^{1/2} \\ J_1 &< \frac{3}{2} \int_0^1 [x^{1/2} dx/(e^{Dtx} - 1)] < \frac{3}{2}(1/Dt)^{3/2} \int_0^{\infty} [y^{1/2} dy/(e^y - 1)] \\ &= \frac{3}{2}[1/(Dt)^{3/2}] \zeta(\frac{3}{2}) \end{aligned} \tag{53}$$

$$J_2 = \int_1^{\infty} [(1 + x)^{1/2} dx/(e^{Dtx} - 1)]:$$

for $x > 1$, we have $(1 + x)^{1/2} \leq (2x)^{1/2}$, and accordingly

$$\begin{aligned} J_2 &< \int_1^{\infty} [(2x)^{1/2} dx/(e^{Dtx} - 1)] < \int_0^{\infty} [(2x)^{1/2} dx/(e^{Dtx} - 1)] \\ &= [2^{3/2}/(Dt)^{3/2}] \zeta(\frac{3}{2}) \end{aligned} \tag{54}$$

These inequalities could be considerably sharpened, but they suffice to show that, for those values of t ($\sim N^{-2/3}$) in which we are primarily interested, we have

$$\int_0^\infty g dx \dot{\chi} = (V/\lambda^3)\{\zeta(3/2) + [Nt^{3/2}/\Gamma(5/2)] + \mathcal{O}(N^{-1/2})\} \quad (55)$$

This gives a saddle point

$$t \sim (\lambda^2/V^{2/3})[1 - (T/T_E)^{3/2}]$$

which has the right order of magnitude, but the proportionality factor comes out somewhat too small because our density function g exaggerates the weight of the lowest quantum state by more than a factor 2 ($\int_0^{\beta\epsilon_0} g dx = 2.7$). The most natural improvement of this approximation is therefore London's procedure⁽⁵⁾ to exempt the ground state from the integration (47), writing

$$N = \bar{n}_0 + (V/\lambda^3)[1/\Gamma(3/2)] \int_{x_0}^\infty g(x) dx \dot{\chi}(x - t) \quad (56)$$

where the lower limit x_0 has to be chosen in such a way that the integral approximates the sum over the energies $\epsilon > \epsilon_0$ as closely as possible. We shall show that:

$$[1/\Gamma(3/2)] \int_{x_0}^\infty g(x) dx \dot{\chi}(x - t) = \zeta(3/2) + \text{negligible terms} \quad (57)$$

Proof. Assuming tentatively that $x_0 < t$, we can write

$$\int_{x_0}^\infty = \left[(-1/2) \int_C - \int_0^{x_0} \right] f(x - t) x^{1/2} dx - P \int_{x_0}^\infty [Dx^{1/2} dx / (e^{D(x-t)} - 1)]$$

By the same substitutions as in (52), one then obtains

$$\begin{aligned} \int_0^{x_0} f(x - t) x^{1/2} dx &= -\frac{2}{3} x_0^{3/2} - \int_{t-x_0}^t f(z)(t-z)^{1/2} dz \\ P \int_{x_0}^\infty Df(D[x-t]) x^{1/2} dx &= D \int_0^{x-t_0} \frac{(t+\xi)^{1/2} - (t-\xi)^{1/2}}{e^{D\xi} - 1} d\xi \\ &\quad + D\xi \int_{t-x_0}^\infty \frac{(t+z)^{1/2}}{e^{Dz} - 1} dz + D \frac{2}{3} [x_0^{3/2} - t^{3/2}] \end{aligned}$$

or, taken together,

$$\begin{aligned} \left\{ \int_0^{x_0} f(x-t) + P \int Df(D[x-t]) \right\} x^{1/2} dx &= -\frac{2}{3} [Dt^{3/2} - Nx^{3/2}] \\ &\quad + D \int_0^{t-x_0} \frac{(t+\xi)^{1/2} - (t-\xi)^{1/2}}{e^{D\xi} - 1} d\xi \\ &\quad + \int_{t-x_0}^t \left\{ \frac{D(t+\xi)^{1/2}}{e^{D\xi} - 1} - \frac{(t-\xi)^{1/2}}{e^\xi - 1} \right\} d\xi \\ &\quad + D \int_t^\infty \frac{(t+\xi)^{1/2}}{e^{D\xi} - 1} d\xi \end{aligned}$$

If instead we assume $x_0 > t$, we get

$$P \int_0^{x_0} x^{1/2} f(x-t) dx = -\frac{2}{3} t^{3/2} + \int_0^{x_0-t} \frac{(t+\xi)^{1/2} - (t-\xi)^{1/2}}{e^\xi - 1} d\xi \\ - \int_{x_0-t}^t f(\xi)(t-\xi)^{1/2} d\xi \\ \int_{x_0}^{\infty} x^{1/2} Df(D[x-t]) dx = D \int_{x_0-t}^{\infty} \frac{(t+\xi)^{1/2}}{e^{D\xi} - 1} d\xi$$

or, taken together,

$$P \int_0^{x_0} + \int_{x_0}^{\infty} = -\frac{2}{3} t^{3/2} + \int_0^{x_0-t} \frac{(t+\xi)^{1/2} - (t-\xi)^{1/2}}{e^\xi - 1} d\xi + \int_t^{\infty} \frac{D(t+\xi)^{1/2}}{e^{D\xi} - 1} d\xi \\ + \int_{t_0-t}^t \left\{ \frac{D(t+\xi)^{1/2}}{e^D - 1} - \frac{(t-\xi)^{1/2}}{e^\xi - 1} \right\} d\xi$$

This can be written

$$-\frac{2}{3} t^{3/2} + \int_0^t \frac{(t+\xi)^{1/2} - (t-\xi)^{1/2}}{e^\xi - 1} d\xi - \int_t^{\infty} \frac{D(t+\xi)^{1/2}}{e^{D\xi} - 1} d\xi - \int_{x_0-t}^t \chi(\xi)(t+\xi)^{1/2} d\xi$$

where in the most interesting range of temperatures $t \sim N^{-2/3}$

$$\int_t^{\infty} [D(t+\xi)^{1/2} d\xi / (e^{D\xi} - 1)] = Dt^{3/2} J_2 \sim N^{-1/2}$$

cf. Eq. (54);

$$\int_0^t \{[(t+\xi)^{1/2} - (t-\xi)^{1/2}] d\xi / (e^\xi - 1)\} < \frac{3}{2} t^{-1/2} \int_0^t [\xi d\xi / (e^\xi - 1)] < \frac{3}{2} t^{1/2} \sim N^{-1/3}$$

cf. Eq. (53);

$$\int_{x_0-t}^t \chi(\xi)(t+\xi)^{1/2} d\xi = [(1-\vartheta)x_0 + 2\vartheta t]^{1/2} [\chi(x_0-t) - \chi(t)] \sim N^{-1/3} \ln N$$

cf. Eq. (56). Similarly, for $x_0 < t$,

$$\left\{ \int_0^{x_0} f(x-t) + P \int_{x_0}^{\infty} Df(D[x-t]) \right\} x^{1/2} dx = -\frac{2}{3} (Dt^{3/2} - Nx_0^{3/2}) + Dt^{3/2} (J_1 + J_2) \\ - \int_{t-x_0}^t \chi(\xi)(t-\xi)^{1/2} d\xi$$

Having already established the smallness of the two latter terms, we need only consider the first term,

$$\frac{2}{3} (Dt^{3/2} - Nx_0^{3/2}) = \frac{2}{3} t^{3/2} + N[\vartheta t + (1-\vartheta)x_0]^{1/2} (t-x_0)$$

This is negligible for the following reason: By supposition, we have

$$0 < t - x_0 \leq t - \beta\epsilon_0$$

and $t - \beta\epsilon_0 = o(N^{-2/3})$ (except of course for the extreme temperatures $T \sim N^{-2/3}T_E$, where the thermal energy is of the same order as the spacing of the energy levels. Accordingly, the term $N[t^{3/2} - x_0^{3/2}]$ is $o(1)$ and can also be neglected.

Therefore, whether we have $x_0 > t$ or $x_0 < t$ for the lower limit of the continuous energies, we may write the equation for the saddle point:

$$N = \chi_0 + (V/\lambda^3) \zeta(3/2) + o(N) \quad (58)$$

where

$$\begin{aligned} \chi_0 = \bar{n}_0 &= [1/(e^z - 1)] - [D/(e^{Dz} - 1)], & z &= \beta\epsilon_0 - t \\ (V/\lambda^3) \zeta(3/2) &= N(T/T_E)^{3/2} \end{aligned} \quad (59)$$

which is London's equation (27).

APPENDIX C. CONTINUOUS ENERGY SPECTRUM

Labeling the one-particle energy levels by a single parameter s , we have, in the discrete case, expressions of the form

$$\Phi = \sum_s g_s \varphi(\beta\epsilon_s - t) \quad (60)$$

and their partial derivatives

$$\partial\Phi/\partial\beta\epsilon_r = g_r \varphi'(\beta\epsilon_r - t) - (\partial t/\partial\beta\epsilon_r) \sum_s g_s \dot{\varphi}(\beta\epsilon_s - t) \quad (61)$$

where φ is a universal function.

When the energy spectrum is continuous, the expression corresponding to Φ will be an integral

$$\Phi = \int ds \gamma(s) \varphi(\beta\epsilon(s) - t) \quad (62)$$

and the partial differential quotient (61) becomes a Volterra derivative

$$\delta\Phi/\delta\beta\epsilon(r) = \gamma(r) \varphi'(\beta\epsilon(r) - t) - [\delta t/\delta\beta\epsilon(r)] \int ds \gamma(s) \dot{\varphi}(\beta\epsilon(s) - t) \quad (63)$$

Both cases can be comprised by

$$\Phi = \int g(x) dx \varphi(x - t) \quad (64)$$

One has only to take

$$g(x) = \begin{cases} \sum_s g_s \delta(x - \beta\epsilon_s) & \text{discrete spectrum} \\ \int \gamma(s) \delta(x - \beta\epsilon(s)) & \text{continuous spectrum} \end{cases} \quad (65)$$

If the continuum description is merely an asymptotic approximation in the sense that

$$\sum_s \rightarrow \int ds \quad \text{when} \quad V \rightarrow \infty$$

the choice of parameter s suggests itself. For example, in the case of the ideal gas,

$$\epsilon_s = (h^2/8mV^{2/3}) s^2, \quad \gamma(s) \sim (1/8) 4\pi s^2 \quad (66)$$

With $\lambda = \beta h^2/2\pi m$, this gives for the density function g according to (65)

$$\begin{aligned} g(x) &= \gamma(s)(ds/d\beta\epsilon)|_{\beta\epsilon(s)=x} \\ &= (V/\lambda^3) x^{1/2}/\Gamma(3/2) \end{aligned} \quad (67)$$

There are, however, many ways of parametrization, and the simplest for our purposes is to choose it in such a way that $d(\text{parameter})/d\beta\epsilon = 1$, that is, to let functional argument and parameter coincide. In order not to confound them, we may for a moment write

$$g([\epsilon]; x) = \int \gamma(\xi) d\xi \delta(x - \beta\epsilon(\xi)) \quad (68)$$

Since we have now $\gamma \equiv g$ and $\beta\epsilon = \xi$, this is certainly a circumstantial way of writing a trivial identity. However, it serves to emphasize that g is a functional of the energy spectrum and this is necessary to keep in mind when carrying out the differentiations. We thus have, according to (68),

$$\delta g/\delta\beta\epsilon(y) = -g(y) \delta'(x - y) \quad (69)$$

and

$$\begin{aligned} \delta\Phi/\delta\beta\epsilon(y) &= \int dx [\delta g/\delta\beta\epsilon(y)] \varphi(x - t) - [\delta t/\delta\beta\epsilon(y)] \int dx g\dot{\varphi}(x - t) \\ &= g(y) \varphi'(y - t) - [\delta t/\delta\beta\epsilon(y)] \int dx g\dot{\varphi} \end{aligned} \quad (70)$$

The equations of the saddle-point approximation will now be

$$\ln Z = -Nt + \int g(x) dx \dot{\chi}(x - t) \quad (71)$$

$$0 = -N + \int g(x) dx \dot{\chi}(x - t) \quad (72)$$

$$-\delta(\ln Z)/\delta\beta\epsilon = \left(N - \int g\dot{\chi} dx \right) (\delta t/\delta\beta\epsilon) + g(\beta\epsilon) \dot{\chi}(\beta\epsilon - t) \quad (73)$$

or, since the parenthesis is zero, the average number of particles per energy interval around ϵ will be

$$\overline{dN(\epsilon)}/d\epsilon = \beta g(\beta\epsilon) \dot{\chi}(\beta\epsilon - t) \quad (74)$$

In order to obtain the fluctuations, we need the functional derivative $\delta t/\delta\beta\epsilon$; varying Eq. (72) for the saddle point with respect to the spectrum, we have

$$\begin{aligned}\delta \int g\dot{\chi} dx &= \delta N = 0 \\ &= \int \{[\delta g/\delta\beta\epsilon(y)] \delta\beta\epsilon(y) dy \dot{\chi} + g\ddot{\chi} \delta t\} dx \\ &= - \int_0^\infty dy g(y) \ddot{\chi}(y-t) \delta\beta\epsilon(y) + \delta t \int_0^\infty dx g(x) \ddot{\chi}(x-t)\end{aligned}$$

or

$$(\delta t/\delta\beta\epsilon)_N = \ddot{\chi}g / \int_0^\infty \ddot{\chi}g dx \quad (75)$$

Let us consider the fluctuation in the number of particles with energies below ϵ . By Eq. (73), their average is

$$\overline{N(\epsilon)} = \int_0^{\beta\epsilon} dx g(x) \dot{\chi}(x-t) \quad (76)$$

The average of their square is given by

$$\overline{ZN^2} = \int_0^{\beta\epsilon} d\xi [\delta/\delta\beta\epsilon(\xi)] \int_0^{\beta\epsilon} d\eta [\delta Z/\delta\beta\epsilon(\eta)] \quad (77)$$

as one sees from the definition (5) of Z and transition to the continuum. Using (74) and (76), we have

$$\begin{aligned}ZN^2 &= \int d\xi [\delta/\delta\beta\epsilon(\xi)] [-ZN(\epsilon)] \\ &= Z(\overline{N})^2 - Z \int_0^{\beta\epsilon} d\xi [\delta\overline{N}/\delta\beta\epsilon(\xi)]\end{aligned} \quad (78)$$

and, by Eq. (76),

$$\begin{aligned}\delta\overline{N}/\delta\beta\epsilon(\xi) &= \int_0^{\beta\epsilon} [\delta g/\delta\beta\epsilon(\xi)] dx \dot{\chi}(x-t) + [\delta t/\delta\beta\epsilon(\xi)] \int_0^{\beta\epsilon} g dx \dot{\chi}(x-t) \\ &= -g(\xi) \ddot{\chi}(\xi-t) + [\delta t/\delta\beta\epsilon(\xi)] \int_0^{\beta\epsilon} g dx \ddot{\chi}(x-t)\end{aligned}$$

Integrating,

$$\begin{aligned}\int d\xi [\delta\overline{N}/\delta\beta\epsilon(\xi)] &= - \int_0^{\beta\epsilon} g\ddot{\chi} dx \left\{ 1 - \int_0^{\beta\epsilon} d\xi [\delta t/\delta\beta\epsilon(\xi)] \right\} \\ &= - \int_0^{\beta\epsilon} g\ddot{\chi} dx \left[1 - \left(\int_0^{\beta\epsilon} g\ddot{\chi} dx / \int_0^\infty g\ddot{\chi} dx \right) \right]\end{aligned}$$

we have finally

$$\overline{N(\epsilon)^2} - [\overline{N(\epsilon)}]^2 = \int_0^{\beta\epsilon} \ddot{\chi}g dx \left[1 - \left(\int_0^{\beta\epsilon} \ddot{\chi}g dx / \int_0^\infty \ddot{\chi}g dx \right) \right] \quad (79)$$

APPENDIX D. ORDER OF MAGNITUDE OF $\partial t/\partial\beta\epsilon$ AND $\ddot{\chi}_0$ FOR THE IDEAL GAS

In the fluctuation formula (16), we need an estimate of

$$\partial t/\partial\beta\epsilon_0 = \ddot{\chi}_0 / \sum \ddot{\chi}_s \quad (80)$$

In the denominator, we split off, as before, the term $\ddot{\chi}_0$ and approximate the sum over the excited levels by an integral

$$\sum_{s>0} \approx \int_t^\infty \ddot{\chi}(x-t) g(x) dx$$

Drawing a diameter and a tangent to the parabola

$$g(x) = (V/\lambda^3) x^{1/2}/\Gamma(3/2)$$

through the point $x = t$, $g(t)$ and remembering the properties of the function $\ddot{\chi}$ (Appendix A), it is seen that

$$g(t) \int_t^\infty \ddot{\chi} dx < \int_t^\infty \ddot{\chi} g dx < \int_t^\infty \ddot{\chi} \cdot (g'(t)[x-t] + g(t)) dx \quad (81)$$

Carrying out the integrations and inserting

$$\dot{\chi}(0) = N/2, \quad \chi(0) = \ln D; \quad t \sim \lambda^2/V^{2/3}$$

it follows that

$$\int_t^\infty g(x) \ddot{\chi}(x-t) dx \sim N(V/\lambda^3)^{2/3} \quad (82)$$

with an error $\sim (V/\lambda^3)^{4/3} \ln N$. Since V/λ^3 is at most of order N , this error is always of smaller order than the main term. We may thus write

$$\partial t/\partial\beta\epsilon \sim \ddot{\chi}_0 / [\ddot{\chi}_0 + N(V/\lambda^3)^{2/3}] \quad (83)$$

When t is positive, it is natural in the continuum description of the energies to associate the states $\epsilon < t$ with the Einstein condensate. Since

$$\int_0^t g dx \sim 1$$

we have in fact by the mean value theorem

$$\begin{aligned} \int_0^t \dot{\chi} g dx &\sim \dot{\chi}(-\vartheta t) \sim \bar{n}_0, & 0 < \vartheta < 1 \\ \int \ddot{\chi} g dx &\sim \ddot{\chi}(-\Theta t) \sim \ddot{\chi}_0, & 0 < \Theta < 1 \end{aligned}$$

This shows that one will recover the same results even if the lowest level is not segregated from the rest. It is thus possible to treat the energy spectrum of the ideal

gas altogether as continuous, and this description holds good well below the Einstein transition point ($V\lambda^3 \sim N$). It does not really break down before $V/\lambda^3 = \mathcal{O}(1)$, that is, when $T \lesssim T_E N^{-2/3}$. Einstein's theory of the ideal Bose gas can therefore in principle be formulated without invoking quantization of the translation energies. This is gratifying because the ratio (thermal energy/level spacing) is such an enormous number at all measurable temperatures that it seems very artificial to consider the spectrum as discrete.

The most convenient expressions for $\ddot{\chi}_0$, however, are obtained by combining Eqs. (45) and (46):

$$\ddot{\chi}_0 \sim \begin{cases} \bar{n}_0^2, & t = 0 & (z = \beta\epsilon_0) \\ N^2, & t \approx \beta\epsilon_0 & [\mathcal{O}(z) = N^{-1}] \\ (N - \bar{n}_0)^2, & t > \beta\epsilon_0 & [\mathcal{O}(z) > N^{-1}] \end{cases} \quad (84)$$

with London's equation (27) in the form

$$(N - \bar{n}_0) \sim V/\lambda^3, \quad t > 0 \quad (85)$$

At the transition point itself, $T = T_E$, \bar{n}_0 is not zero, as might be indicated by Eq. (27). Here, we have

$$t = 0, \quad \therefore z = \beta\epsilon_0 \sim N^{-2/3}$$

and accordingly

$$\begin{aligned} \bar{n}_0 &= \ddot{\chi}_0(z) \approx 1/z \sim N^{2/3} \\ \ddot{\chi}_0 &\sim \bar{n}_0^2 \sim \bar{N}^{4/3} \end{aligned} \quad (86)$$

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