

# The Saddle-Point Method for Condensed Bose Gases

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The application of the conventional saddle-point approximation to condensed Bose gases is thwarted by the approach of the saddle-point to the ground-state singularity of the grand canonical partition function. We develop and test a variant of the saddle-point method which takes proper care of this complication, and provides accurate, flexible, and computationally efficient access to both canonical and microcanonical statistics. Remarkably, the error committed when naively employing the conventional approximation in the condensate regime turns out to be universal, that is, independent of the system's single-particle spectrum. The new scheme is able to cover all temperatures, including the critical temperature interval that marks the onset of Bose–Einstein condensation, and reveals in analytical detail how this onset leads to sharp features in gases with a fixed number of particles. In particular, within the canonical ensemble the crossover from the high-temperature asymptotics to the condensate regime occurs in an error-function-like manner; this error function reduces to a step function when the particle number becomes large. Our saddle-point formulas for occupation numbers and their fluctuations, verified by numerical calculations, clearly bring out the special role played by the ground state. © 1999 Academic Press

## 1. INTRODUCTION

The saddle-point method is one of the most essential tools in statistical physics [1, 2]. When comparing different statistical ensembles, it is used with overwhelming success in both fundamental theoretical considerations and practical calculations [3, 4]. Yet, the conventional form of this usually easy-to-handle approximation fails in the case of condensed ideal Bose gases [5–7]; for instance, it does not yield the correct fluctuation of the number of condensate particles [8, 9].

To elucidate the reason for this failure we consider an ideal Bose gas with single-particle energies  $\varepsilon_\nu$ , with  $\nu = 0, 1, 2, \dots$  labeling the individual energy eigenvalues.

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Since the grand canonical partition function  $\Xi(\beta, z)$  generates the canonical partition functions  $Z_N(\beta)$  by means of the expansion

$$\begin{aligned}\Xi(\beta, z) &= \prod_{v=0}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_v)} \\ &= \sum_{N=0}^{\infty} z^N Z_N(\beta),\end{aligned}\quad (1)$$

each  $N$ -particle partition function  $Z_N(\beta)$  can be represented, according to Cauchy's theorem, by a contour integral in the complex  $z$ -plane,

$$Z_N(\beta) = \frac{1}{2\pi i} \oint dz \frac{\Xi(\beta, z)}{z^{N+1}}, \quad (2)$$

where the path of integration encircles the origin counter-clockwise. As usual,  $\beta = 1/(k_B T)$  is the inverse temperature. Denoting the negative logarithm of the integrand as  $\bar{F}(z)$ , i.e., writing

$$\frac{1}{z^{N+1}} \prod_{v=0}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_v)} \equiv \exp(-\bar{F}(z)) \quad (3)$$

or

$$\bar{F}(z) = (N+1) \ln z + \sum_{v=0}^{\infty} \ln(1 - z e^{-\beta \varepsilon_v}), \quad (4)$$

the saddle-point  $z_0$  is determined by the requirement that this function becomes stationary,

$$\left. \frac{\partial \bar{F}(z)}{\partial z} \right|_{z=z_0} = 0, \quad (5)$$

giving

$$N+1 = \sum_{v=0}^{\infty} \frac{1}{z_0^{-1} e^{\beta \varepsilon_v} - 1}. \quad (6)$$

Apart from the appearance of one extra particle on the left hand side, this is just the grand canonical relation between particle number  $N$  and fugacity  $z_0$ .

Proceeding according to folk wisdom, one then expands the logarithm  $\bar{F}(z)$  quadratically around  $z_0$  and leads the path of integration parallel to the imaginary axis over the saddle, relying on the fact that for large  $N$  the main contribution to the integral (2) is collected in the immediate vicinity of the saddle-point [2], so that the quadratic expansion should prove sufficient. Doing the remaining Gaussian

integral, one arrives at the standard saddle-point approximation  $\tilde{Z}_N^{(\text{s.p.})}$  to the canonical partition functions,

$$\begin{aligned}\tilde{Z}_N^{(\text{s.p.})}(\beta) &= \frac{1}{2\pi i} \int_{z_0 - i\infty}^{z_0 + i\infty} dz \exp \left( -\bar{F}^{(0)} - \frac{1}{2} \bar{F}^{(2)}(z - z_0)^2 \right) \\ &= \frac{1}{2\pi} \exp(-\bar{F}^{(0)}) \int_{-\infty}^{+\infty} du \exp \left( +\frac{1}{2} \bar{F}^{(2)} u^2 \right) \\ &= \frac{\exp(-\bar{F}^{(0)})}{\sqrt{-2\pi \bar{F}^{(2)}}}.\end{aligned}\quad (7)$$

Here and in the following we write  $f^{(n)}$  for the  $n$ th derivative of a function  $f$  at a saddle-point; we have used  $\bar{F}^{(2)} < 0$ . Hence, one finds

$$\begin{aligned}\ln \tilde{Z}_N^{(\text{s.p.})}(\beta) &= -\frac{1}{2} \ln 2\pi - (N+1) \ln z_0 - \sum_{v=0}^{\infty} \ln(1 - z_0 e^{-\beta \varepsilon_v}) \\ &\quad - \frac{1}{2} \ln \sum_{v=0}^{\infty} \frac{z_0^{-1} e^{-\beta \varepsilon_v}}{(1 - z_0 e^{-\beta \varepsilon_v})^2},\end{aligned}\quad (8)$$

from which the canonical occupation number  $\langle n_\alpha \rangle_{\text{cn}}$  of the state  $\alpha$  is obtained by differentiating once with respect to  $(-\beta \varepsilon_\alpha)$ ,

$$\langle n_\alpha \rangle_{\text{cn}} = \frac{\partial \ln \tilde{Z}_N^{(\text{s.p.})}}{\partial(-\beta \varepsilon_\alpha)} + \frac{\partial \ln \tilde{Z}_N^{(\text{s.p.})}}{\partial z_0} \frac{\partial z_0}{\partial(-\beta \varepsilon_\alpha)}.\quad (9)$$

As long as the gas is not condensed, the fourth term in the approximation (8) remains small in comparison to the third, and therefore may be neglected. Then the partial derivative  $\partial \ln \tilde{Z}_N^{(\text{s.p.})} / \partial z_0$  vanishes as a consequence of the saddle-point equation (6), and one is left with

$$\begin{aligned}\langle n_\alpha \rangle_{\text{cn}} &= \frac{\partial \ln \tilde{Z}_N^{(\text{s.p.})}}{\partial(-\beta \varepsilon_\alpha)} \\ &= \frac{1}{z_0^{-1} e^{\beta \varepsilon_\alpha} - 1},\end{aligned}\quad (10)$$

so that within these approximations the canonical occupation numbers equal their grand canonical counterparts.

However, this reasoning breaks down for temperatures below the onset of Bose–Einstein condensation, where Eq. (6) requires that  $z_0^{-1} e^{\beta \varepsilon_0} - 1$  be on the order of  $1/N$ , so that the third and the fourth terms on the right hand side of Eq. (8) are of comparable magnitude, namely of the order  $O(\ln N)$ . Hence, the argument that

led to the familiar formula (10) becomes invalid. Moreover, inspecting the higher derivatives of  $\bar{F}(z)$  at the saddle-point,

$$\bar{F}^{(n)} = -\frac{(n-1)!}{z_0^n} \left[ (-1)^n (N+1) + \sum_{v=0}^{\infty} \left( \frac{1}{z_0^{-1} e^{\beta \varepsilon_v} - 1} \right)^n \right], \quad (11)$$

one finds that in the condensate regime these derivatives grow dramatically with increasing  $n$ ,  $\bar{F}^{(n)} = O(N^n)$ , casting doubt on the validity of the saddle-point approximation even if higher-order terms are included [5]. However, for the derivation of an asymptotic series the convergence properties of the formal Taylor series of  $\bar{F}(z)$  are irrelevant [10]; what actually endangers the approximation scheme (7) in the condensate regime is the narrow approach of the saddle-point to the ground-state singularity  $z = e^{\beta \varepsilon_0}$  of the grand canonical partition function (1). Namely, the Gaussian integral (7) can well represent the exact expression (2) only if the function  $\bar{F}(z)$  is free of singularities at least in those intervals where the Gaussian is still large, i.e., where  $-\bar{F}^{(2)}(z - z_0)^2/2$  is on the order of unity. Since  $\bar{F}^{(2)} = O(N^2)$ , this observation translates into the requirement that *the function  $\bar{F}(z)$  should be regular at least in an interval of order  $O(1/N)$  around  $z_0$* . On the other hand, *in the condensate regime the singularity at  $z = e^{\beta \varepsilon_0}$  falls within a distance of order  $O(1/N)$  from the saddle-point  $z_0$* , again as a consequence of Eq. (6). It is this conflict, *not* the poor behavior of the Taylor expansion of  $\bar{F}(z)$ , which necessitates an approach to the contour integral (2) that is essentially more careful than the standard scheme (7). Interestingly, though, the dilemma does not appear to be overly severe—the magnitude of both conflicting intervals being of the *same* order  $O(1/N)$ —and one might wonder already at this point whether the usual procedure can be saved by simple means.

The failure of the saddle-point approximation (7) for condensed Bose gases has been the subject of a long debate in the literature [5–7], with notable early contributions by Dingle [11] and Fraser [12]. Various schemes have been designed for computing the number of condensate particles, and its fluctuation, for gases with a fixed number  $N$  of particles, *without* resorting to the saddle-point method. Quite recently, Navez *et al.* have suggested a statistical ensemble within which one regards the condensate as an infinite particle reservoir for the excited-states subsystem [13], thus putting into shape an idea already expressed by Fierz [14]. In a mathematical setting, each excited single-particle level  $\varepsilon_\alpha$  then becomes formally equivalent to a harmonic oscillator with frequency  $(\varepsilon_\alpha - \varepsilon_0)/h$ , which allows one to derive elegant integral representations for canonical and microcanonical expectation values: Setting  $\varepsilon_0 = 0$  for convenience, restricting oneself to temperatures below the onset of condensation, and introducing the spectral Zeta function

$$Z(\beta, t) = \sum_{v=1}^{\infty} \frac{1}{(\beta \varepsilon_v)^t}, \quad (12)$$

with the sum running over the excited states only, the canonical number of condensate particles can be written as [15]

$$\langle n_0 \rangle_{\text{cn}} = N - \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt \Gamma(t) Z(\beta, t) \zeta(t), \quad (13)$$

where  $\zeta(t)$  is the Riemann Zeta function. The path of integration up the complex  $t$ -plane lies to the right of all poles of the integrand, so that the residues of these poles, taken from right to left, yield a systematic expansion of the integral [15]. Similarly, the canonical mean-square fluctuation of the number of condensate particles takes the form

$$\langle \delta^2 n_0 \rangle_{\text{cn}} = \frac{1}{2\pi i} \int_{\tau - i\infty}^{\tau + i\infty} dt \Gamma(t) Z(\beta, t) \zeta(t-1), \quad (14)$$

and the difference between canonical and microcanonical fluctuations is given by

$$\langle \delta^2 n_0 \rangle_{\text{cn}} - \langle \delta^2 n_0 \rangle_{\text{mc}} = \frac{[1/2\pi i \int_{\tau - i\infty}^{\tau + i\infty} dt \Gamma(t) Z(\beta, t-1) \zeta(t-1)]^2}{1/2\pi i \int_{\tau - i\infty}^{\tau + i\infty} dt \Gamma(t) Z(\beta, t-2) \zeta(t-1)}. \quad (15)$$

Yet, there are at least two reasons not to be content with this state of affairs. Firstly, since Eqs. (13), (14), and (15) rely on the presence of a reservoir of condensate particles, they are blind to the onset of Bose–Einstein condensation, that is, to the sudden appearance of this reservoir; as a consequence of this underlying “oscillator approximation,” they do not allow one to discuss just how such a sharp feature can emerge in a Bose gas with a large, fixed number of particles. Second, for a given single-particle spectrum the integrals may not always be straightforward to evaluate; already the treatment of an anisotropic harmonic oscillator potential, in which case  $Z(\beta, t)$  is related to Zeta functions of the Barnes type [15], requires quite some analytical skills. Therefore, one desires a tool that works, in principle, for all temperatures, and is easy to use in practical calculations.

The development of such a tool is the objective of the present paper. Following a trail pioneered by Dingle [10], we work out and test a variant of the saddle-point method that fulfills the above two requirements. Our guiding maxim is the same which already governed London’s classic analysis [16] of the condensation phenomenon: If the ground state is causing trouble, single it out and give it a special treatment—which, in our case, means to exempt the ground-state factor of the grand canonical partition function (1) from the quadratic expansion performed in the usual scheme (7), and to treat that factor exactly. As will be demonstrated in detail, this natural strategy leads to an approach to the canonical and the microcanonical statistics of condensed Bose gases which is both extremely accurate and unsurpassed in computational ease.

We proceed as follows: In the next section we will first explain *why* and *how* this proper saddle-point approximation works for the calculation of the canonical partition functions, and how known limiting cases are recovered, concentrating key

technical details in Appendices A and B. We then apply the method to computing canonical occupation numbers and their fluctuations, illustrating the analytical results by numerical calculations for an ideal Bose gas confined by an isotropic harmonic potential. In Section III we turn to the microcanonical ensemble and show how the very same refined saddle-point approach allows one to obtain the interesting quantities almost without further effort. The final Section IV summarizes the most important findings.

Although our discussion is led along the lines of the ideal Bose gas, and although some interesting physical insights will turn up—in particular, it will become clear why the canonical occupation numbers are well described by the expression (10), and thus essentially equal to their grand canonical analogues, even for temperatures below the onset of condensation, where the previous argument had failed—this is not primarily a work on the ideal Bose gas as such. Rather, major emphasis lies on the mathematics of saddle-point integrals with a singular integrand, of which condensed Bose gases provide perhaps the most prominent examples; we hope that the detailed exposition presented here will prove fruitful also in other areas of mathematical physics where similar problems arise.

## II. THE CANONICAL ENSEMBLE

### A. The Canonical Partition Function

Since the conventional approximation (7) is thwarted by the fact that the saddle-point  $z_0$ , i.e., the solution to Eq. (6), approaches the ground-state singularity  $z = e^{\beta\epsilon_0}$  of the integrand (3) within order  $O(1/N)$  in the condensate regime, we now exclude the ground-state contribution from the quadratic expansion of the logarithm (4). That is, we define

$$\begin{aligned} F(z) &= \bar{F}(z) - \ln(1 - ze^{-\beta\epsilon_0}) \\ &= (N+1) \ln z + \sum_{v=1}^{\infty} \ln(1 - ze^{-\beta\epsilon_v}), \end{aligned} \quad (16)$$

and write the canonical  $N$ -particle partition function as

$$Z_N(\beta) = \frac{1}{2\pi i} \oint dz \frac{\exp(-F(z))}{1 - ze^{-\beta\epsilon_0}}. \quad (17)$$

The key idea for treating integrals of this kind, due to Dingle [10], is to let the potentially dangerous denominator stand as it is, and to expand only the tempered function  $F(z)$  around the saddle-point  $z_0$ . The resulting approximation to  $Z_N(\beta)$  will then be valid for *all* temperatures: For high  $T$ , when the saddle-point moves away from the singularity, it is of no concern whether or not the denominator is included in the Gaussian approximation; in the condensate regime its exclusion is crucial.

Let us first check the behavior of the derivatives  $F^{(n)}$ . When omitting the ground-state term ( $v=0$ ) from the sum in Eq. (11), the behavior of the remaining sum is governed in the condensate regime by the following terms ( $v=1, 2, 3, \dots$ ), each of them being about proportional to the  $n$ th power of temperature. Hence,

$$\left[ \sum_{v=1}^{\infty} \left( \frac{1}{z_0^{-1} e^{\beta \varepsilon_v} - 1} \right)^n \right]^{1/n} \propto k_B T, \quad (18)$$

with approximate  $T$ -proportionality holding the better, the larger  $n$ , since large  $n$  emphasize the low-lying states. Now we focus on systems with single-particle energies of the form [17]

$$\varepsilon_{\{v_i\}} = \varepsilon_0 + \varepsilon_1 \sum_{i=1}^d c_i v_i^s, \quad (19)$$

where  $v_i=0, 1, 2, \dots$  are integer quantum numbers. The dimensionless anisotropy coefficients  $c_i$  should be of comparable magnitude, the lowest of them equaling unity. This class of systems contains, e.g., a gas of  $N$  ideal Bose particles confined by a  $d$ -dimensional harmonic oscillator potential ( $s=1$ ), or by a  $d$ -dimensional hard box ( $s=2$ ). For  $d/s > 1$  and large  $N$  there is a sharp onset of Bose–Einstein condensation, with

$$k_B T \propto \langle N_{\text{ex}} \rangle_{\text{cn}}^{s/d} \quad (20)$$

in the condensate regime;  $\langle N_{\text{ex}} \rangle_{\text{cn}} \equiv N - \langle n_0 \rangle_{\text{cn}}$  is the total number of excited particles [18, 19]. Thus, for largish  $n$  the Eqs. (18) and (20) give

$$S_n \equiv \sum_{v=1}^{\infty} \left( \frac{1}{z_0^{-1} e^{\beta \varepsilon_v} - 1} \right)^n \propto \langle N_{\text{ex}} \rangle_{\text{cn}}^{ns/d} \quad \text{for } d/s > 1, \quad (21)$$

resulting, by virtue of Eq. (11), in

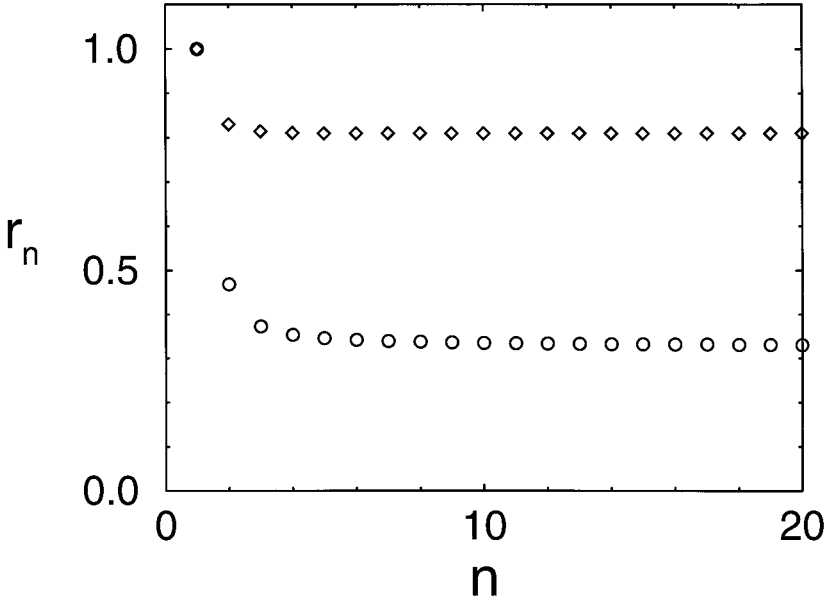
$$F^{(n)} = O(N^{\xi(n)}) \quad \text{with } \xi(n) = \max\{1, ns/d\}, \quad (22)$$

as long as, besides  $\langle n_0 \rangle_{\text{cn}} = O(N)$ , also  $\langle N_{\text{ex}} \rangle_{\text{cn}} = O(N)$ . To confirm this relation, the case  $n=2$  of which will be of particular interest later, Fig. 1 shows the numerically computed quantities

$$r_n \equiv \frac{\ln S_n}{n \ln \langle N_{\text{ex}} \rangle_{\text{cn}}} \quad (23)$$

(which, in the general case, should approach  $s/d$  for large  $n$ ) for a gas of  $N=10^6$  ideal Bose particles kept at temperature  $T=0.5 T_0^{(3)}$  in a three-dimensional isotropic harmonic oscillator potential, with

$$T_0^{(3)} = \frac{\hbar \omega}{k_B} \left( \frac{N}{\zeta(3)} \right)^{1/3} \quad (24)$$



**FIG. 1.** Circles: ratios  $r_n$ , as defined by Eqs. (21) and (23), for a gas of  $N=10^6$  ideal Bose particles with temperature  $T=0.5\,T_0^{(3)}$  which is confined by an isotropic three-dimensional harmonic oscillator potential. According to Eq. (21), one expects  $r_n \approx 1/3$  for largish  $n$ . The diamonds indicate the corresponding data for a gas with same number of particles kept at  $T=0.5\,T_0^{(1)}$  in a one-dimensional harmonic trap.

denoting the condensation temperature in the large- $N$ -limit [17];  $\omega$  is the oscillator frequency. As expected,  $r_n$  approaches the value  $1/3$  fairly rapidly with  $n$ . For comparison, Fig. 1 also shows the corresponding data for a gas with the same number of particles which is stored in a one-dimensional harmonic potential. Its temperature is  $T=0.5\,T_0^{(1)}$ , where

$$T_0^{(1)} = \frac{\hbar\omega}{k_B} \frac{N}{\ln N}. \tag{25}$$

This is a borderline case: For  $d=s=1$  there is no sharp onset of Bose–Einstein condensation, so that  $T_0^{(1)}$  merely plays the role of a characteristic temperature below which the ground-state population becomes significant. There are logarithmic corrections [15] which keep the ratios  $r_n$  below the value  $s/d=1$  also for large  $n$ , but, as seen in the figure, even now  $r_n$  rapidly approaches a constant not too far from unity. We conclude that for systems of the type (19), with  $d/s > 1$ , the  $O(N^n)$ -growth of  $\bar{F}^{(n)}$  in the condensate regime is replaced by the somewhat milder  $O(N^{ns/d})$ -growth of  $F^{(n)}$  when going from  $\bar{F}(z)$  to its ground-state-amputated



descendant  $F(z)$ , so that also the formal Taylor expansion of  $F(z)$  around the saddle-point  $z_0$  is ill-behaved.

But as already indicated, the properties of the Taylor series of  $F(z)$  are only of secondary importance. What really matters is that this function does not share the ground-state singularity; the singular point to be watched now is the one at  $z = e^{\beta\epsilon_1}$ . Since  $z_0 < e^{\beta\epsilon_0}$ , the saddle-point remains separated from that singularity by at least the  $N$ -independent gap  $e^{\beta\epsilon_1} - e^{\beta\epsilon_0} \approx (\epsilon_1 - \epsilon_0)/k_B T$ . This guarantees that when quadratically expanding the amputated function  $F(z)$ , rather than  $\bar{F}(z)$ , around  $z_0$ , an interval of the required order  $O(1/\sqrt{-F^{(2)}}) = O(N^{-\xi(2)/2})$  becomes singularity-free for sufficiently large  $N$ ; the higher the temperature (while remaining in the condensate regime), the smaller the gap, and the larger the particle number has to be. Then the Gaussian approximation to  $\exp(-F(z))$  is safe. As shown in detail in Appendix A, the subsequently emerging saddle-point integral for the canonical partition function (17) can be done exactly, yielding (cf. Eq. (A14) with  $\sigma = 1$ )

$$Z_N^{(\text{s.p.})}(\beta) = \frac{1}{\sqrt{2\pi}} \exp\left(\beta\epsilon_0 - F^{(0)} - 1 + \frac{1}{2}\eta^2 - \frac{1}{4}\bar{\eta}^2\right) D_{-1}(\bar{\eta}), \quad (26)$$

where

$$\eta = (e^{\beta\epsilon_0} - z_0) \sqrt{-F^{(2)}}, \quad (27)$$

$$\bar{\eta} = \eta - \frac{1}{\eta}, \quad (28)$$

and  $D_{-1}(\bar{\eta})$  is a parabolic cylinder function, employing Whittaker's notation [20, 21]. For discussing this unfamiliar-looking expression (26), which, as already remarked above, is valid for *all* temperatures, we observe [21] that  $D_{-1}$  is related to the complementary error function  $\text{erfc}$ ,

$$D_{-1}(\bar{\eta}) = \exp\left(\frac{1}{4}\bar{\eta}^2\right) \sqrt{\frac{\pi}{2}} \text{erfc}\left(\frac{\bar{\eta}}{\sqrt{2}}\right); \quad (29)$$

hence

$$Z_N^{(\text{s.p.})}(\beta) = \exp\left(\beta\epsilon_0 - F^{(0)} - 1 + \frac{1}{2}\eta^2\right) \frac{1}{2} \text{erfc}\left(\frac{\bar{\eta}}{\sqrt{2}}\right). \quad (30)$$

For high temperatures, well above the condensation point,  $z_0$  approaches zero, so that the parameter  $\eta$ , and as a consequence also  $\bar{\eta}$ , grows without bound when  $N$  becomes large. Then we may replace the complementary error function by the leading term of its asymptotic expansion for large *positive* arguments [22],

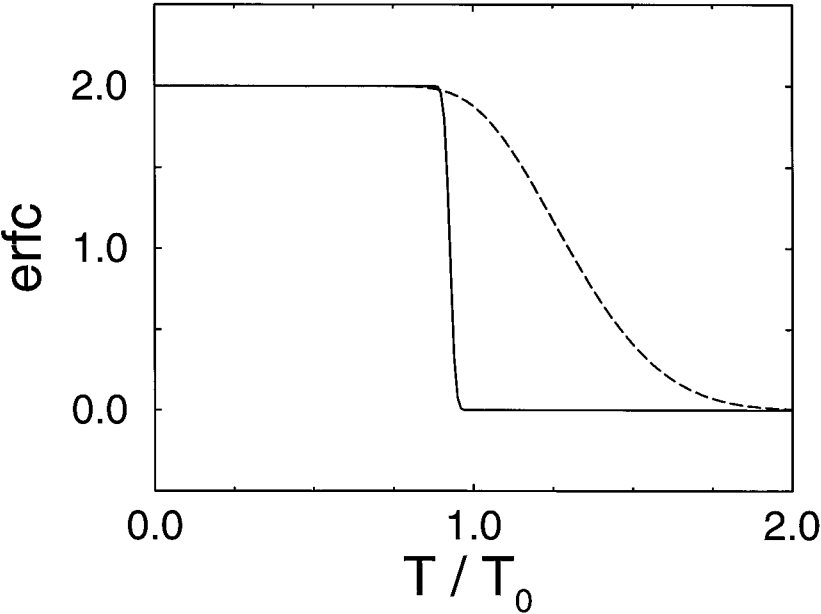
$$\text{erfc}\left(\frac{\bar{\eta}}{\sqrt{2}}\right) \sim \sqrt{\frac{2}{\pi}} \frac{\exp(-\bar{\eta}^2/2)}{\bar{\eta}}. \quad (31)$$

This is a special case of the approximation (B1) introduced in Appendix B, and implies, together with the further approximations (B2)–(B5), that the general expression (26) correctly approaches the standard saddle-point result (7) outside the condensate phase,

$$Z_N^{(\text{s.p.})}(\beta) \sim \tilde{Z}_N^{(\text{s.p.})}(\beta) \quad \text{for high } T. \tag{32}$$

This was to be expected, since when the denominator in the integrand (17) does not become small, it doesn't matter whether it is included in the quadratic approximation, as in the scheme (7), or treated exactly, as in the derivation of Eq. (26).

In the condensate regime, where  $e^{\beta\epsilon_0} - z_0 = O(1/N)$  and  $F^{(2)} = O(N^{\xi(2)})$  as specified by Eq. (22), the definition (27) of the parameter  $\eta$  implies either  $\eta = O(N^{-1/2})$  or  $\eta = O(N^{s/d-1})$ , whichever is larger. Since we require  $d/s > 1$ , we conclude that in either case  $\eta$  approaches zero for large  $N$ , so that now  $\bar{\eta} = \eta - \eta^{-1}$  is a large *negative* number. Therefore, we may safely use the approximation  $\text{erfc}(\bar{\eta}/\sqrt{2}) \approx 2$ , and arrive at



**FIG. 2.** Complementary error function  $\text{erfc}(\bar{\eta}/\sqrt{2})$ , with the temperature-dependent parameter  $\bar{\eta}$  defined by Eqs. (27) and (28), for a gas of  $N = 10^3$  ideal Bose particles in a *three*-dimensional isotropic harmonic oscillator potential (full line; here the reference temperature  $T_0$  equals  $T_0^{(3)}$  as given by Eq. (24)), and in a *one*-dimensional harmonic potential (dashed line; with  $T_0 = T_0^{(1)}$  as in Eq. (25)). When  $\text{erfc}(\bar{\eta}/\sqrt{2})$  approaches zero, the standard high-temperature result (7) holds; when it approaches two, Eq. (33) provides the correct partition function.

$$\begin{aligned}
Z_N^{(\text{s.p.})}(\beta) &\sim \exp(\beta\epsilon_0 - F^{(0)} - 1) \\
&= \frac{e^{\beta\epsilon_0 - 1}}{z_0^{N+1}} \prod_{v=1}^{\infty} \frac{1}{1 - z_0 \exp(-\beta\epsilon_v)}.
\end{aligned} \tag{33}$$

Even when the particle number  $N$  is merely moderately large, the decrease of the parameter  $\bar{\eta}$  with temperature from large positive to large negative values can be fairly rapid, so that the complementary error function in the canonical  $N$ -particle partition function (30) acts as a switch, meaning that the transition from the high-temperature asymptotics (7) to the condensate asymptotics (33) becomes quite sharp. This is confirmed by Fig. 2, which depicts  $\text{erfc}(\bar{\eta}/\sqrt{2})$  as function of temperature for a gas of  $N=10^3$  ideal Bosons in a three-dimensional isotropic harmonic potential. In the borderline case of the one-dimensional harmonic potential, also indicated in the figure, there is no such sharp transition.

It is worthwhile to discuss the condensate partition function (33) a little further. Anticipating that, despite the incorrect reasoning, the expression (10) for the canonical occupation numbers will remain valid approximately even in the condensate regime, we have

$$z_0^{-1} e^{\beta\epsilon_0} = 1 + \langle n_0 \rangle_{\text{cn}}^{-1}. \tag{34}$$

Hence, we may eliminate the saddle-point  $z_0$  by setting

$$\begin{aligned}
\left(\frac{1}{z_0}\right)^{N+1} &= e^{-(N+1)\beta\epsilon_0} (1 + \langle n_0 \rangle_{\text{cn}}^{-1})^{N+1} \\
&\sim e^{-(N+1)\beta\epsilon_0} e^{N/\langle n_0 \rangle_{\text{cn}}},
\end{aligned} \tag{35}$$

yielding

$$Z_N^{(\text{s.p.})}(\beta) \sim \exp(N/\langle n_0 \rangle_{\text{cn}} - 1 - N\beta\epsilon_0) \prod_{v=1}^{\infty} \frac{1}{1 - \exp(\beta[\epsilon_0 - \epsilon_v])}. \tag{36}$$

The infinite product on the right hand side, describing the excited-states subsystem, equals the canonical partition function of a collection of infinitely many, distinguishable harmonic oscillators with frequencies  $(\epsilon_v - \epsilon_0)/\hbar$  (where  $v=1, 2, 3, \dots$ ), thus leading back to the “oscillator approximation” which has been the starting point for the derivation of the integral representations (13), (14), and (15) in Ref. [15]. In contrast, the value of the present approximation (36) lies in the fact that it is not restricted to the excited states, but also contains the ground state explicitly.

Taking the derivatives with respect to  $-\beta\varepsilon_\alpha$ , with  $\alpha \neq 0$ , one then finds occupation numbers

$$\begin{aligned}\langle n_\alpha \rangle_{\text{cn}} &= \frac{\partial \ln Z_N^{(\text{s.p.})}}{\partial(-\beta\varepsilon_\alpha)} \\ &= \frac{1}{e^{\beta(\varepsilon_\alpha - \varepsilon_0)} - 1}\end{aligned}\quad (37)$$

and mean-square fluctuations

$$\begin{aligned}\langle \delta^2 n_\alpha \rangle_{\text{cn}} &= \frac{\partial^2 \ln Z_N^{(\text{s.p.})}}{\partial(-\beta\varepsilon_\alpha)^2} \\ &= \langle n_\alpha \rangle_{\text{cn}} (\langle n_\alpha \rangle_{\text{cn}} + 1)\end{aligned}\quad (38)$$

of the excited states, while differentiating the logarithm of Eq. (36) with respect to  $-\beta\varepsilon_0$  produces first the obvious identity

$$\langle n_0 \rangle_{\text{cn}} = N - \sum_{\nu=1}^{\infty} \langle n_\nu \rangle_{\text{cn}} \quad (39)$$

and then the important equation

$$\langle \delta^2 n_0 \rangle_{\text{cn}} = \sum_{\nu=1}^{\infty} \langle \delta^2 n_\nu \rangle_{\text{cn}}; \quad (40)$$

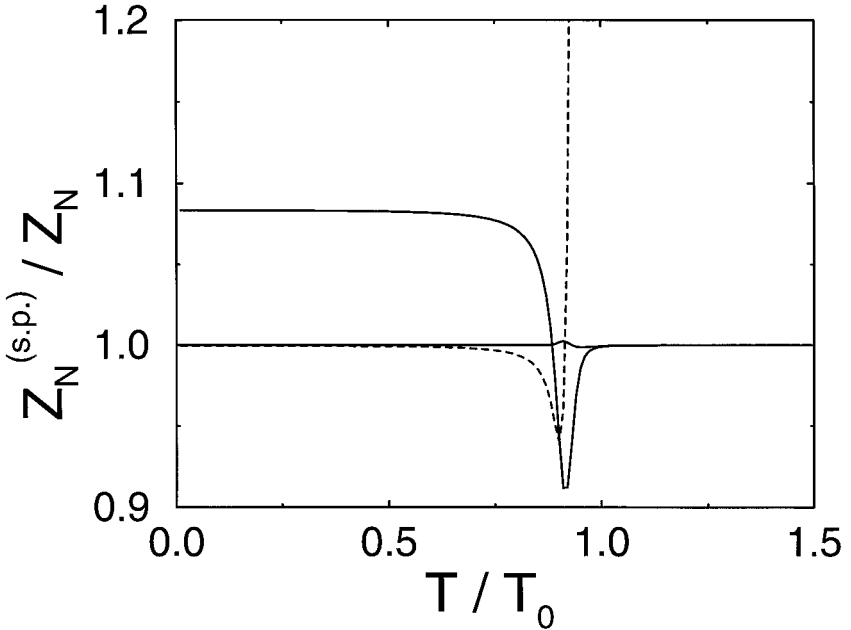
stating that, in the condensate regime and subject to the above approximations, within the canonical ensemble the occupation numbers of the excited states are *uncorrelated* stochastic variables [11, 12, 15].

Remarkably, the error one would have committed had one naively employed the standard approximation (7) in the condensate regime, and which can be quantified only now, is not devastating. As explained in Appendix B (cf. Eq. (B11)), *in the low-temperature, large- $N$ -regime the incorrect partition function  $\tilde{Z}_N^{(\text{s.p.})}(\beta)$  exceeds the correct partition function by merely the temperature-independent factor  $1/R_1 \approx 1.08444$ , regardless of the single-particle spectrum*, that is, regardless of the trapping potential—implying that the error might even go unnoticed when carelessly taking derivatives of  $\ln \tilde{Z}_N^{(\text{s.p.})}(\beta)$ . This finding is illustrated in Fig. 3, again for an ideal Bose gas with  $N=1000$  particles in a three-dimensional isotropic harmonic potential. The figure shows the ratios of  $\tilde{Z}_N^{(\text{s.p.})}(\beta)$ , computed according to the scheme (7), of the correct approximation (26), and of its condensate descendant (33), to the exact canonical partition function, the latter having been obtained from the

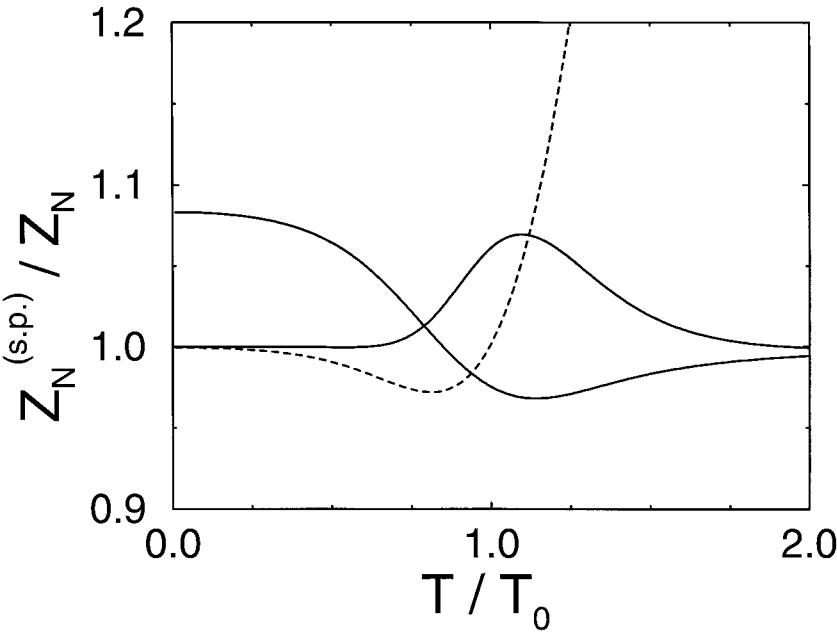
one-particle partition function  $Z_1(\beta)$  by means of the familiar recursion formula [19, 23–26]

$$Z_N(\beta) = \frac{1}{N} \sum_{k=1}^N Z_1(k\beta) Z_{N-k}(\beta), \quad Z_0(\beta) \equiv 1. \quad (41)$$

As witnessed by Fig. 3, the quality of the proper approximation (26) is outstanding for all temperatures, its low-temperature variant (33) performs bravely where it is expected to, and the standard approximation (7) is good at high temperatures, but fails by the predicted factor  $1/R_1$  in the condensate regime. For comparison, Fig. 4 shows the corresponding data for the one-dimensional case; here the exact  $N$ -particle partition function is known in closed form [27, 28]. We find features that are qualitatively similar to those in the preceding figure, although, with  $N=1000$ , the approximation (26) is not quite as good at intermediate  $T$ . The standard scheme (7) again is off by the same, universal factor  $1/R_1$  at low temperatures.



**FIG. 3.** Ratio of the standard saddle-point result (7) (solid line approaching the value  $1/R_1 \approx 1.08444$  at low temperatures), of the proper approximation (26) (solid line everywhere close to unity), and of its low-temperature descendant (33) (dashed line), to the *exact* canonical partition function  $Z_N(\beta)$ , for a gas of  $N=1000$  ideal Bose particles in a three-dimensional isotropic harmonic potential. The reference temperature  $T_0$  is given by Eq. (24). Note the impressive overall performance of the approximation (26).



**FIG. 4.** The same as Fig. 3, now for a gas of  $N=1000$  ideal Bose particles in a one-dimensional harmonic potential. The reference temperature  $T_0$  is given by Eq. (25). Note that for  $T/T_0 \rightarrow 0$  the ratio of the standard approximation (7) and the exact data approaches the same value  $1/R_1 \approx 1.08444$  as met in the three-dimensional case.

B. Canonical Occupation Numbers

The derivation of the expressions (37) and (39) from the condensate approximation (33) to the canonical partition function serves to render that partition function plausible, but it is not the best one can do, since we have simply *assumed* the validity of Eq. (34). An accurate and fully consistent computation of these occupation numbers starts from the identity

$$\begin{aligned} \langle n_\alpha \rangle_{\text{cn}} &= \frac{\partial}{\partial(-\beta \varepsilon_\alpha)} \ln Z_N(\beta) \\ &= \frac{1}{Z_N(\beta)} \frac{1}{2\pi i} \oint dz \frac{1}{z^N} \prod_{v=0}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_v)} \frac{\exp(-\beta \varepsilon_\alpha)}{1 - z \exp(-\beta \varepsilon_\alpha)} \\ &\equiv \frac{1}{Z_N(\beta)} \frac{1}{2\pi i} \oint dz \exp(-\bar{G}(z)), \end{aligned} \tag{42}$$

with

$$\bar{G}(z) = N \ln z + \sum_{v=0}^{\infty} \ln(1 - ze^{-\beta \varepsilon_v}) + \ln(1 - ze^{-\beta \varepsilon_\alpha}) + \beta \varepsilon_\alpha. \tag{43}$$

The equation that determines the saddle-point  $z_1$  for the new contour integral (42), namely

$$N = \sum_{v=0}^{\infty} \frac{1}{z_1^{-1} e^{\beta \varepsilon_v} - 1} + \frac{1}{z_1^{-1} e^{\beta \varepsilon_\alpha} - 1}, \quad (44)$$

formally looks like the grand canonical relation between particle number  $N$  and fugacity  $z_1$  for a system with an extra energy level  $\varepsilon_\alpha$ . Now we have to distinguish two cases.

If  $\alpha \neq 0$ , we merely have to copy the steps made in the derivation of the proper canonical partition function (26). That is, we separate the ground-state contribution from the exponent  $\bar{G}(z)$  by defining the tempered function

$$G(z) = \bar{G}(z) - \ln(1 - ze^{-\beta \varepsilon_0}), \quad (45)$$

and obtain

$$\begin{aligned} \frac{\partial}{\partial(-\beta \varepsilon_\alpha)} Z_N(\beta) &= \frac{1}{2\pi i} \oint dz \frac{\exp(-G(z))}{1 - ze^{-\beta \varepsilon_0}} \\ &\sim \exp(\beta \varepsilon_0 - G^{(0)} - 1), \end{aligned} \quad (46)$$

proceeding at once to temperatures below the onset of condensation. Then Eq. (42), together with the previous result (33) for  $Z_N(\beta)$ , yields the expression

$$\langle n_\alpha \rangle_{\text{cn}} = \exp(F(z_0) - G(z_1)) \quad (\alpha \neq 0) \quad (47)$$

for the canonical occupation numbers of the excited states in the condensate regime. This accurate result is well approximated by the previous formula (37): Since the level that has artificially been doubled differs from the ground state, we may set  $z_0 \approx z_1 \approx e^{\beta \varepsilon_0}$  in Eq. (47), and obtain

$$\begin{aligned} \langle n_\alpha \rangle_{\text{cn}} &\approx \exp(\ln z_0 - \ln(1 - z_0 e^{-\beta \varepsilon_\alpha}) - \beta \varepsilon_\alpha) \\ &\approx \frac{1}{e^{\beta(\varepsilon_\alpha - \varepsilon_0)} - 1}, \end{aligned} \quad (48)$$

using the definitions (16) and (45) of the functions  $F$  and  $G$ .

If, however,  $\alpha = 0$ , the exponent  $\bar{G}(z)$  in Eq. (42) corresponds to a system with a doubled ground state. Hence, we have to temper this function accordingly, and define

$$G(z) = \bar{G}(z) - \ln(e^{\beta \varepsilon_0} [1 - ze^{-\beta \varepsilon_0}]^2). \quad (49)$$

This leads to

$$\begin{aligned}\frac{\partial}{\partial(-\beta\varepsilon_0)}Z_N(\beta)&=\frac{1}{2\pi i}\oint dz\frac{\exp(-G(z)-\beta\varepsilon_0)}{(1-ze^{-\beta\varepsilon_0})^2}\\&\sim\frac{2}{e^{\beta\varepsilon_0}-z_1}\exp(\beta\varepsilon_0-G^{(0)}-2),\end{aligned}\tag{50}$$

where we have employed the condensate approximation (B9) to the general saddle-point formula (A14), with  $\sigma=2$ . Thus, in the condensate regime the canonical ground-state occupation number is given by

$$\langle n_0 \rangle_{\text{cn}} = \frac{2}{z_1^{-1}e^{\beta\varepsilon_0}-1}\exp(F(z_0)-G(z_1)-1-\ln z_1).\tag{51}$$

For showing that this cumbersome expression actually is consistent with the familiar grand-canonical result in the large- $N$ -limit, we now have to carefully keep track of the two different parameters  $z_0$  and  $z_1$ . That is, we may set

$$\frac{1}{z_0^{-1}e^{\beta\varepsilon_0}-1}\approx\langle n_0 \rangle_{\text{cn}},\tag{52}$$

whereas

$$\frac{1}{z_1^{-1}e^{\beta\varepsilon_0}-1}\approx\frac{\langle n_0 \rangle_{\text{cn}}}{2},\tag{53}$$

reflecting the double appearance of the ground state in Eq. (44). Hence, the argument of the exponential in the ground-state occupation formula (51) should be approximately equal to zero. This follows by observing

$$\begin{aligned}F(z_0)-G(z_1)-1-\ln z_1&=(N+1)\ln\frac{z_0}{z_1}-1+\sum_{v=1}^\infty\ln\left(\frac{1-z_0e^{-\beta\varepsilon_v}}{1-z_1e^{-\beta\varepsilon_v}}\right)\\&\approx(N+1)\ln\frac{z_0}{z_1}-1-\left(1-\frac{z_1}{z_0}\right)\sum_{v=1}^\infty\frac{1}{z_0^{-1}e^{\beta\varepsilon_0}-1}\\&=(N+1)\ln\frac{z_0}{z_1}-1-\left(1-\frac{z_1}{z_0}\right)(N+1-\langle n_0 \rangle_{\text{cn}}),\end{aligned}\tag{54}$$

which, upon inserting

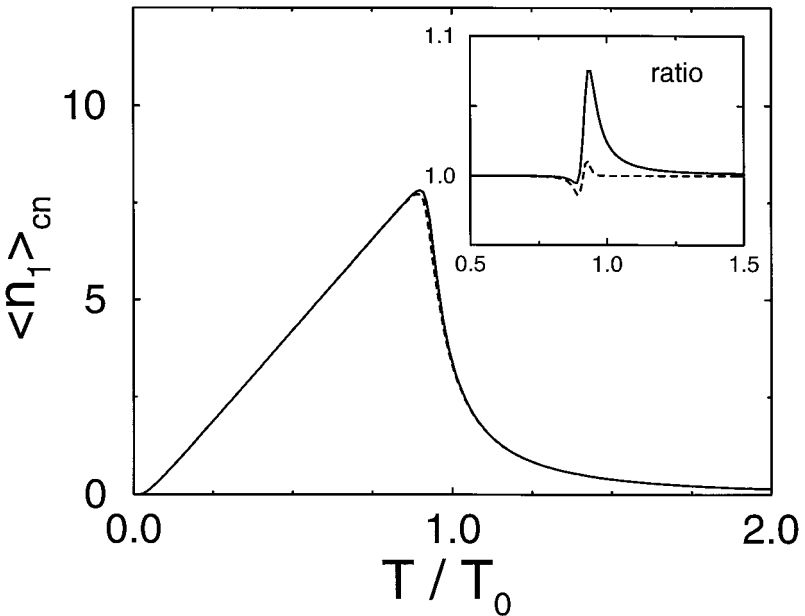
$$\frac{z_0}{z_1}\approx 1+\frac{1}{\langle n_0 \rangle_{\text{cn}}}\tag{55}$$



as obtained from Eqs. (52) and (53), indeed gives the required relation

$$F(z_0) - G(z_1) - 1 - \ln z_1 \approx 0. \quad (56)$$

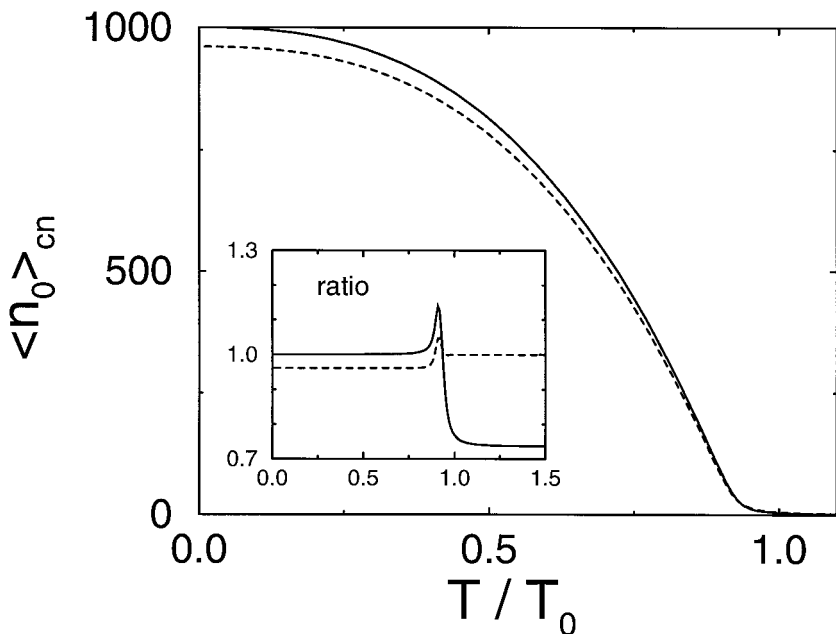
For demonstrating the accuracy of the canonical formulas (47) and (51), we resort once more to a gas of  $N=1000$  ideal Bose particles in a three-dimensional harmonic oscillator potential. Figure 5 shows the occupation number  $\langle n_1 \rangle_{\text{cn}}$  as a function of temperature, computed according to Eq. (47), and compares these data to those that are obtained if  $Z_N(\beta)$  and  $\partial Z_N(\beta)/\partial(-\beta\varepsilon_1)$  are naively calculated from the standard saddle-point formula. The inset quantifies the ratios of these approximate occupation numbers to the exact ones, which have again been computed recursively. In the condensate regime, the naive approximation to *both*  $Z_N(\beta)$  and  $\partial Z_N(\beta)/\partial(-\beta\varepsilon_1)$  is off by the same universal factor  $1/R_1$  derived in Appendix B, so that this error cancels when forming their ratio: The standard saddle-point scheme accidentally yields the correct canonical occupation numbers of the excited states both above and below the onset of condensation. On the other



**FIG. 5.** Canonical occupation number  $\langle n_1 \rangle_{\text{cn}}$  as obtained from Eq. (47) (full line), and from the ratio of  $\partial Z_N(\beta)/\partial(-\beta\varepsilon_1)$  to  $Z_N(\beta)$ , both computed from the standard saddle-point formula (dashed line), for  $N=1000$  ideal Bose particles in an isotropic three-dimensional harmonic potential. The inset shows the respective ratios of these approximate occupation numbers to the exact ones. The energy level  $\varepsilon_1$  is three-fold degenerate; the data shown here correspond to an individual state. In this and all following figures, the reference temperature  $T_0$  is given by Eq. (24).

hand, if one uses even at high temperatures the approximations (33) and (46), each of which is correct in the condensate regime only, it follows from Eq. (B14) that the ratio of the individual errors is given by the square root of  $\bar{G}^{(2)}/\bar{F}^{(2)}$ . Since this ratio approaches unity in the large- $N$ , high- $T$ -regime, Eq. (47) actually is correct also at high temperatures.

This accidental correctness is no longer met in the case of the ground-state occupation number  $\langle n_0 \rangle_{\text{cn}}$ , depicted in Fig. 6. Now the error introduced when computing  $\partial Z_N(\beta)/\partial(-\beta\epsilon_0)$  at low temperatures within the standard scheme is given by the factor  $1/R_2$  (see Appendix B), so that the resulting value of  $\langle n_0 \rangle_{\text{cn}}$  is too small by the constant factor  $R_1/R_2 \approx 0.96106$  in the condensate regime, whereas Eq. (51) yields the correct data. Outside the condensate regime the standard approximation becomes correct, whereas Eq. (B14) reveals that the condensate approximation (51) is wrong by the factor  $M_2/M_1 \sim R_2/(R_1\sqrt{2}) \approx 0.73576$ . Needless to say, if one deduces the canonical occupation numbers directly from the ratios of the saddle-point approximations (A14) to the respective contour integrals, instead of invoking their high- and low-temperature limits (B6) and (B9), one obtains expressions that are valid for all temperatures.



**FIG. 6.** Canonical occupation number  $\langle n_0 \rangle_{\text{cn}}$  as obtained from Eq. (51) (full line), and from the ratio of  $\partial Z_N(\beta)/\partial(-\beta\epsilon_0)$  to  $Z_N(\beta)$ , both computed from the standard saddle-point formula (dashed line), for the same system as considered in Fig. 5. The inset shows the respective ratios of these approximate occupation numbers to the exact ones. The error of the standard approximation in the condensate regime is determined by the ratio  $R_1/R_2 \approx 0.96106$ ; the error of the condensate approximation (51) in the high-temperature regime is given by the factor  $R_2/(R_1\sqrt{2}) \approx 0.73576$ .

### C. Canonical Fluctuations

The calculation of the canonical mean-square fluctuations  $\langle \delta^2 n_\alpha \rangle_{\text{cn}}$  of the occupation numbers now directly parallels that of the occupation numbers themselves: Starting from the identity

$$\begin{aligned} \langle \delta^2 n_\alpha \rangle_{\text{cn}} &= \frac{\partial^2 \ln Z_N}{\partial (-\beta \varepsilon_\alpha)^2} \\ &= \frac{1}{Z_N} \frac{\partial Z_N}{\partial (-\beta \varepsilon_\alpha)} - \left( \frac{1}{Z_N} \frac{\partial Z_N}{\partial (-\beta \varepsilon_\alpha)} \right)^2 + \frac{2}{Z_N} \frac{1}{2\pi i} \oint dz \exp(-\bar{H}(z)), \end{aligned} \quad (57)$$

we are left with the task to evaluate the further contour integral

$$\frac{1}{2\pi i} \oint dz \exp(-\bar{H}(z)) \equiv \frac{1}{2\pi i} \oint dz \frac{1}{z^{N-1}} \prod_{v=0}^{\infty} \frac{1}{1 - z \exp(-\beta \varepsilon_v)} \frac{\exp(-2\beta \varepsilon_\alpha)}{[1 - z \exp(-\beta \varepsilon_\alpha)]^2}, \quad (58)$$

where

$$\bar{H}(z) = (N-1) \ln z + \sum_{v=0}^{\infty} \ln(1 - z e^{-\beta \varepsilon_v}) + 2 \ln(1 - z e^{-\beta \varepsilon_\alpha}) + 2\beta \varepsilon_\alpha. \quad (59)$$

As a consequence of the second derivative performed in Eq. (57), the state with energy  $\varepsilon_\alpha$  now has formally been tripled, giving the equation

$$N-1 = \sum_{v=0}^{\infty} \frac{1}{z_2^{-1} e^{\beta \varepsilon_v} - 1} + \frac{2}{z_2^{-1} e^{\beta \varepsilon_\alpha} - 1} \quad (60)$$

for the new saddle-point  $z_2$ . Thus, for  $\alpha \neq 0$  the tempered version of the function  $\bar{H}(z)$  becomes

$$H(z) = \bar{H}(z) - \ln(1 - z e^{-\beta \varepsilon_0}), \quad (61)$$

implying

$$\begin{aligned} \frac{1}{2\pi i} \oint dz \exp(-\bar{H}(z)) &= \frac{1}{2\pi i} \oint dz \frac{\exp(-H(z))}{1 - z e^{-\beta \varepsilon_0}} \\ &\sim \exp(\beta \varepsilon_0 - H^{(0)} - 1) \end{aligned} \quad (62)$$

in the condensate regime; hence

$$\langle \delta^2 n_\alpha \rangle_{\text{cn}} = \langle n_\alpha \rangle_{\text{cn}} - \langle n_\alpha \rangle_{\text{cn}}^2 + 2 \exp(F(z_0) - H(z_2)) \quad (\alpha \neq 0). \quad (63)$$

Setting  $z_0 \approx z_2 \approx e^{\beta\epsilon_0}$ , similar to the reasoning underlying Eq. (48), it can be seen that the third term on the right hand side is close to  $2\langle n_\alpha \rangle_{\text{cn}}^2$ , so that this expression (63) properly reduces to the familiar Eq. (38).

If  $\alpha = 0$ , we disentangle the three-fold ground-state contribution from  $\bar{H}(z)$  by defining

$$H(z) = \bar{H}(z) - \ln(e^{2\beta\epsilon_0}[1 - ze^{-\beta\epsilon_0}]^3), \quad (64)$$

and get

$$\begin{aligned} \frac{1}{2\pi i} \oint dz \exp(-\bar{H}(z)) &= \frac{1}{2\pi i} \oint dz \frac{\exp(-H(z) - 2\beta\epsilon_0)}{(1 - ze^{-\beta\epsilon_0})^3} \\ &\sim \frac{1}{2} \left( \frac{3}{e^{\beta\epsilon_0} - z_2} \right)^2 \exp(\beta\epsilon_0 - H^{(0)} - 3), \end{aligned} \quad (65)$$

employing the condensate approximation (B9) with  $\sigma = 3$ . Therefore, the canonical fluctuation of the number of condensate particles now takes the form

$$\langle \delta^2 n_0 \rangle_{\text{cn}} = \langle n_0 \rangle_{\text{cn}} - \langle n_0 \rangle_{\text{cn}}^2 + \frac{9}{(e^{\beta\epsilon_0} - z_2)^2} \exp(F(z_0) - H(z_2) - 2). \quad (66)$$

We check the results (63) and (66) again for  $N = 1000$  ideal Bosons in an isotropic harmonic oscillator potential. Figure 7 shows the root-mean-square fluctuation  $\langle \delta n_1 \rangle_{\text{cn}} \equiv \langle \delta^2 n_1 \rangle_{\text{cn}}^{1/2}$  as obtained from Eq. (63), and from the standard saddle-point approximations to the three individual terms on the right hand side of the identity (57). For each term we have the same accidental correctness of the standard saddle-point result in the condensate regime, and of the condensate approximation at high temperatures, as already described for the occupation numbers of the excited states; the inset, which depicts the ratios of the two approximations to the recursively calculated exact fluctuation, confirms that either approximation is correct at both high and low temperatures.

In the case of the condensate fluctuation, however, the situation is quite different. As witnessed by the inset in Fig. 8, our formula (66) gives the correct fluctuation of the number of ground-state particles in the condensate regime. Since the canonical mean-square fluctuation  $\langle \delta^2 n_0 \rangle_{\text{cn}}$  has to vanish for zero temperature, when all  $N$  particles occupy the ground state, the third term on the right hand side of Eq. (66) approaches  $N^2 - N$  for  $T \rightarrow 0$ . When naively using the standard saddle-point scheme, the results for the individual terms in Eq. (57) are incorrect by factors  $R_1/R_2$ ,  $(R_1/R_2)^2$ , and  $R_1/R_3$ , respectively, with the universal numbers  $R_\sigma$  determined in Appendix B. Hence, the naive scheme yields spurious mean-square ground-state fluctuations

$$\begin{aligned} \langle \delta^2 n_0 \rangle_{\text{cn}}^{\text{spur}} &= [R_1/R_3 - (R_1/R_2)^2] N^2 + [R_1/R_2 - R_1/R_3] N \\ &\approx 0.02438 N^2 + 0.01304 N \end{aligned} \quad (67)$$

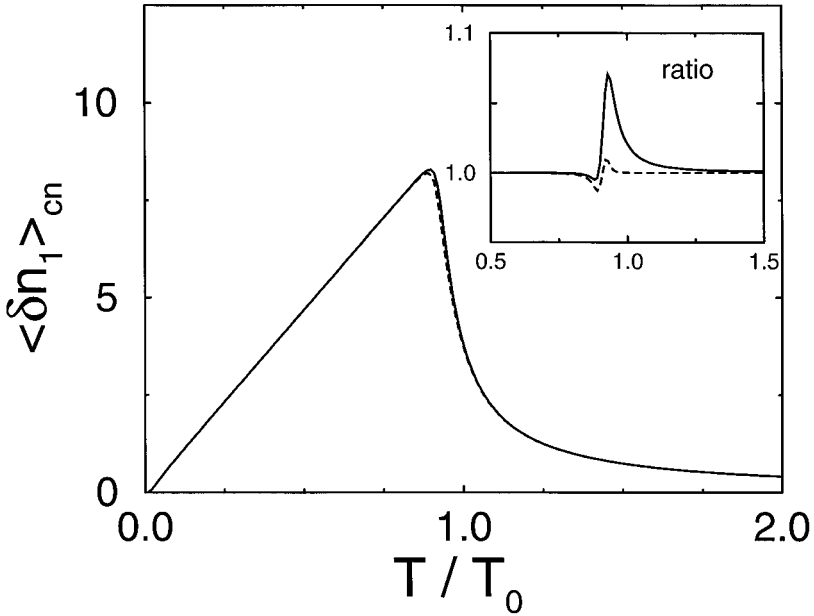
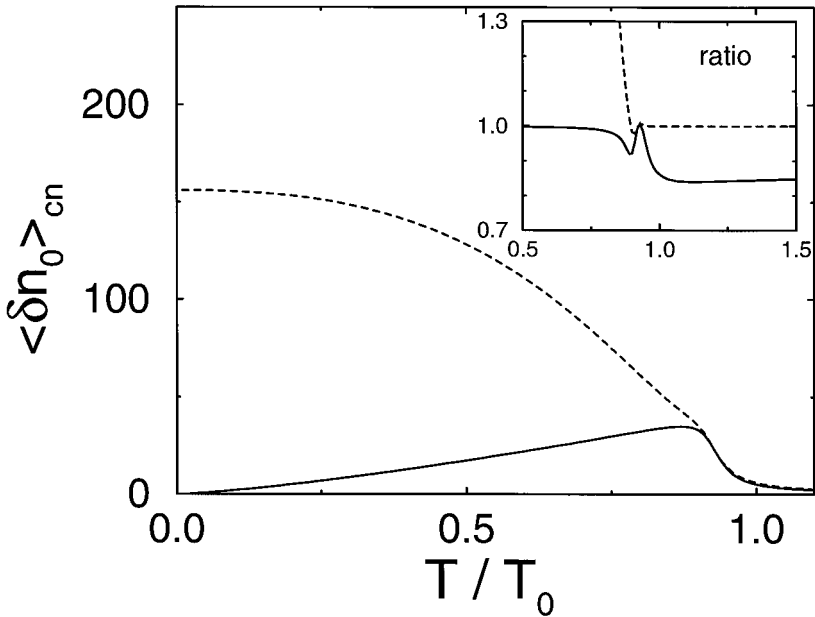


FIG. 7. Canonical r.m.s.-fluctuation  $\langle \delta n_1 \rangle_{\text{cn}}$  as obtained from Eq. (63) (full line), and from the standard saddle-point approximations to the individual terms in Eq. (57) (dashed line), for the same system as considered in Fig. 5. The inset shows the respective ratios of these approximate fluctuations to the recursively computed exact one. As in Fig. 5, the data refer to only one of the three states with energy  $\varepsilon_1$ .

for  $T \rightarrow 0$ , giving, for instance, the incorrect r.m.s.-fluctuation  $\langle \delta n_0 \rangle_{\text{cn}}^{\text{spur}} \approx 156$  for  $N=1000$ , in precise agreement with what is observed in Fig. 8. In the opposite regime, that is, for high temperatures, the standard scheme becomes correct. Then, since  $\langle n_0 \rangle_{\text{cn}} \ll 1$ , the condensate approximation (66) is off by roughly the same factor  $R_2/(R_1 \sqrt{2}) \approx 0.73576$  that also determines the error of  $\langle n_0 \rangle_{\text{cn}}$  itself.

It is now also illuminating to compare the saddle-point scheme developed here to the oscillator approximation that has led in Ref. [15] to the integral representations (13)–(15). This latter approximation cannot cope with the Bose–Einstein transition, that is, its validity remains restricted to the condensate regime, since it rests on the fiction of an infinite reservoir of condensate particles [13]. This very feature, however, is what allows one to derive closed expressions for the condensate fluctuations, provided the pole structure of the spectral Zeta function (12) in the complex  $t$ -plane is known. For an ideal Bose gas in a three-dimensional isotropic harmonic potential, this function can be written in terms of Riemann Zeta functions,

$$Z(\beta, t) = (\beta \hbar \omega)^{-t} \left[ \frac{1}{2} \zeta(t-2) + \frac{3}{2} \zeta(t-1) + \zeta(t) \right], \quad (68)$$

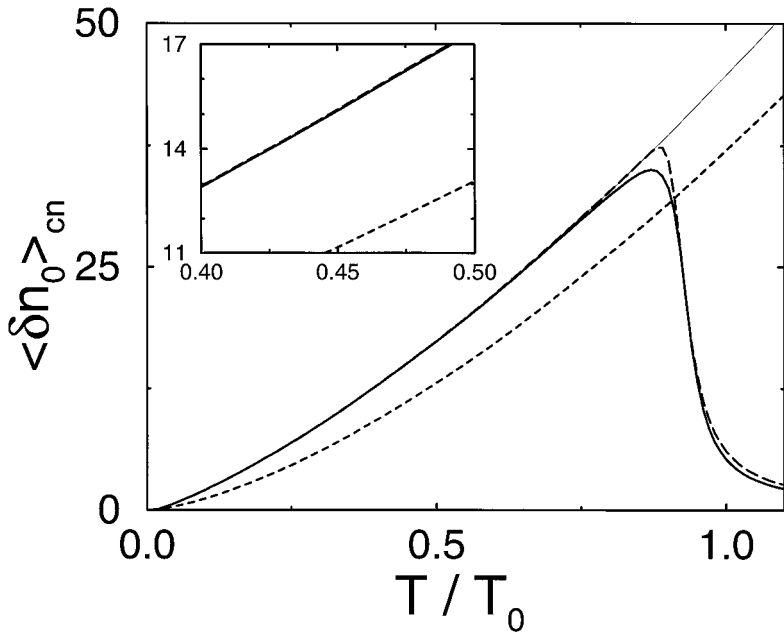


**FIG. 8.** Canonical r.m.s.-fluctuation  $\langle \delta n_0 \rangle_{\text{cn}}$  as obtained from Eq. (66) (full line), and from the standard saddle-point approximations to the individual terms in Eq. (57) (dashed line), for the same system as considered in Fig. 5. The inset shows the respective ratios of these approximate fluctuations to the recursively computed exact one. The error of the standard scheme for  $T \rightarrow 0$  is determined by Eq. (67), whereas the error of the condensate approximation for high temperatures is given by the factor  $(R_2/(R_1 \sqrt{2}))^{1/2} \approx 0.85776$ .

having shifted the ground-state energy to  $\varepsilon_0 = 0$ . Taking into account the three rightmost poles of the product  $\Gamma(t) Z(\beta, t) \zeta(t-1)$ , located at  $t = 3$ ,  $t = 2$ , and  $t = 1$ , Eq. (14) then gives

$$\begin{aligned}
 \langle \delta^2 n_0 \rangle_{\text{cn}} &= \left( \frac{k_B T}{\hbar \omega} \right)^3 \zeta(2) \\
 &+ \left( \frac{k_B T}{\hbar \omega} \right)^2 \left[ \frac{3}{2} \ln \left( \frac{k_B T}{\hbar \omega} \right) + \frac{3}{2} \gamma + \frac{5}{4} + \zeta(2) \right] \\
 &+ \frac{k_B T}{\hbar \omega} \left( -\frac{1}{2} \right)
 \end{aligned} \tag{69}$$

for  $k_B T/(\hbar \omega) \gg 1$ , where  $\gamma \approx 0.57722$  is Euler's constant. In contrast, the saddle-point approach requires the numerical determination of the three saddle-point parameters  $z_0$ ,  $z_1$ , and  $z_2$  from Eqs. (6), (44), and (60), respectively, but this effort is rewarded by the possibility to monitor the fluctuations for all temperatures, including the transition regime. As detailed in Fig. 9, sufficiently below the onset of



**FIG. 9.** Canonical r.m.s-fluctuation  $\langle \delta n_0 \rangle_{\text{cn}}$  for the same system as considered in Fig. 5. The exact, recursively computed fluctuation (long-dashed line) is compared to the data obtained from the saddle-point formula (66) (heavy full line), to the approximation provided by the leading,  $T^3$ -proportional term in Eq. (69) (short-dashed line), and to the prediction made by the oscillator approximation (69) with terms up to order  $T$  (thin line). The inset emphasizes the outstanding accuracy of both the proper saddle-point method and the oscillator approximation.

condensation both the saddle-point approximation (66) and the oscillator approximation (69) yield excellent agreement with the exact condensate fluctuation, even for particle numbers as low as  $N = 1000$ .

### III. THE MICROCANONICAL ENSEMBLE

#### A. The Microcanonical Partition Function

For extending the techniques developed in the previous section to the microcanonical ensemble, we write the grand canonical partition function (1) as

$$\prod_{v=0}^{\infty} \frac{1}{1 - z \exp(-\beta \epsilon_v)} = \sum_{N=0}^{\infty} z^N \sum_E e^{-\beta E} \tilde{\Omega}(E, N), \quad (70)$$

where the microcanonical partition functions  $\tilde{\Omega}(E, N)$  denote the number of microstates accessible to a thermally isolated  $N$ -particle system with total excitation

energy  $E$ . Setting the ground-state energy equal to zero, we now assume that all single-particle energies  $\varepsilon_v$ , and hence also all possible excitation energies, can be represented reasonably well as integer multiples of a basic quantum  $\hbar\omega$ . Introducing the variable

$$x = e^{-\beta\hbar\omega} \quad (71)$$

and writing  $E/(\hbar\omega) = m$ , Eq. (70) takes the form of a double power series,

$$\begin{aligned} \prod_{v=0}^{\infty} \frac{1}{(1 - zx^v)^{g_v}} &= \sum_{N=0}^{\infty} z^N \sum_{m=0}^{\infty} x^m \Omega(m, N) \\ &\equiv \Xi(x, z), \end{aligned} \quad (72)$$

with  $g_v$  indicating the degree of degeneracy of the single-particle energy level  $v\hbar\omega$ , and  $\Omega(m, N) \equiv \tilde{\Omega}(m\hbar\omega, N)$ . With the help of two suitable contours which encircle the origin of the complex  $x$ - and  $z$ -plane, respectively, the desired partition functions can be isolated from this series by means of the identity

$$\begin{aligned} \Omega(m, N) &= \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{1}{x^{m+1} z^{N+1}} \prod_{v=0}^{\infty} \frac{1}{(1 - zx^v)^{g_v}} \\ &\equiv \frac{1}{(2\pi i)^2} \oint dx \oint dz \exp(-\bar{F}(x, z)), \end{aligned} \quad (73)$$

where

$$\bar{F}(x, z) = (m+1) \ln x + (N+1) \ln z + \sum_{v=0}^{\infty} g_v \ln(1 - zx^v). \quad (74)$$

The saddle-point  $(x_0, z_0)$  for the double contour integral (73) now is determined by the simultaneous solution of the two equations

$$\left. \frac{\partial \bar{F}(x, z)}{\partial x} \right|_{x=x_0, z=z_0} = 0, \quad \left. \frac{\partial \bar{F}(x, z)}{\partial z} \right|_{x=x_0, z=z_0} = 0, \quad (75)$$

reading explicitly

$$\begin{aligned} m+1 &= \sum_{v=0}^{\infty} g_v \frac{v}{z_0^{-1} x_0^{-v} - 1} \\ N+1 &= \sum_{v=0}^{\infty} g_v \frac{1}{z_0^{-1} x_0^{-v} - 1}. \end{aligned} \quad (76)$$



As long as the gas is not condensed, we may safely use the standard approximation scheme [8]. That is, we may expand the function (74) quadratically around the saddle-point,

$$\bar{F}(x, z) \approx \bar{F}(x_0, z_0) + \frac{1}{2} \bar{F}^{(2,0)}(x - x_0)^2 + \bar{F}^{(1,1)}(x - x_0)(z - z_0) + \frac{1}{2} \bar{F}^{(0,2)}(z - z_0)^2 \quad (77)$$

with

$$\bar{F}^{(r,s)} \equiv \frac{\partial^{r+s} \bar{F}(x, z)}{\partial x^r \partial z^s} \bigg|_{x=x_0, z=z_0},$$

substitute  $x - x_0 = iw$  and  $z - z_0 = iu$ , and get

$$\begin{aligned} \Omega(m, N) &\sim \frac{1}{(2\pi)^2} \exp(-\bar{F}(x_0, z_0)) \\ &\quad \times \int_{-\infty}^{+\infty} dw \int_{-\infty}^{+\infty} du \exp\left(\frac{1}{2} \bar{F}^{(2,0)} w^2 + \bar{F}^{(1,1)} wu + \frac{1}{2} \bar{F}^{(0,2)} u^2\right) \\ &= \frac{1}{2\pi\sqrt{D}} \exp(-\bar{F}(x_0, z_0)), \end{aligned} \quad (78)$$

where  $D$  is the functional determinant

$$D = \det \begin{pmatrix} \bar{F}^{(2,0)} & \bar{F}^{(1,1)} \\ \bar{F}^{(1,1)} & \bar{F}^{(0,2)} \end{pmatrix} = \bar{F}^{(2,0)} \bar{F}^{(0,2)} - (\bar{F}^{(1,1)})^2. \quad (79)$$

For temperatures below the onset of condensation, however, this procedure is invalid, because then the second of the saddle-point equations (76) dictates that  $z_0$  differs from the ground-state singularity  $z = 1$  of the grand canonical partition function (72) merely by a quantity of order  $O(1/N)$ , exactly as in the canonical case. Hence, we have to proceed according to the insight accumulated there for computing  $\Omega(m, N)$  in the condensate regime, and have to exempt the ground-state factor from the quadratic expansion: Defining

$$F(x, z) = \bar{F}(x, z) - \ln(1 - z), \quad (80)$$

we have to start from the representation

$$\Omega(m, N) = \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{\exp(-F(x, z))}{1 - z}. \quad (81)$$

The expansion of the tempered function  $F(x, z)$  around  $(x_0, z_0)$  then yields

$$\begin{aligned} F(x, z) \approx & F(x_0, z_0) + \tfrac{1}{2}F^{(2,0)}(x-x_0)^2 \\ & + [F^{(0,1)} + F^{(1,1)}(x-x_0)](z-z_0) + \tfrac{1}{2}F^{(0,2)}(z-z_0)^2, \end{aligned} \tag{82}$$

where we have used

$$F^{(1,0)} = 0. \tag{83}$$

It is now of key interest to compare the magnitude of the two terms in the square brackets of Eq. (82), which constitute the coefficient of  $(z-z_0)$ . On the one hand, we have

$$F^{(0,1)} = -\frac{\partial}{\partial z} \ln(1-z)|_{z=z_0} = \frac{1}{1-z_0}; \tag{84}$$

hence  $F^{(0,1)} = O(N)$  in the condensate regime. On the other hand, relevant contributions to the integral over  $x$  are collected from an interval of order  $O(1/\sqrt{-F^{(2,0)}})$  around  $x_0$ . Thus, the relevant  $F^{(1,1)}(x-x_0)$  are on the order of  $F^{(1,1)}/\sqrt{-F^{(2,0)}}$ , with

$$\begin{aligned} F^{(1,1)} &= -\sum_{\nu=1}^\infty g_\nu \frac{\nu x_0^{\nu-1}}{(1-z_0 x_0^\nu)^2}, \\ F^{(2,0)} &= -\sum_{\nu=1}^\infty g_\nu \frac{\nu^2 z_0 x_0^{\nu-2}}{(1-z_0 x_0^\nu)^2}. \end{aligned} \tag{85}$$

If we focus again on systems of the type (19)—i.e., if both the quantum  $\hbar\omega$  and the weights  $g_\nu$  have been adjusted accordingly—we may repeat the reasoning that has led to the canonical estimate (21), and conclude that both  $F^{(1,1)}$  and  $F^{(2,0)}$  are of the order  $O(N^{2s/d})$ . Therefore,  $F^{(1,1)}(x-x_0) = O(N^{s/d})$  for relevant  $x$ . To be honest, this can be taken as a rather crude guideline only, in the same sense as the quantities  $r_n$  displayed in Fig. 1 have not yet approached the expected value  $1/3$  for  $n=2$ . In fact, numerical calculations for the three-dimensional isotropic harmonic oscillator potential reveal that for reasonably large  $N$  the expression  $F^{(1,1)}/\sqrt{-F^{(2,0)}}$  is about proportional to  $\langle N_{\text{ex}} \rangle_{\text{mc}}^{1/2}$ , the square root of the total number of excited particles in a microcanonical setting, instead of being proportional to  $\langle N_{\text{ex}} \rangle_{\text{mc}}^{1/3}$ . Nonetheless, the above estimate indicates that for  $d/s > 1$  and large  $N$  we may neglect  $F^{(1,1)}(x-x_0)$  against  $F^{(0,1)}$ . This implies a drastic simplification of the analysis, because then the remaining saddle-point integral factorizes: Leading both contours parallel to the respective imaginary axis over the saddle, we are left with

$$\Omega(m, N) \sim \frac{\exp(-F(x_0, z_0))}{2\pi i} \int_{x_0 - i\infty}^{x_0 + i\infty} dx \exp\left(-\frac{1}{2}F^{(2,0)}(x - x_0)^2\right) \\ \times \frac{1}{2\pi i} \int_{z_0 - i\infty}^{z_0 + i\infty} dz \frac{\exp(-F^{(0,1)}(z - z_0) - \frac{1}{2}F^{(0,2)}(z - z_0)^2)}{1 - z}. \quad (86)$$

The first of these integrals is standard, the second is precisely of the type worked out in Appendices A and B. Thus, without any further labor we obtain

$$\Omega(m, N) \sim \frac{\exp(-F(x_0, z_0) - 1)}{\sqrt{-2\pi F^{(2,0)}}}, \quad (87)$$

the saddle-point approximation to the microcanonical partition functions in the condensate regime.

### B. Microcanonical Occupation Numbers and Their Fluctuations

The computation of microcanonical occupation numbers  $\langle n_\alpha \rangle_{\text{mc}}$  in the condensate regime is a matter of routine by now, so we merely need to sketch the main steps. Denoting the number of microstates of an isolated  $N$ -particle system with total excitation energy  $m\hbar\omega$  and with exactly  $n_\alpha$  particles occupying a given single-particle state with energy  $\alpha\hbar\omega$  as  $\Gamma_\alpha(n_\alpha; m, N)$ , we have

$$\sum_{n_\alpha=0}^N \Gamma_\alpha(n_\alpha; m, N) = \Omega(m, N) \quad (88)$$

and

$$\langle n_\alpha \rangle_{\text{mc}} = \frac{\sum_{n_\alpha=0}^N n_\alpha \Gamma_\alpha(n_\alpha; m, N)}{\Omega(m, N)}. \quad (89)$$

Introducing the symbol  $\bar{\partial}/\partial(x^\alpha)$ , where the overbar is meant to indicate that the partial derivative acts on only *one* of the  $g_\alpha$ -fold degenerate states with energy  $\alpha\hbar\omega$ , the first microcanonical moments are generated from the grand canonical partition function (72) by means of the identity

$$x^\alpha \frac{\bar{\partial}}{\partial(x^\alpha)} \Xi(x, z) = \sum_{N=0}^{\infty} z^N \sum_{m=0}^{\infty} x^m \left( \sum_{n_\alpha=0}^N n_\alpha \Gamma_\alpha(n_\alpha; m, N) \right). \quad (90)$$

Hence,

$$\sum_{n_\alpha=0}^N n_\alpha \Gamma_\alpha(n_\alpha; m, N) = \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{x^\alpha}{x^{m+1} z^{N+1}} \frac{\bar{\partial}}{\partial(x^\alpha)} \Xi(x, z) \\ \equiv \frac{1}{(2\pi i)^2} \oint dx \oint dz \exp(-\bar{G}(x, z)), \quad (91)$$

where

$$\bar{G}(x, z) = (m + 1 - \alpha) \ln x + N \ln z + \sum_{v=0}^{\infty} g_v \ln(1 - zx^v) + \ln(1 - zx^\alpha). \quad (92)$$

The evaluation of the integral (91) first requires the knowledge of its saddle-point  $(x_1, z_1)$ , obtained by simultaneously solving the two equations

$$\begin{aligned} m + 1 - \alpha &= \sum_{v=0}^{\infty} g_v \frac{v}{z_1^{-1} x_1^{-v} - 1} + \frac{\alpha}{z_1^{-1} x_1^{-\alpha} - 1}, \\ N &= \sum_{v=0}^{\infty} g_v \frac{1}{z_1^{-1} x_1^{-v} - 1} + \frac{1}{z_1^{-1} x_1^{-\alpha} - 1}. \end{aligned} \quad (93)$$

If then  $\alpha \neq 0$ , we define the tempered function

$$G(x, z) = \bar{G}(x, z) - \ln(1 - z), \quad (94)$$

yielding

$$\begin{aligned} \sum_{n_x=0}^N n_x \Gamma_\alpha(n_x; m, N) &= \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{\exp(-G(x, z))}{1 - z} \\ &\sim \frac{\exp(-G(x_1, z_1) - 1)}{\sqrt{-2\pi G^{(2,0)}}} \end{aligned} \quad (95)$$

in direct analogy to Eq. (87), with

$$G^{(2,0)} = - \sum_{v=1}^{\infty} g_v \frac{v^2 z_1 x_1^{v-2}}{(1 - z_1 x_1^v)^2} - \frac{\alpha^2 z_1 x_1^{\alpha-2}}{(1 - z_1 x_1^\alpha)^2}. \quad (96)$$

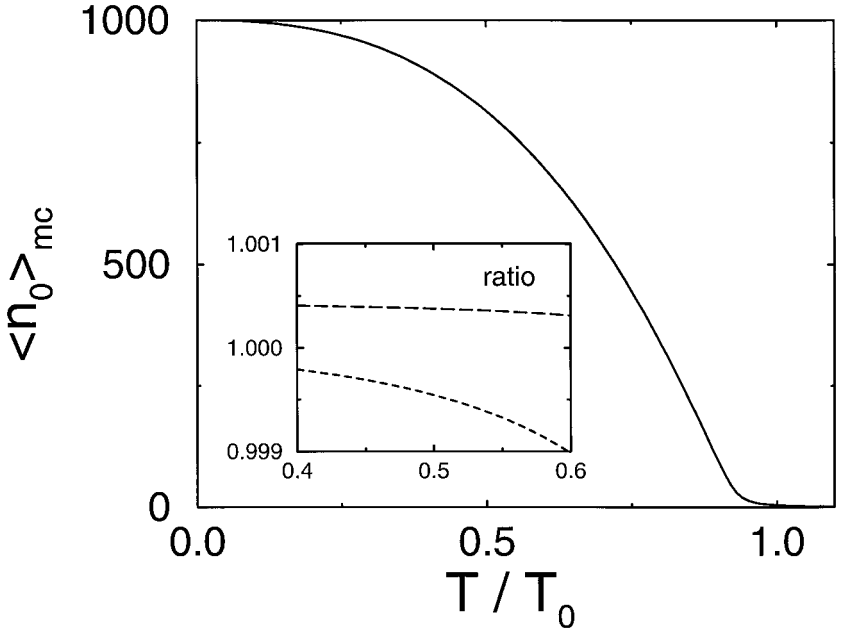
If, however,  $\alpha = 0$ , we have to account for ground-state doubling. In this case we define

$$G(x, z) = \bar{G}(x, z) - 2 \ln(1 - z) \quad (97)$$

and invoke Eq. (B9) with  $\sigma = 2$ , resulting in

$$\begin{aligned} \sum_{n_0=0}^N n_0 \Gamma_0(n_0; m, N) &= \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{\exp(-G(x, z))}{(1 - z)^2} \\ &\sim \frac{2}{1 - z_1} \frac{\exp(-G(x_1, z_1) - 2)}{\sqrt{-2\pi G^{(2,0)}}}. \end{aligned} \quad (98)$$

To give at least one application of these formulas, Fig. 10 shows the microcanonical ground-state occupation number  $\langle n_0 \rangle_{\text{mc}}$  as a function of the microcanonical temperature for  $N = 1000$  ideal Bose particles in an isotropic harmonic oscillator potential, as computed from Eqs. (87) and (98) according to Eq. (89). The



**FIG. 10.** Microcanonical ground-state occupation number  $\langle n_0 \rangle_{mc}$  for a gas of  $N=1000$  ideal Bosons in a three-dimensional isotropic harmonic oscillator potential, as computed from the saddle-point approximations (87) and (98). The inset shows the ratio  $\langle n_0 \rangle_{cn}/\langle n_0 \rangle_{gc}$  of the canonical to the grand canonical occupation numbers (short dashes; with exact, recursively computed canonical data), and the ratio  $\langle n_0 \rangle_{mc}/\langle n_0 \rangle_{gc}$  of the microcanonical to the grand canonical values (long dashes).

microcanonical temperature does not differ significantly from the canonical one [8]; the inset quantifies the ratio of canonical to grand canonical, and of microcanonical to grand canonical occupation numbers. As expected, the relative differences between the ground-state occupation numbers in the three ensembles are on the order of  $1/N$ .

For calculating the corresponding microcanonical mean-square fluctuations  $\langle \delta^2 n_\alpha \rangle_{mc}$  within the saddle-point approximation, we exploit the identity

$$\begin{aligned} \left( x^\alpha \frac{\bar{\partial}}{\partial(x^\alpha)} \right)^2 \Xi(x, z) &= x^\alpha \frac{\bar{\partial}}{\partial(x^\alpha)} \Xi(x, z) + x^{2\alpha} \frac{\bar{\partial}^2}{\partial(x^\alpha)^2} \Xi(x, z) \\ &= \sum_{N=0}^{\infty} z^N \sum_{m=0}^{\infty} x^m \left( \sum_{n_\alpha=0}^N n_\alpha^2 \Gamma_\alpha(n_\alpha; m, N) \right) \end{aligned} \quad (99)$$

which immediately leads to the analogue of Eq. (57), namely

$$\langle \delta^2 n_\alpha \rangle_{mc} = \langle n_\alpha \rangle_{mc} - \langle n_\alpha \rangle_{mc}^2 + \frac{2}{\Omega(m, N)} \frac{1}{(2\pi i)^2} \oint dx \oint dz \exp(-\bar{H}(x, z)). \quad (100)$$

The newly appearing integral is defined by

$$\begin{aligned} & \frac{1}{(2\pi i)^2} \oint dx \oint dz \exp(-\bar{H}(x, z)) \\ & \equiv \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{(1/2) x^{2\alpha}}{x^{m+1} z^{N+1}} \frac{\bar{\partial}^2}{\partial(x^\alpha)^2} \Xi(x, z), \end{aligned} \quad (101)$$

giving

$$\bar{H}(x, z) = (m+1-2\alpha) \ln x + (N-1) \ln z + \sum_{v=0}^{\infty} g_v \ln(1-zx^v) + 2 \ln(1-zx^\alpha). \quad (102)$$

Hence, its saddle-point  $(x_2, z_2)$  is found by simultaneously solving the two equations

$$\begin{aligned} m+1-2\alpha &= \sum_{v=0}^{\infty} g_v \frac{v}{z_2^{-1} x_2^{-v} - 1} + \frac{2\alpha}{z_2^{-1} x_2^{-\alpha} - 1}, \\ N-1 &= \sum_{v=0}^{\infty} g_v \frac{1}{z_2^{-1} x_2^{-v} - 1} + \frac{2}{z_2^{-1} x_2^{-\alpha} - 1}. \end{aligned} \quad (103)$$

The usual distinction follows: If  $\alpha \neq 0$ , extracting the ground-state contribution from the function (102) means introducing

$$H(x, z) = \bar{H}(x, z) - \ln(1-z), \quad (104)$$

resulting in

$$\frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{\exp(-H(x, z))}{1-z} \sim \frac{\exp(-H(x_2, z_2) - 1)}{\sqrt{-2\pi H^{(2,0)}}} \quad (105)$$

with

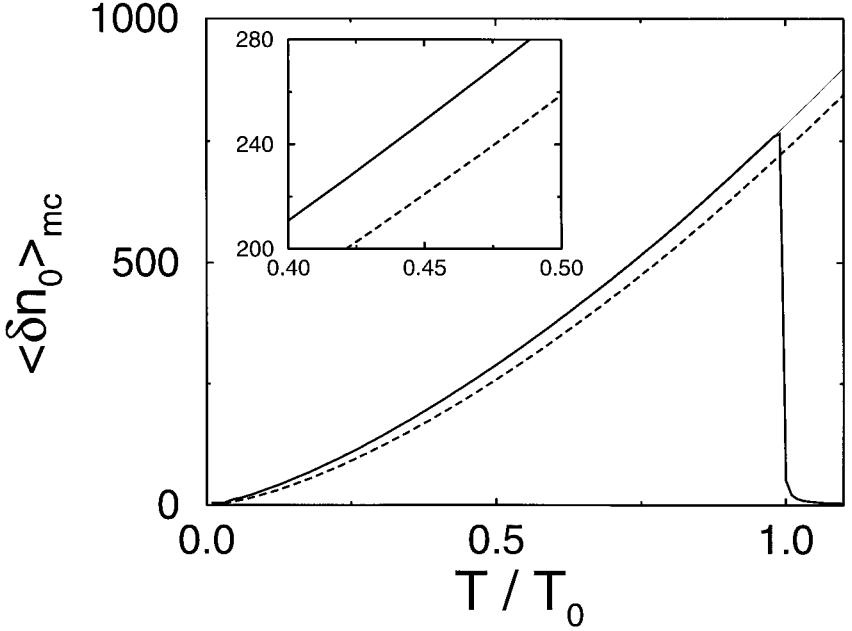
$$H^{(2,0)} = - \sum_{v=1}^{\infty} g_v \frac{v^2 z_2 x_2^{v-2}}{(1-z_2 x_2^v)^2} - 2 \frac{\alpha^2 z_2 x_2^{\alpha-2}}{(1-z_2 x_2^\alpha)^2}. \quad (106)$$

If  $\alpha = 0$ , we define instead

$$H(x, z) = \bar{H}(x, z) - 3 \ln(1-z), \quad (107)$$

and invoke Eq. (B9) once more, now for  $\sigma = 3$ , to arrive at

$$\begin{aligned} & \frac{1}{(2\pi i)^2} \oint dx \oint dz \frac{\exp(-H(x, z))}{(1-z)^3} \\ & \sim \frac{1}{2} \frac{9}{(1-z_2)^2} \frac{\exp(-H(x_2, z_2) - 3)}{\sqrt{-2\pi H^{(2,0)}}}. \end{aligned} \quad (108)$$



**FIG. 11.** Microcanonical r.m.s.-condensate fluctuation  $\langle \delta n_0 \rangle_{\text{mc}}$  for a gas of  $N = 10^6$  ideal Bosons in a three-dimensional isotropic harmonic potential, as computed from the saddle-point approximation (full line). The dashed line corresponds to only the leading term of the oscillator approximation, cf. Eq. (110); the thin line, visible only in the upper right corner, also takes the next-to-leading term into account. Even in the inset, the result of the saddle-point calculation is indistinguishable from this oscillator approximation.

Collecting the results (87), (95), and (105) for  $\alpha \neq 0$ , or (87), (98), and (108) for  $\alpha = 0$ , Eq. (100) then allows one to determine the fluctuations. An example for such a calculation is depicted in Fig. 11: The heavy solid line is the root-mean-square fluctuation  $\langle \delta n_0 \rangle_{\text{mc}} \equiv \langle \delta^2 n_0 \rangle_{\text{mc}}^{1/2}$  as obtained from the above saddle-point scheme for a gas of  $10^6$  ideal Bosons in the usual isotropic oscillator potential. For comparison, when evaluating for the same system the formula (15) for the difference  $\langle \delta^2 n_0 \rangle_{\text{cn}} - \langle \delta^2 n_0 \rangle_{\text{mc}}$  up to terms of the order  $k_B T / (\hbar \omega)$ , one finds

$$\begin{aligned}
 & \langle \delta^2 n_0 \rangle_{\text{cn}} - \langle \delta^2 n_0 \rangle_{\text{mc}} \\
 &= \left( \frac{k_B T}{\hbar \omega} \right)^3 \frac{3}{4} \frac{\zeta^2(3)}{\zeta(4)} \\
 &+ \left( \frac{k_B T}{\hbar \omega} \right)^2 \left[ \frac{3}{2} \frac{\zeta(2) \zeta(3)}{\zeta(4)} - \frac{9}{16} \frac{\zeta^3(3)}{\zeta^2(4)} \right] \\
 &+ \frac{k_B T}{\hbar \omega} \frac{\zeta(3)}{2 \zeta(4)} \left[ \ln \left( \frac{k_B T}{\hbar \omega} \right) + \gamma + \frac{5}{24} + \frac{27}{32} \frac{\zeta^3(3)}{\zeta^2(4)} - \frac{5}{2} \frac{\zeta(2) \zeta(3)}{\zeta(4)} + \frac{3}{2} \frac{\zeta^2(2)}{\zeta(3)} \right]. \quad (109)
 \end{aligned}$$

This, together with Eq. (69), yields a closed expression for the microcanonical condensate fluctuations of an ideal Bose gas in a three-dimensional isotropic harmonic trap in the oscillator approximation, that is, under the assumption of an infinite reservoir of condensate particles:

$$\begin{aligned} \langle \delta^2 n_0 \rangle_{\text{mc}} \approx & 0.64366 \left( \frac{k_B T}{\hbar \omega} \right)^3 + \left[ 1.5 \ln \left( \frac{k_B T}{\hbar \omega} \right) + 1.85443 \right] \left( \frac{k_B T}{\hbar \omega} \right)^2 \\ & - \left[ 0.55531 \ln \left( \frac{k_B T}{\hbar \omega} \right) + 0.96969 \right] \frac{k_B T}{\hbar \omega}. \end{aligned} \quad (110)$$

The dashed line in Fig. 11 corresponds to the leading term of this approximation [13], whereas the thin line also takes the next-to-leading order into account. Even for  $10^6$  particles, finite-size effects are still visible in the condensate fluctuation; the leading-order term of Eq. (110) alone yields only modest agreement with the saddle-point result. After accounting for the dominant corrections, the agreement becomes close to perfect: Even on the scale of the inset, the saddle-point result is indistinguishable from the oscillator approximation (110).

#### IV. DISCUSSION

The necessity to abandon the usual saddle-point scheme when exploring canonical or microcanonical statistics of condensed Bose gases with  $N$  particles is brought about by a characteristic dilemma. On the one hand, the approach of the saddle-point to the ground-state singularity at  $z = e^{\beta \epsilon_0}$  of the grand canonical partition function within order  $O(1/N)$  may be taken as the very hallmark of Bose–Einstein condensation; on the other hand, the customary Gaussian approximation requires that intervals of order  $O(1/N)$  around the saddle-point stay clear of singularities. The solution to this problem almost suggests itself: If one exempts the ground-state factor of the grand canonical partition function from the Gaussian expansion and treats that factor exactly, but proceeds as usual otherwise, then the singular point that now decides the fate of the approximation is the one produced by the first excited state at  $z = e^{\beta \epsilon_1}$ . Since the saddle-point remains pinned below  $e^{\beta \epsilon_0}$ , it remains separated from the decisive singularity at  $z = e^{\beta \epsilon_1}$  by an  $N$ -independent gap. This gap is wide enough to get the approximation going if the particle number is sufficiently large, because the required interval of regularity shrinks with increasing  $N$ . The representation (17) of the canonical partition functions can be viewed as the prototype integral expressing this strategy; the other canonical and microcanonical quantities computed in this work constitute nothing but variations of the same mathematical theme.

The success of this amended saddle-point method hinges on the fact that the emerging integrals with singular integrands can be done exactly; as explained in Appendix A, they lead directly to parabolic cylinder functions. Thus, we have



accomplished the two goals set in the Introduction: The results (A14) are easy to use and provide bona fide approximations to partition functions, occupation numbers, and their fluctuations which are valid at all temperatures—not only in the high-temperature limit or in the condensate regime, but also in the critical temperature range that witnesses the onset of condensation. In particular, the sharpness of the drop of the complementary error function contained in the canonical partition function (30) allows one to precisely assess the sharpness of this onset in a Bose gas with a finite, fixed number of particles.

The observation that the interval of regularity claimed by the Gaussian expansion around the saddle-point is of the same order  $O(1/N)$  as the distance of the saddle-point from the ground-state singularity, meaning that the original conflict is not too large, reflects itself in the noteworthy fact that the error of the conventional scheme in the condensate regime is merely a temperature- and system-independent multiplicative constant. The discovery, made in Appendix B, that this constant approaches unity when the multiplicity of the ground-state pole is increased fits in nicely: Increasing that multiplicity amounts to considering a Bose gas with a multiple-degenerate ground state and thus drives the saddle-point away from the ground-state singularity—the occupation number of each individual of the degenerate states is lowered—thereby lessening the error of the naive approach.

It is also of interest to compare the workload implied by the proper saddle-point method to that required by other techniques aiming at canonical or microcanonical statistics. Exact recursion relations like Eq. (41) or their microcanonical analogues are invaluable for treating relatively small samples with not substantially more than about 1000 particles [19, 26], but the computation of, e.g., microcanonical condensate fluctuations by such means for a gas with  $10^6$  Bosons, as presented in Fig. 11, is entirely out of the question. The integral representations (13)–(15), on the other hand, immediately yield analytical expressions for condensate occupation numbers and fluctuations, *provided* the pole structure of the spectral Zeta function (12) is known, but they do not allow one to monitor the system at the onset of condensation. In contrast, saddle-point techniques always require one numerical step—finding the saddle-point as the root of the respective saddle-point equation—, but once this has been done, the formalism yields all quantities of interest, by means of the ever-same formulas, without further hardship. Therefore, we may conclude that despite all reservations [6, 7] piled up in more than half a century since Schubert's incisive comments [5], it really is the saddle-point method which, if executed properly, provides the most powerful approach to the statistical mechanics of isolated, condensed ideal Bose gases.

Having an instrument that reliable and flexible at one's disposal is certainly not merely of mathematical value, but may also have some bearing on experiments with Bose–Einstein condensates of dilute atomic vapors which are now becoming routine. These experiments are mainly done in isolated harmonic traps, in the regime of vapor densities where the atomic interactions, quantified by the  $s$ -wave scattering length  $a$ , can be considered as weak: Denoting the atom mass as  $m$  and the characteristic trap frequency as  $\omega$ , and defining the oscillator length

$L = \sqrt{\hbar/(m\omega)}$  which quantifies the extension of the trap's ground state, one has  $N(a/L)^3 \ll 1$  under typical conditions. For example,  $a = 5.4$  nm for  $^{87}\text{Rb}$  [29], giving  $N(a/L)^3 = 8 \cdot 10^{-3}$  for a sample of  $N = 10^6$  condensate atoms in a shallow trap with  $\omega = 100 \text{ s}^{-1}$ , while  $Na/L = 2 \cdot 10^3$ . These two relations place the system in the Bogoliubov regime, traditionally associated with the notion of a weakly interacting Bose gas. However, it is feasible to prepare even more weakly interacting samples, either by tuning the scattering length with the help of external magnetic fields [30], or by working with spin-polarized atomic hydrogen [31], which features the unusually low triplet scattering length  $a = 0.0648$  nm [32]. Thus,  $a/L = 2.6 \cdot 10^{-6}$  in a harmonic trap with  $\omega = 100 \text{ s}^{-1}$ , so that even for  $N \approx 400\,000$  hydrogen atoms one finds  $Na/L \approx 1$ , indicating the crossover regime from the ideal to the Bogoliubov gas. This crossover should manifest itself, in a non-trivial manner, in the behavior of the condensate fluctuations [33], which also determine what one may aptly term “the minimum linewidth of an atom laser” [34, 35]. It would therefore be of substantial importance to study condensate fluctuations of *very weakly interacting Bose gases*, that is, of systems intermediate between the ideal gas and the Bogoliubov gas, and to probe whether the difference (109) between the canonical and the microcanonical ensemble remains visible there; in general, this difference should show a pronounced dependence on the trap type [15]. In this way, an old, apparently purely academic issue—the non-equivalence of statistical ensembles in the condensate regime—suddenly pops up at the forefront of topical research, in the theory of the atom laser. Seen from the experimental angle, such an enterprise is on the verge of becoming possible; on the theoretical side, the first requirement is a tool for routinely computing ideal condensate fluctuations within the different ensembles, for traps with various geometries. This tool is available now.

## APPENDIX A

### *Accurate Saddle-Point Approximations for Bose-Type Integrals*

In Section II we have met contour integrals of the form

$$I_\sigma \equiv \frac{1}{2\pi i} \oint dz \frac{\exp(-f(z) - (\sigma - 1)\beta\epsilon_0)}{(1 - ze^{-\beta\epsilon_0})^\sigma}, \quad (\text{A1})$$

with positive integer  $\sigma$ , and a saddle-point lying too close to the singularity at  $z = e^{\beta\epsilon_0}$  for the standard approximation (7) to be viable. In this appendix we derive the proper saddle-point approximation to these integrals, following a suggestion by Dingle [10].

Writing, in accordance with our previous notation, the negative logarithm of the full integrand as  $\bar{f}(z)$ ,

$$\bar{f}(z) = f(z) + (\sigma - 1)\beta\epsilon_0 + \sigma \ln(1 - ze^{-\beta\epsilon_0}), \quad (\text{A2})$$

the saddle-point  $z_*$  is determined by the equation

$$\left. \frac{d\bar{f}(z)}{dz} \right|_{z=z_*} = 0. \quad (\text{A3})$$

In the large- $N$ -limit, this equation corresponds to the grand canonical relation between particle number  $N$  and fugacity  $z_*$  for a system with a  $\sigma$ -fold degenerate ground state.

Substituting  $z = z_* + u$ , so that the saddle-point is found at  $u = 0$ , and writing the difference between the singular point and the saddle-point as

$$u_0 \equiv e^{\beta\epsilon_0} - z_*, \quad (\text{A4})$$

we have

$$\bar{f}(z_* + u) = f(z_* + u) - \beta\epsilon_0 + \sigma \ln(u_0 - u) \quad (\text{A5})$$

and

$$I_\sigma = \frac{e^{\beta\epsilon_0}}{2\pi i} \oint du \frac{\exp(-f(z_* + u))}{(u_0 - u)^\sigma}. \quad (\text{A6})$$

Defining  $f^{(n)} \equiv f^{(n)}(z_*)$ , Eqs. (A3) and (A5) immediately yield

$$\begin{aligned} f^{(1)} &= -\sigma \frac{d}{du} \ln(u_0 - u)|_{u=0} \\ &= \frac{\sigma}{u_0}; \end{aligned} \quad (\text{A7})$$

moreover, we require  $f^{(2)} \ll 0$ . Expanding  $f(z_* + u)$  up to second order around the saddle-point—with a first derivative  $f^{(1)}$  which does not, as in the conventional approximation (7), vanish, but instead becomes *large* when  $u_0$  is small, as in the condensate regime—then leading the path of integration over the saddle at  $u = 0$ , we obtain the approximation

$$\begin{aligned} 2\pi i I_\sigma^{(\text{s.p.})} &= (-1)^\sigma \exp(\beta\epsilon_0 - f^{(0)}) \\ &\times \int_{-i\infty}^{+i\infty} du \exp\left(-\frac{\sigma u}{u_0} - \frac{1}{2} f^{(2)} u^2\right) (u - u_0)^{-\sigma}, \end{aligned} \quad (\text{A8})$$

which, upon substituting

$$u = i \frac{v}{\sqrt{-f^{(2)}}} + u_0, \quad (\text{A9})$$

becomes

$$2\pi i I_{\sigma}^{(\text{s.p.})} = (-1)^{\sigma} \exp\left(\beta\varepsilon_0 - f^{(0)} - \sigma + \frac{1}{2}\eta^2\right) \left(\frac{\sqrt{-f^{(2)}}}{i}\right)^{\sigma-1} \times \int_{-\infty+i\eta}^{+\infty+i\eta} dv \exp(i\bar{\eta}v - \frac{1}{2}v^2) v^{-\sigma}, \quad (\text{A10})$$

with

$$\eta \equiv u_0 \sqrt{-f^{(2)}} \quad (\text{A11})$$

$$\bar{\eta} \equiv \eta - \frac{\sigma}{\eta}. \quad (\text{A12})$$

The integral occurring here is closely related to Whittaker's parabolic cylinder function  $D_{-\sigma}(\bar{\eta})$ , namely<sup>1</sup>

$$\int_C dv \exp(i\bar{\eta}v - \frac{1}{2}v^2) v^{-\sigma} = \sqrt{2\pi} i^{-\sigma} e^{-(1/4)\bar{\eta}^2} D_{-\sigma}(\bar{\eta}), \quad (\text{A13})$$

where  $C$  runs from  $-\infty$  to  $+\infty$ , passing  $v=0$  from above. Thus, the saddle-point approximation to the integrals (A1) finally takes the form

$$I_{\sigma}^{(\text{s.p.})} = \frac{1}{\sqrt{2\pi}} (\sqrt{-f^{(2)}})^{\sigma-1} \times \exp\left(\beta\varepsilon_0 - f^{(0)} - \sigma + \frac{1}{2}\eta^2 - \frac{1}{4}\bar{\eta}^2\right) D_{-\sigma}(\bar{\eta}). \quad (\text{A14})$$

## APPENDIX B

### *High- and Low-Temperature Approximations for Bose-Type Integrals*

The approximation (A14) is valid regardless whether or not the saddle-point  $z_*$  lies close to  $e^{\beta\varepsilon_0}$ , that is, for all temperatures. Therefore, it should adopt a more simple form in the condensate regime, where  $z_*^{-1}e^{\beta\varepsilon_0} - 1$  is of the order  $O(\sigma/N)$ , and should merge into the standard saddle-point formula in the high-temperature limit, where  $z_*$  approaches zero.

In the case of high temperatures, the saddle-point moves away from the ground-state singularity; the distance  $u_0$  defined in Eq. (A4) approaches unity,  $u_0 \rightarrow 1$ . Hence, both parameters  $\eta$  and  $\bar{\eta} = \eta - \sigma/\eta$  introduced in Eqs. (A11) and (A12)

<sup>1</sup> This integral representation can be obtained from Eq. (19.5.4) in Ref. [22], observing that the parabolic cylinder function  $U(a, z)$  equals the Whittaker function  $D_{-a-1/2}(z)$ .

adopt large positive values. Then the asymptotic expansion of the parabolic cylinder functions gives [20]

$$D_{-\sigma}(\bar{\eta}) \sim \frac{\exp(-\bar{\eta}^2/4)}{\bar{\eta}^\sigma}; \quad (\text{B1})$$

moreover, we have

$$\frac{1}{2}\eta^2 - \frac{1}{2}\bar{\eta}^2 \sim \sigma. \quad (\text{B2})$$

Observing that, as a consequence of  $u_0 \rightarrow 1$ ,

$$\bar{\eta} \sim \eta \sim \sqrt{-f^{(2)}}, \quad (\text{B3})$$

$$\bar{f}^{(0)} \sim f^{(0)} - \beta\epsilon_0, \quad (\text{B4})$$

$$\bar{f}^{(2)} = f^{(2)} - \sigma u_0^{-2} \sim f^{(2)}, \quad (\text{B5})$$

we find

$$\begin{aligned} I_\sigma^{(\text{s.p.})} &\sim \frac{1}{\sqrt{-2\pi f^{(2)}}} \exp(\beta\epsilon_0 - f^{(0)}) \\ &\sim \frac{\exp(-\bar{f}^{(0)})}{\sqrt{-2\pi \bar{f}^{(2)}}}. \end{aligned} \quad (\text{B6})$$

This is just the expected result: For high temperatures, i.e., when  $z_*$  stays sufficiently far away from  $e^{\beta\epsilon_0}$ , we recover the formula provided by the usual approximation scheme (7).

In the opposite limit, that is, in the condensate regime, we infer  $\sqrt{-f^{(2)}} = O(N^{\xi(2)/2})$  from Eq. (22), whereas  $u_0$  is of order  $O(\sigma/N)$ . Since  $\xi(2)/2 = \max\{1/2, s/d\}$  for systems of the type (19), and we have required  $s/d < 1$ , we find that  $u_0$  goes to zero faster than  $\sqrt{-f^{(2)}}$  increases when  $N$  becomes large. Hence,  $\eta = u_0 \sqrt{-f^{(2)}}$  approaches zero for large  $N$ . This, in turn, implies that the argument  $\bar{\eta}$  of the parabolic cylinder functions now is a large negative number, so that [20]

$$D_{-\sigma}(\bar{\eta}) \sim \frac{\sqrt{2\pi}}{(\sigma-1)!} (-\bar{\eta})^{\sigma-1} \exp(\bar{\eta}^2/4). \quad (\text{B7})$$

Since

$$-\bar{\eta} \sim \frac{\sigma}{u_0 \sqrt{-f^{(2)}}}, \quad (\text{B8})$$

the low-temperature limit of the approximation (A14) becomes

$$I_{\sigma}^{(\text{s.p.})} \sim \frac{1}{(\sigma-1)!} \left( \frac{\sigma}{u_0} \right)^{\sigma-1} \exp(\beta \varepsilon_0 - f^{(0)} - \sigma), \quad (\text{B9})$$

which has been used heavily in Sections II and III.

It is of interest to recast this expression (B9) into a form which lends itself to a direct comparison with the now incorrect standard saddle-point formula. To this end we exploit that, since  $u_0 \rightarrow 0$ , the second derivative of the full function  $\bar{f}$  at the saddle-point will be dominated by the singular ground-state contribution, giving

$$\bar{f}^{(2)} \sim -\frac{\sigma}{u_0^2}. \quad (\text{B10})$$

With this additional approximation, and utilizing the identity  $\bar{f}^{(0)} = f^{(0)} - \beta \varepsilon_0 + \sigma \ln u_0$ , Eq. (B9) yields

$$\begin{aligned} I_{\sigma}^{(\text{s.p.})} &\sim \frac{\sigma^{\sigma-1}}{(\sigma-1)!} u_0 \exp(-\bar{f}^{(0)} - \sigma) \\ &\sim \frac{\sigma^{\sigma-1} e^{-\sigma}}{(\sigma-1)!} \sqrt{2\pi\sigma} \frac{\exp(-\bar{f}^{(0)})}{\sqrt{-2\pi\bar{f}^{(2)}}} \\ &\equiv R_{\sigma} \frac{\exp(-\bar{f}^{(0)})}{\sqrt{-2\pi\bar{f}^{(2)}}}. \end{aligned} \quad (\text{B11})$$

This is a most intriguing observation: In the large- $N$ , low-temperature limit, i.e., in the condensate regime, the result of the properly executed saddle-point approximation to the Bose-type integral (A1) differs from the standard saddle-point formula by a *temperature- and system-independent* factor  $R_{\sigma}$ , namely

$$R_{\sigma} = \sqrt{2\pi\sigma} \frac{\sigma^{\sigma-1} e^{-\sigma}}{(\sigma-1)!}; \quad (\text{B12})$$

some numerical values of  $R_{\sigma}$  are listed in the following table.

$\sigma$	$R_{\sigma}$
1	0.92214
2	0.95950
3	0.97270
5	0.98349
10	0.99170

Recalling Stirling's formula for  $(\sigma-1)!$ , one immediately realizes that these universal renormalization factors  $R_{\sigma}$  approach unity when the singularity index  $\sigma$

is increased. This finding, which might appear paradoxical at first, has a simple explanation: In a system with a  $\sigma$ -fold degenerate ground state, each individual of these states takes only  $1/\sigma$ th of the particles that a non-degenerate ground state would have to carry. Therefore,  $z_*^{-1}e^{\beta\epsilon_0} - 1$  is of the order  $O(\sigma/N)$ : The larger  $\sigma$ , the farther away is the saddle-point  $z_*$  from the singularity at  $z = e^{\beta\epsilon_0}$ , and the better is the standard procedure.

On the other hand, in the high-temperature regime, where  $u_0 \rightarrow 1$ , the left hand side of Eq. (B9) can be written as

$$\frac{\sigma^{\sigma-1}e^{-\sigma}}{(\sigma-1)!}\exp(-\bar{f}^{(0)}) \equiv M_\sigma \frac{\exp(-\bar{f}^{(0)})}{\sqrt{-2\pi\bar{f}^{(2)}}}. \quad (\text{B13})$$

Thus, when using the low-temperature approximation (B9) in the high-temperature regime, the result is incorrect by the factor

$$M_\sigma = R_\sigma \sqrt{-\bar{f}^{(2)}/\sigma}. \quad (\text{B14})$$

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