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Statistical mechanics of ideal Bose atoms in a harmonic trap

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For ideal Bose atoms in an isotropic harmonic trap, we consider thermodynamic variables obtained from microcanonical, canonical, and grand canonical ensembles, each with certain variables specified and other variables fluctuating. For the first two of these ensembles, we derive recursion relations that link partition functions for different dimensions. We discuss fluctuations in general, and obtain expressions for variances of the atom number N, the chemical potential μ, and the temperature T for small, Gaussian fluctuations in the grand canonical ensemble. Then from our recursion relations and others given elsewhere, we obtain probability distributions for N, for ground-state occupation number n_0, for μ, and for T. Below the critical temperature, the shape of the distributions for N, n_0, and μ are definitely not Gaussian for the grand canonical ensemble. For given temperature and small N, we find that the chemical potential values pertaining to the three ensembles differ. We compare the specific-heat function $C_N(T)$ for the three ensembles and propose to use the minimum of dC_N/dT to define the critical temperature to facilitate comparisons with similar configurations of interacting atoms. [S1050-2947(98)01309-2]

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I. INTRODUCTION

There are many different statistical ensembles used in statistical mechanics; nevertheless, only one thermodynamics is known. The equivalence of the results given by the different ensembles describing this thermodynamics is exhibited as the ''thermodynamic limit'' [1], which is equivalent to the saddle-point approximation. If the system is homogeneous, the convergence of the viewpoints of the different ensembles occurs through a limiting process in which the number of particles and the volume both tend to infinity, in such a manner that their ratio, the density, is constant.

For inhomogeneous systems the usual argument for the universal equivalence of different statistical ensembles needs to be reconsidered. Of course, there are special cases of inhomogeneous systems when the equilibrium system can be divided into (essentially) homogeneous layers, and each layer can be subjected to its own limiting process. This, however, requires that the volume of each homogeneous layer can be made infinite without changing the physical situation. For example, in a constant gravitational field, the system can be divided into thin layers by planar equipotential surfaces. The thin layers between the planes can be made infinite in extent, enclosing regions of uniform density without altering the physics of the problem. If a finite number of particles is confined in a harmonic potential (thus *not* in a finite volume independent of dynamics), the problem must be analyzed anew. Here the system contains only a finite number of particles. It is also inhomogeneous, and the regions of approximately constant density are finite. The usual limiting process cannot be applied. Of course, this is of small consequence if we do not wish to have a thermodynamic description. Then, however, thermodynamic variables can no longer be used.

If we insist on a statistical mechanical description of thermodynamic variables, immediate difficulties arise. The quantities used in the constructions of thermodynamical variables will in general fluctuate, and their statistics will be different for different Gibbsian ensembles. Moreover, there is a question whether we should associate the physically observed quantities with mean values, most probable values, or some other type of statistical average.

For this reason, it seems to us of interest to compute the relevant thermodynamical quantities exactly in the standard ensembles, and also some nonthermodynamical quantities such as occupation numbers and fluctuations. We will therefore compare results in three Gibbsian ensembles [2] for an ideal Bose gas confined in an isotropic harmonic potential when the particle numbers are small.

For a microcanonical ensemble [3–5], the total number of particles N and the total energy E are prescribed, and all configurations satisfying the given N and E are considered equally probable. Explicit enumeration of these configurations is possible if the number of particles is less than 100 or so. Using recursion relations given below, computation of $W(N,K)$, the number of configurations, is possible up to $N=1000$ or so. For the canonical ensemble, the system is assumed to be in thermal contact with a heat bath of given temperature T, so that the prescribed parameters become T and N. For the grand canonical ensemble, the system exchanges particles as well as energy with a bath. The chemical potential μ and T of the bath itself are now the control variables. This simplifies the analysis immensely, and therefore the grand canonical ensemble is the most convenient and most commonly used statistical ensemble.

However, atoms confined in a trap exchange neither particles nor energy with a surrounding heat bath, after evaporative cooling is turned off. (Loss of atoms due to collisions with background gas atoms cannot be considered an equilibrating process.) With no heat bath, the total energy, rather than T, and N, rather than μ, are the experimentally determined variables, as in the microcanonical ensemble. (Even if not accurately known, the energy and total atom number of an isolated system will not fluctuate.) Though long known [6,4], there has been increasing concern with this point, and a number of authors have recently considered the canonical ensemble (CE) [7,8], microcanonical ensemble (MCE) [9–12], as well as a newly defined ''Maxwell Demon'' ensemble [13,12] in which particles, but not energy, are ex-

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changed with an infinite reservoir of ground state atoms. New and useful results have been obtained, but these ensembles remain difficult to work with, and the properties of these ensembles for finite numbers of atoms in an inhomogeneous (harmonic) potential warrant further study.

Grossmann and Holthaus have examined these questions on several levels [14,9,12,15]. They initially used asymptotic expressions to consider the microcanonical ensemble in one dimension, and more recently [12,15] have used the MD ensemble and the low-temperature properties of the microcanonical ensemble to obtain results for three dimensions. Chase, Mekjian, and Zamick [16] have derived recursion relations for the CE (actually obtained earlier by Landsberg [17]) and the MCE, and made comparisons of the specific heat, and of the mean ground-state occupation number $\langle n_0 \rangle$ for the three ensembles. Weiss and Wilkens [11] have presented the distribution over n_0 as well as the fluctuation of n_0 for the three primary ensembles. Although for given N or $\langle N \rangle$, the average value $\langle n_0 \rangle$ is nearly the same in the different ensembles, below T_c the shape of the distribution over n_0 is quite different, and the fluctuation is much less for the CE than for the GCE, and less for the MCE than for the CE. Also it has been established that for the CE [6,7] and MCE [9,13,11], the fluctuation of n_0 goes to zero with T, as one would expect. Gajda and Rzazewski [10] obtained analytic results for the MCE for a 3D harmonic trap from the saddle-point approximation, replacing the sum over eigenenergies by an integral and the Euler-McLaurin expansion. There are various possibilities for expanding these results about $T=0$ or about $T=\infty$ (or about $1/T=0$), or even about some intermediate value.

As are many of the above cited works, this study is concerned exclusively with ideal, noninteracting atoms in an isotropic harmonic potential. We use the previously derived recursion relations, and also present new recursion relations for both the CE and the MCE that link the partition functions in one, two, and three dimensions (Sec. II). In Sec. III, we discuss average values and fluctuations in general, and obtain variances of temperature and chemical potential in the GCE point of view. We then in Sec. IV use the CE and MCE recursion relations to obtain distributions over N, n_0, μ, and T. These distributions highlight the contrasting natures of the different ensembles. Finally (Sec. V), we consider the specific heat obtained from the various ensembles, especially as a means of establishing a definition for the critical temperature T_c that may be extended from ideal to real gases.

A secondary goal of interest would be to assess the accuracy of the analytic approximations developed for the MCE in [10], and the ''Maxwell Demon'' ensemble [13,12], but because of the multitude of possibilities, we will not address these questions in this report.

II. PARTITION FUNCTIONS

We consider N identical Bose particles in a harmonic oscillator potential of frequency $\omega/2\pi$. For dimension $d>1$, we will consider only the simplest case in which the potential is isotropic. If the ground-state energy is taken to be zero, then the single-particle energies ϵ_k are integral multiples of $\hbar\omega$; $\epsilon_k = k\hbar\omega, k=0,1,2,3,\ldots$. The degeneracy of each level k is $g_k(d)=(k+d-1)!/k!(d-1)!$. Thus $g_k(1)=1, g_k(2)=k+1, g_k(3)=(k+1)(k+2)/2$. An allowed configuration is completely characterized by an occupation number set $n_0, n_1, n_2, \ldots$, denoted by $\{n_i\}$, which satisfy the side conditions

$$N=\sum_k n_k, \tag{1}$$

$$E=\sum_k n_k \epsilon_k = \sum_k n_k \hbar\omega k = \hbar\omega K, \quad \text{or} \quad K=\sum_k n_k k. \tag{2}$$

In the present case the value of the total energy E is an integer, K, times $\hbar\omega$.

The microcanonical partition function for N atoms with total energy $E=K\hbar\omega$ in d dimensions, $W(d,N,K)$, is a function of N and K only, and is given by a sum over all allowed configurations:

$$W(d,N,K)=\sum_{\{n_i\}}{}'' \prod_k C(d,n_k), \tag{3}$$

where $C(d,n_k)=[n_k+g_k(d)-1]!/n_k![g_k(d)-1]!$ is the number of ways n_k atoms can be placed into g_k states. The summation is over all possible occupation number sets $n_0, n_1, n_2, \ldots$ that satisfy the side conditions, Eq. (1) and (2), indicated by the two primes on the summation sign.

The canonical partition function, $Z(d,N,v)$, where $v \equiv \exp(-\beta)$, $\beta=\hbar\omega/kT$, is a function of N and T. The grand canonical partition function, $R(d,u,v)$, depends on the chemical potential, μ, and on T as independent variables via the parameters $u \equiv \exp(\beta\mu)$ (the fugacity) and v. (Note that both $v<1$ and $u<1$ for an ideal Bose gas.) Thus

$W(d,N,K)$ is the microcanonical partition function, (4)

$$Z(d,N,v)=\sum_{K=0}^{\infty} v^K W(d,N,K)$$

is the canonical partition function, (5)

$$R(d,u,v)=\sum_{N=0}^{\infty} u^N Z(d,N,v)$$

is the grand canonical partition function. (6)

A. Grand canonical ensemble

In the standard way, $R(d,u,v)$ can be obtained from Eqs. (3) and (6) after summing over N so that the constraints are removed. For an isotropic harmonic oscillator, a relatively simple expression results:

$$\begin{aligned} R(d,u,v) &= \sum_{N,K} u^N v^K W(d,N,K) \\ &= \prod_k \sum_{n_k=0} u^{n_k} v^{k n_k} C(d,n_k) = \prod_k \frac{1}{(1-uv^k)^{g_k(d)}} \end{aligned} \tag{7}$$

since u and v are less than unity. R can also be considered a generating function associated with W. For the special case of an isotropic harmonic oscillator, the degeneracies are such as to yield the relation

$$R(d,uv,v)R(d-1,u,v)=R(d,u,v), \tag{8}$$

which will play an important role in the following discussion. The properties of the grand canonical ensemble for atoms in a harmonic potential have been studied in detail recently by Grossmann and Holthaus [14].

B. Canonical ensemble

Recursion relations lead to computationally efficient methods for computing $Z(d,N,v)$ and $W(d,N,K)$. The following recursion relation has been known for some time [17], and recently rediscovered [18,16,12,11]:

$$Z(d,N,v)=\frac{1}{N}\sum_{k=1}^{N} Z(d,1,v^k)Z(d,N-k,v). \tag{9}$$

Another recursion relation that connects the $Z(d,N,v)$ for different d can be developed by substituting Eq. (6) in Eq. (8):

$$\sum_{N=0}^{\infty} u^N Z(d,N,v)=\sum_{N'=0}^{\infty} u^{N'}v^{N'}Z(d,N',v)\times\sum_{N''=0}^{\infty} u^{N''}Z(d-1,N'',v). \tag{10}$$

The coefficient of u^N on both sides is

$$Z(d,N,v)=\sum_{N'=0}^{N} v^{N'}Z(d,N',v)Z(d-1,N-N',v). \tag{11}$$

In order to use this result, we recognize that it is consistent with Eq. (7) to take

$$R(0,u,v)=\frac{1}{1-u}=\sum_{N=0} u^N Z(0,N,v), \tag{12}$$

which implies $Z(0,N,v)=1$, for $N=0,1,2,\ \dots$. As a check, the following identity may be confirmed by taking $N=0,1,\dots$:

$$Z(1,N,v)=\sum_{N'=0}^{N} v^{N'}Z(1,N',v). \tag{13}$$

Taking into account also the result for no atoms, $Z(d,0,v)=1$ (below), the above recursion relation may be written

$$Z(d,N,v)=\frac{1}{1-v^N}\sum_{N'=0}^{N-1} v^{N'}Z(d,N',v)Z(d-1,N-N',v),\quad d=1,\dots\ . \tag{14}$$

C. Microcanonical ensemble

Analogous to Eq. (9), recently [16,11] the following recursion relation has been obtained:

$$W(d,N,K)=\frac{1}{N}\sum_{k=1}^{N}\sum_{j=1}^{K/k} g_k(d)W(d,N-k,K-kj), \tag{15}$$

with the condition $W(d,0,K)=\delta(0,K)$. From this condition it follows that $Z(d,0,v)=1$ for all d, as above.

To obtain a recursion relation joining $W(d,N,K)$ for different values of d, we recognize that $W(1,N,K)$ is the number of partitions of K into N parts and is given by the coefficients of the expansion of

$$Z(1,N,v)=\prod_{i=1}^{N}\frac{1}{1-v^i}=\sum_{K=0}^{\infty} v^K W(1,N,K) \tag{16}$$

and thus $Z(1,N,v)=Z(1,N-1,v)/(1-v^N)$. Therefore, for $N>0$,

$$(1-v^N)\sum_{K=0}^{\infty} v^K W(1,N,K)=\sum_{K'=0}^{\infty} v^{K'}W(1,N-1,K') \tag{17}$$

or

$$\sum_{K=0}^{\infty} v^K W(1,N,K)=\sum_{K'=0}^{\infty} v^{K'}W(1,N-1,K')+\sum_{K''=N}^{\infty} v^K W(1,N,K''-N). \tag{18}$$

By equating coefficients of v^K in Eq. (18), we find that below the diagonal in the $N-K$ plane, $W(1,N,K)$ is independent of N:

$$W(1,N,K)=W(1,N-1,K),\quad N>K. \tag{19}$$

On the diagonal,

$$W(1,N,N)=W(1,N-1,N)+W(1,N,0)=W(1,N-1,N)+1 \tag{20}$$

and, above the diagonal,

$$W(1,N,K)=W(1,N-1,K)+W(1,N,K-N),\quad K>N. \tag{21}$$

To develop analogous recursion relations for $d>1$, we substitute Eq. (6) into Eq. (8):

$$\left[\sum_{N=0}^{\infty}(uv)^N Z(d,N,v)\right]\left[\sum_{N'=0}^{\infty}u^{N'}Z(d-1,N',v)\right]=\sum_{N''=0}^{\infty}u^{N''}Z(d,N'',v). \tag{22}$$

Equating terms in u^N, we have

$$(1-v^N)Z(d,N,v)=\sum_{M=1}^{N}v^{N-M}Z(d,N-M,v)Z(d-1,M,v). \tag{23}$$

Substituting from Eq. (5),

$$\sum_{K=0}^{\infty}v^K W(d,N,K)-\sum_{K'=0}^{\infty}v^{K'+N}W(d,N,K')=\sum_{M=1}^{N}v^{N-M}\left[\sum_{K''=0}^{\infty}v^{K''}W(d-1,M,K'')\right]\left[\sum_{K'=0}^{\infty}v^{K'}W(d,N-M,K')\right]. \tag{24}$$

Equating terms in v^K,

$$W(d,N,K)=W(d,N,K-N)+\sum_{M=1}^{N}\sum_{K'=0}^{K+M-N}W(d,N-M,K')W(d-1,M,K+M-N-K'). \tag{25}$$

Once $W(d,N,K)$ has been computed, $Z(d,N,v)$ can be obtained from Eq. (5). However, we have found numerically that Eq. (5) is sensitive to round-off error, even for small N, whereas Eq. (14) is not.

III. AVERAGES AND FLUCTUATIONS

A. Classical ensemble averages

In the different ensembles, different thermodynamical quantities can fluctuate. Since these fluctuations are important if the number of particles is small, it is useful to study these differences. We present two approaches to fluctuations in the next two subsections. To simplify the discussion, the classical phase space density, $\Omega(E,N)$, will be considered in place of the quantum degeneracy, $W(E,N)$, discussed above. Discretization is by no means a trivial step and will be discussed in Sec. IV C 1.

The *thermodynamical* description admits no fluctuation of thermodynamical quantities. The fundamental thermodynamical quantities are the extensive ones, since the combined first and second laws establish a linear relation between them; the intensive quantities are the coefficients in the linear relation. For atoms in a harmonic trap, the mechanical work terms are missing, and thus this relation is simply

$$dS=(1/T)dE-(\mu/T)dN. \tag{26}$$

Then $1/T$ and μ/T are given as derivatives of the function $S(E,N)$:

$$\left(\frac{\partial S}{\partial E}\right)_N=\frac{1}{T}, \quad \left(\frac{\partial S}{\partial N}\right)_E=-\frac{\mu}{T}. \tag{27}$$

In the *microcanonical ensemble* no thermodynamical variable fluctuates. Statistical mechanics simply specifies the entropy in terms of mechanical quantities. In classical mechanics, we have $S=\ln[\Omega(E,N)]$, the logarithm of the phase space density, $\Omega(E,N)$, or, in quantum mechanics, $S=\ln[W(E,N)]$, where $W(E,N)$ is the degeneracy at the total energy E for N particles. Consequently in the microcanonical ensemble, no thermodynamical quantity, extensive or intensive, can fluctuate. (Nonthermodynamical quantities, such as the occupation numbers of the single-particle energy states in a noninteracting gas, can fluctuate.)

In the *canonical ensemble* the energy becomes a *random* variable with a probability distribution. Thus the energy will fluctuate. Physically we interpret this as a consequence of the system being attached to a heat bath. For example, in a classical gas, the probability distribution will be $\Omega(E,N)\exp(-\beta E)dE/C$,where $C=\int dE\ \Omega(E,N)\exp(-\beta E)$. ($\beta$ is a characteristic parameter associated with the heat bath to which the system is attached.) The reciprocal temperature of the system in the microcanonical description is $\beta_{\text{system}}=(1/T)_{\text{system}}=\partial\ln\Omega/\partial E$. Its average in a canonical ensemble is

$$\langle\beta_{\text{system}}\rangle_{\beta,N}=\int dE(\partial\ln\Omega/\partial E)\Omega\exp(-\beta E)/C=\int dE(\partial\Omega/\partial E)\exp(-\beta E)/C=\beta, \tag{28}$$

where in the last step we performed an integration by parts. Thus the physical meaning of the bath parameter β is given as the *average* of the reciprocal system temperature, which is a fluctuating quantity. The usual *thermodynamical* equilibrium condition for combined systems, the equality of the temperature of its parts, is then to be interpreted for the *average*. (The bath temperature does not fluctuate, since the bath is supposed to be large.)

The mean square fluctuation of β_{system} in the canonical ensemble is given as

$$\begin{aligned}\langle(\beta_{\text{system}})^2\rangle_{\beta,N}=\langle(\partial \ln \Omega/\partial E)^2\rangle_{\beta,N}&=\int dE(\Omega'/\Omega)(\Omega'/\Omega)\Omega\exp(-\beta E)/C\\ &=\int dE\ \Omega'[(\Omega'/\Omega)\exp(-\beta E)]/C=-\int dE\ \Omega[(\Omega'/\Omega)\exp(-\beta E)]'/C\\ &=-\int dE\ \Omega[(\Omega'/\Omega)]'\exp(-\beta E)/C+\beta\int dE\ \Omega(\Omega'/\Omega)\exp(-\beta E)/C=-\langle\partial(1/T_{\text{system}})/\partial E\rangle_{\beta,N}+\beta^2.\end{aligned}$$

(The primes indicate derivatives with respect to E.)

The dispersion around the mean $\langle(\Delta(1/T_{\text{system}})^2\rangle_{\beta,N}=\langle(\beta_{\text{system}}-\beta)^2\rangle_{\beta,N}$ becomes

$$\langle(\beta_{\text{system}})^2\rangle_{\beta,N}-(\beta)^2=-\langle\partial(\beta_{\text{system}})/\partial E\rangle_{\beta,N}. \tag{29}$$

The calculation was simple because we computed the fluctuation of the *reciprocal* temperature. If the fluctuations are small, however, one can reexpress the above result in terms of the system temperature fluctuation itself:

$$\begin{aligned}\langle[\Delta(1/T_{\text{system}})]^2\rangle_{\beta,N}&=\langle(\beta_{\text{system}})^4(\Delta T_{\text{system}})^2\rangle_{\beta,N}\\ &=-\langle(\partial\beta_{\text{system}}/\partial E\rangle_{\beta,N}.\end{aligned} \tag{30}$$

If we approximate in this relation the averages of the products with the averages of the factors we obtain immediately

$$\langle(\Delta T_{\text{system}})^2\rangle_{\beta,N}=(1/\beta)^2/C_N, \tag{31}$$

where C_N is the specific heat for a given number of atoms. This is the usual result for small (and thereby also Gaussian) fluctuations.

In the *grand canonical* ensemble both E and N become random variables with the joint probability distribution $\Omega\exp(-\beta E+\alpha N)/C$, where C is another normalizing factor, and α is a new bath or reservoir parameter, controlling the coupling with the particle reservoir. Its physical meaning must be identified by a suitable average. If we treat N as a continuous variable we can follow the previous discussion for temperature fluctuations, replacing there E with N, β with $-\alpha$, and introducing $\alpha_{\text{system}}=(-\mu/T)_{\text{system}}=\partial \ln \Omega/\partial N$. Consequently the bath parameter α must be identified with the grand canonical average $\langle(-\mu/T)_{\text{system}}\rangle_{\beta,\mu}$, while the mean square fluctuation of α_{system}, $\langle(\Delta\alpha_{\text{system}})^2\rangle_{\beta,\mu}$is $\langle\partial(\mu/T)_{\text{system}}/\partial N\rangle_{\beta,\mu}$. Breaking the correlations for small fluctuations, this results in $\beta(\partial\mu/\partial N)$ for the dispersion of α. Here, too, the thermal equilibrium condition needs to hold only for the averaged intensive variable, i.e., α. Further discussion of the GCE appears in the next subsection.

In the above discussion, it was assumed that E and N are continuous variables. When E is quantized and N is discrete, one can imagine various procedures for translating the derivative to a differences expression, and it will be shown below that the results can vary greatly, especially for μ and $\alpha=\mu/T$. However, it will be shown in Secs. IV C 1 and IV D that with one particular discretization of the partial derivatives, the grand canonical average of the microcanonical variables $u=\exp(\mu/T)$ and $v=\exp(-1/T)$ are exactly equal to the GCE quantity.

B. Gaussian fluctuations in a grand canonical ensemble

Consistent with the above discussion and with, for example, Ref. [5], we take the point of view that with the grand canonical ensemble, the system values of not only extensive variables, such as E, N, and S, but also the intensive variables T and μ will fluctuate about their mean values. To clarify the discussion, we will call the system variables T_{system} and μ_{system}. The mean values of T_{system} and μ_{system} are precisely the heat bath values. Other authors [19] have taken the point of view that intensive variables, (T,μ), do *not* fluctuate. In any case, in the thermodynamic limit, the fluctuations become negligible, and furthermore, one often considers the thermodynamical equilibrium conditions *(T* constant, μ constant) to hold, neglecting fluctuations. However, for small N, we find that the fluctuations are substantial.

For atoms confined in a harmonic trap, the GCE does not precisely apply, as discussed in the Introduction, and therefore the fluctuations discussed here will not be observable. Furthermore, it has been emphasized [7] that atom-atom interactions will diminish fluctuations, at least in ground-state occupation number. Our interest in fluctuations with the GCE derives from the goal of understanding the statistical implications of the various model ensembles, and in particular of the ensemble that is most commonly used in theoretical work. Also, it may be that future experiments with Bose atoms will involve processes that resemble equilibration of particles and energy with a heat bath, as assumed for the GCE.

Thermodynamical fluctuation theory as presented in [5] has yielded useful expressions for the variances when the fluctuations are small and Gaussian. It is implicit in the discussions in [5] that the grand canonical ensemble is under consideration. Following a much earlier model [20], the fluctuation probability is said to be proportional to $e^{\Delta S_t/k}$, where ΔS_t is the change of total entropy of the system plus bath. This is restated as $\Delta S_t=-R_{\min}/T$, where R_{min} is the minimum work required to carry out such a change. Since the concept of minimum work is inapplicable to trapped atoms, we will derive expressions for the variance of thermodynamic quantities by considering the grand canonical distribution function.

In the grand canonical distribution,

$$P(E,N;\alpha,\beta)=Ce^{\tilde{S}(E,N)-\beta E+\alpha N}dE\ dN, \tag{32}$$

E and N are random variables, while α and β are *fixed* bath variables. $\tilde{S}(E,N)$ is the microcanonical entropy, which is a monotonic nondecreasing function of E. Hence we can solve it for $E=\tilde{E}(S,N)$, where the tilde stresses that E is now a function, and S is now considered a random variable:

$$P(S,N;\alpha,\beta)dS\ dN=Ce^{S-\beta\tilde{E}(S,N)+\alpha N}\left(\frac{d\tilde{E}}{dS}\right)dS\ dN. \tag{33}$$

We will now expand the exponent about its maximum, which occurs at (S^*,N^*), at which

$$1-\beta\left(\frac{\partial\tilde{E}}{\partial S}\right)^*=0,\quad -\beta\left(\frac{\partial\tilde{E}}{\partial N}\right)^*+\alpha=0. \tag{34}$$

But since

$$\left(\frac{\partial\tilde{E}}{\partial S}\right)=T_{\text{system}}(S,N),\quad \left(\frac{\partial\tilde{E}}{\partial N}\right)=\mu_{\text{system}}(S,N), \tag{35}$$

the maximum occurs at such (S^*,N^*) for which $T_{\text{system}}=1/\beta$, and $\beta\mu_{\text{system}}=\alpha$, or $\mu_{\text{system}}/T_{\text{system}}=\alpha$. We now introduce the random variables $\Delta S,\Delta N$, such that $S=S^*(\alpha,\beta)+\Delta S, N=N^*(\alpha,\beta)+\Delta N$, and expand the exponent up to quadratic terms. In what follows, all increments will be relative to the maximum of the exponent. In view of Eq. (34), the linear terms vanish, only the quadratic terms survive, and the α,β dependence becomes partly implicit. For the exponent, labeled Y, one now has

$$Y=-\frac{\beta}{2}\left[\left(\frac{\partial^2\tilde{E}}{\partial S^2}\right)^*(\Delta S)^2+2\left(\frac{\partial^2\tilde{E}}{\partial S\partial N}\right)^*\Delta S\Delta N+\left(\frac{\partial^2\tilde{E}}{\partial N^2}\right)^*(\Delta N)^2\right]. \tag{36}$$

If we now consider increments ΔS and ΔN in S and N at S^* and N^*, the increments of the derivatives $\partial\tilde{E}/\partial S$ and $\partial\tilde{E}/\partial N$ will be

$$\Delta\left(\frac{\partial\tilde{E}}{\partial S}\right)_{S^*,N^*}=\left(\frac{\partial^2\tilde{E}}{\partial S^2}\right)^*\Delta S+\left(\frac{\partial^2\tilde{E}}{\partial N\partial S}\right)^*\Delta N=\Delta T_{\text{system}} \tag{37}$$

$$\Delta\left(\frac{\partial\tilde{E}}{\partial N}\right)_{S^*,N^*}=\left(\frac{\partial^2\tilde{E}}{\partial S\partial N}\right)^*\Delta S+\left(\frac{\partial^2\tilde{E}}{\partial N^2}\right)^*\Delta N=\Delta\mu_{\text{system}}, \tag{38}$$

in terms of which the exponent becomes

$$Y=-\frac{\beta}{2}[\Delta S\Delta T+\Delta N\Delta\mu], \tag{39}$$

where all quantities refer to the *system*, and the increments are changes about the maximum at (S^*,N^*). A similar expression occurs in [5] with $\Delta P\Delta V$ in place of $\Delta N(\Delta\mu)$.

To derive variances for T and N, we could immediately take T and N to be independent variables, and write the probability distribution in Eq. (32) as

$$P(T,N)dT\ dN=Ce^{(\hat{S}(T,N)-\beta\hat{E}(T,N)+\alpha N)}dT\ dN, \tag{40}$$

where $\hat{E}$ and $\hat{S}$ denote functions of T and N, which are different from the functions $\tilde{S}(E,N)$ and $\tilde{E}(S,N)$ defined above. An expansion to second order in T and N will yield the results we desire. However, we will here follow a slightly shorter route closer to that in Ref. [5]. In Eq. (39) we substitute

$$\Delta\mu=\left(\frac{\partial\mu}{\partial T}\right)_N\Delta T+\left(\frac{\partial\mu}{\partial N}\right)_T\Delta N \tag{41}$$

and

$$\Delta S=\left(\frac{\partial S}{\partial T}\right)_N\Delta T+\left(\frac{\partial S}{\partial N}\right)_T\Delta N=\frac{C_N}{T}\Delta T-\left(\frac{\partial\mu}{\partial T}\right)_N\Delta N, \tag{42}$$

in which we have used

$$\left(\frac{\partial S}{\partial N}\right)_T=-\frac{\partial}{\partial N}\left(\frac{\partial F}{\partial T}\right)_N=-\left(\frac{\partial\mu}{\partial T}\right)_N. \tag{43}$$

Then for the exponent Y in the probability $w\propto e^Y$, we obtain

$$Y\approx-\frac{\beta}{2}\left[\frac{C_N}{T}(\Delta T)^2+\left(\frac{\partial\mu}{\partial N}\right)_T(\Delta N)^2\right]. \tag{44}$$

From this the variances follow directly:

$$\langle(\Delta T)^2\rangle=\frac{kT^2}{C_N},\quad \langle(\Delta N)^2\rangle=kT\left(\frac{\partial N}{\partial\mu}\right)_T,\quad \langle\Delta T\Delta N\rangle=0. \tag{45}$$

Thus in this approximation, the fluctuations of T and N are not correlated. By contrast, if we take S and μ as independent variables,

$$\Delta N=\left(\frac{\partial N}{\partial S}\right)_\mu\Delta S+\left(\frac{\partial N}{\partial\mu}\right)_S\Delta\mu \tag{46}$$

and

$$\Delta T=\left(\frac{\partial T}{\partial S}\right)_\mu\Delta S+\left(\frac{\partial T}{\partial\mu}\right)_S\Delta\mu=\frac{T}{C_\mu}\Delta S-\left(\frac{\partial N}{\partial S}\right)_\mu\Delta\mu, \tag{47}$$

where we have introduced $\Lambda=E-\mu N$, $d\Lambda=T\ dS-N\ d\mu$, such that

$$\left(\frac{\partial T}{\partial\mu}\right)_S=\frac{\partial}{\partial\mu}\left(\frac{\partial\Lambda}{\partial S}\right)_\mu=-\left(\frac{\partial N}{\partial S}\right)_\mu \tag{48}$$

and, therefore, the exponent becomes

$$Y\approx-\frac{\beta}{2}\left[\frac{T}{C_\mu}(\Delta S)^2+\left(\frac{\partial N}{\partial\mu}\right)_S(\Delta\mu)^2\right] \tag{49}$$

and the variances are

$$\langle(\Delta S)^2\rangle=kC_\mu,\quad \langle(\Delta\mu)^2\rangle=kT\left(\frac{\partial\mu}{\partial N}\right)_S,\quad \langle\Delta S\Delta\mu\rangle=0. \tag{50}$$

The above expressions for $\langle(\Delta\mu)^2\rangle$ as well as $\langle(\Delta T)^2\rangle$ will be compared with the widths of the corresponding probability distributions in Secs. IV C 2 and IV D.

By selecting the other possible variable pairs, we determine that, to terms of second order,

$$\langle\Delta T\Delta\mu\rangle\neq 0, \quad \langle\Delta S\Delta N\rangle\neq 0. \tag{51}$$

The above fluctuations have been derived with the assumption that the probability distributions are Gaussian. In the following section, we will show that this is not the case below T_c for N and μ.

IV. PROBABILITY DISTRIBUTIONS

A. Atomic number

For the grand canonical ensemble, it is well known that the mean values $\langle N\rangle$ and $\langle n_i\rangle$ can be obtained from

$$\langle N\rangle=\frac{1}{\beta}\frac{\partial\ln R(u,v)}{\partial\mu}=u\frac{\partial\ln R(u,v)}{\partial u}$$
$$=\sum_{i=0}^{\infty}\frac{g(i)}{e^{\beta(i-\mu)}-1}=\sum_{i=0}^{\infty}\langle n_i\rangle, \tag{52}$$

where $u=e^{\alpha}=e^{\mu\beta}$. (Except where noted, the following discussion applies to any value of d, and we will normally omit this variable in the following.) When computing the $\langle n_i\rangle$ for a given atom number N, μ is adjusted so as to fulfill the condition $N=\langle N\rangle$ to the desired precision.

Various approximations have been used for the GCE for atoms in a harmonic trap. One approach is to replace the above sum by a term for the ground state plus an integral over E [14]. The first three terms for $\langle N\rangle$ for the 3D isotropic harmonic trap are then

$$\langle N\rangle=\frac{u}{1-u}+\frac{1}{\beta^3}g_3(u)+\frac{3}{2\beta^2}g_2(u), \tag{53}$$

where the first term is $\langle N_0\rangle$, and $g_n(z)=\Sigma_{l=1}^{\infty}z^l/l^n$. A definition for T_c is obtained by making the approximation $u=1$ and setting $\langle N_0\rangle=0$ in the above approximate expression [14,21]. This leads to the result

$$\frac{kT_c}{\hbar\omega}=\left(\frac{N}{\zeta(3)}\right)^{1/3}-\frac{\zeta(2)}{2\zeta(3)}+\frac{\zeta(2)^2}{4\zeta(3)^{5/3}N^{1/3}}$$
$$=0.94050N^{1/3}-0.684216+0.49777N^{-1/3}, \tag{54}$$

where $\zeta(n)$ is the Riemann ζ function. This expression gives a useful N-dependent critical temperature, T_c, that we will use in the following discussion. However, for values of N such as will be of interest below, neither approximation $u=1$ or $N_0=0$ is precisely correct at $T=T_c$, as is fully recognized in [14].

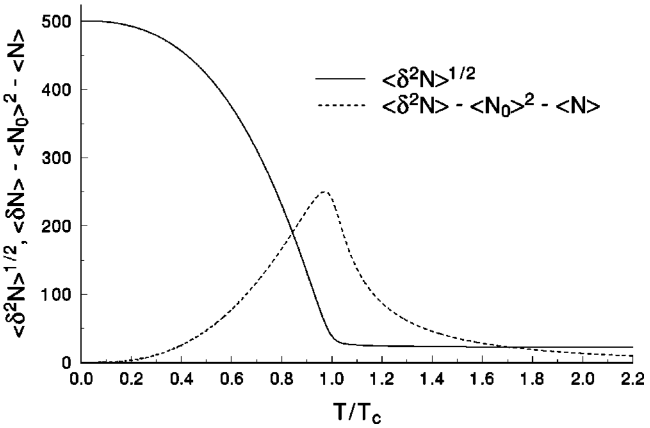

FIG. 1. The mean fluctuation, $\langle\delta^2N\rangle^{1/2}$ of the total atom number, for $N=500$ (solid line) from the grand canonical ensemble. The dashed line shows that the major contributions to $\langle\delta^2N\rangle$ are the terms $\langle n_0\rangle^2+\langle N\rangle$, except near T_c, when the contribution of excited states to the last term of Eq. (55) becomes significant.

The mean square of the fluctuation of N is

$$\langle(\Delta N)^2\rangle=\langle(N-\langle N\rangle)^2\rangle=\left(u\frac{\partial}{\partial u}\right)^2\ln[R(u,v)]$$
$$=\langle N\rangle+\sum_{i=0}^{\infty}\frac{g(i)}{[e^{\beta(i-\mu)}-1]^2}. \tag{55}$$

Figure 1 shows $\langle(\Delta N)^2\rangle^{1/2}$ as a function of T obtained from Eq. (55) by adjusting μ (or u) at each value of T so that $\langle N\rangle=500$ atoms. At low T, $\langle(\delta N)^2\rangle$ is dominated by the $i=0$ term in the final sum of Eq. (55), which is equal to $\langle n_0\rangle^2$, while for $T>T_c$, the $\langle N\rangle$ term dominates. The remaining terms in the sum are shown as the dashed line in Fig. 1. These equations and plots emphasize again that for the GCE, the total atomic number is a fluctuating quantity. As is widely recognized [4,14,9], as $T\rightarrow 0$, $\langle(\delta N)^2\rangle^{1/2}$ approaches $\langle N\rangle$ (hence is not small compared to N), in contrast with the actual physical situation for a collection of trapped atoms. Although the total number is not exactly known, it cannot fluctuate if the trapped cloud does not exchange particles with a surrounding bath.

Going beyond the mean value and the fluctuation of N, it is interesting to consider the probability distribution $P(N|u,v)$ over N, for given u and v. For this purpose, we return to Eq. (6) and obtain

$$P(N|u,v)=u^N Z(N,v)/R(u,v). \tag{56}$$

The partition function for the canonical ensemble, $Z(N,v)$, thus provides a distribution over N for the *grand* canonical ensemble. Numerical calculations of $P(N|u,v)$, shown for $N=500$ in Fig. 2, display qualitatively different behavior over three regimes of temperature. Above T_c (for $N=500$, $kT_c/\hbar\omega=6.78053$), the distribution is Gaussian, centered on $\langle N\rangle$; $P(N)\approx\exp[(N-\langle N\rangle)/\sigma]^2/\sigma\sqrt{\pi}$ with $\sigma^2\approx 2\langle\delta^2N\rangle$. Slightly below T_c (Fig. 2), the peak occurs substantially below the mean, and there is a long tail at high N. Near $T=0$, the peak occurs at N_1, a very small value of N, and the distribution is found to have the form

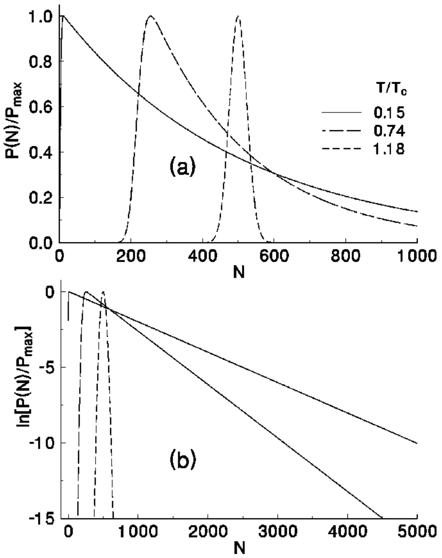

FIG. 2. Probability distributions for $\langle N\rangle=500$ atoms for three values of T/T_c for the GCE, normalized to unity at the maximum. Above T_c, the distribution is a Gaussian centered on $\langle N\rangle$. For $T/T_c \ll 1$, the distribution is exponentially decreasing. (a) Linear scale. (b) Log scale. The straight lines for $T/T_c=0.15$ and 0.74 show that the exponential decrease at these temperatures is nearly exact.

$$P(N|u,v)\approx\frac{1}{\langle N\rangle}e^{-(N-N_1)/\langle N\rangle}, \tag{57}$$

an exponential decrease. Thus for $T<T_c$, ln[$P(N)$] exhibits a linear decrease, as shown in Fig. 2(b), consistent with Eq. (55). Clearly, the shape of this probability distribution must be taken into account when considering any property of the ensemble that depends on $\langle N\rangle$ in a nonlinear way.

B. Occupation numbers

The distribution function for occupation numbers, n_i, and for n_0 in particular is especially relevant for Bose-Einstein condensation phenomena. It is interesting to observe that while the averages of n_i are not thermodynamical quantities, nevertheless they can be obtained with the help of the partition functions alone. For general i, for given u and v, the probability that n_i assumes a particular value is

$$\Pr(n_i|u,v)=R(n_i|u,v)/R(u,v)=u^{n_i}v^{in_i}(1-uv^i)^{g_i}C(n_i). \tag{58}$$

For $i=0$, this assumes a particularly simple form:

$$\Pr(n_0|u)=u^{n_0}(1-u). \tag{59}$$

Note that since $u<1$, $\Pr(n_0|u)$ for the GCE is always a decreasing function of n_0, and does not peak at $n_0=N$ even as $T\rightarrow 0$. From Eq. (59) one obtains the standard results [4] $\langle n_0\rangle=u/(1-u)$ and $\langle(\Delta n_0)^2\rangle=\langle(n_0-\langle n_0\rangle)^2\rangle=\langle n_0^2\rangle-\langle n_0\rangle^2=u/(1-u)^2$. Here again is the so-called ''fluctuation catastrophe'' [9], in that near $T=0$, both the average value and the fluctuation of n_0 are on the order of N, which is inconsistent with the assumption that the number of atoms is fixed at N.

This pathological situation does not arise with the canonical or microcanonical ensembles. For general level i,

$$\Pr(n_i|N,v)=Z(n_i|N,v)/Z(N,v). \tag{60}$$

For the canonical ensemble, we invoke the definitions, which involve a single constraint:

$$Z(N,v)=\prod_k\sum_{n_k}{}'\,C(n_k)v^{kn_k},\qquad \sum_{k=0}n_k=N \tag{61}$$

and

$$Z(n_i|N,v)=C(n_i)v^{in_i}\prod_{k\neq i}\sum_{n_k}{}'\,C(n_k)v^{kn_k}. \tag{62}$$

Then we can write

$$\begin{aligned}\sum_N Pr(n_i|N,v)Z(N,v)u^N\\ &=\sum_N Z(n_i|N,v)u^N=C(n_i)u^{n_i}v^{in_i}\prod_{k\neq i}\sum_{n_k}u^{n_k}C(n_k)v^{kn_k}\\ &=C(n_i)u^{n_i}v^{in_i}\prod_{k\neq i}\frac{1}{(1-uv^k)^{g_k}}\\ &=C(n_i)u^{n_i}v^{in_i}(1-uv^i)^{g_i}\sum_N Z(N,v)u^N.\end{aligned} \tag{63}$$

Equating coefficients of u^N, we obtain

$$\Pr(n_i|N,v)=\frac{C(n_i)}{Z(N,v)}\sum_{l=0}^{g_i}(-1)^l\binom{g_i}{l}Z(N-n_i-l)v^{i(n_i+l)}. \tag{64}$$

For the ground state,

$$\Pr(n_0|N,v)=[Z(N-n_0,v)-Z(N-n_0-1,v)]/Z(N,v), \tag{65}$$

where it is understood that $\Pr(n_0=N|N,v)=1/Z(N,v)$. Equation (65) can be used in conjunction with the above recursion relations.

For the microcanonical ensemble, we again fix n_i to have the value n_i'. The sum over the thus reduced total number of allowed states $W(n_i'|N,K)$ is now given by

$$W(n_i'|N,K)=\sum_{\{n_i\}}{}''\prod_k C(n_k)\delta(n_i-n_i'), \tag{66}$$

where the Kronecker delta assures that now the allowed occupation number sets satisfy the previous constraints with also $n_i=n_i'$. Then the probability that $n_i=n_i'$, $\Pr(n_i'|N,K)$, is given by

$$\Pr(n_i'|N,K)=W(n_i'|N,K)/W(N,K). \tag{67}$$

From this it follows that (the primes are no longer needed)

$$\begin{aligned}\sum_N \sum_K u^N v^K \mathrm{Pr}(n_i|N,K)W(N,K) &= u^{n_i} v^{in_i} C(n_i) \prod_{k\neq i} \sum_{n_k} u^{n_k} v^{kn_k} C(n_k) = u^{n_i} v^{rn_i} C(n_i) \prod_{k \neq i} [1/(1-uv^{\epsilon_k})]^{g_k} \\ &= u^{n_i} v^{in_i} C(n_i)[(1-uv^i)]^{g_r} \prod_k \frac{1}{(1-uv^k)^{g_k}} = u^{n_i} v^{in_i} C(n_i)[(1-uv^i)]^{g_i} R(u,v),\end{aligned} \tag{68}$$

or

$$\sum_N \sum_K u^N v^K \mathrm{Pr}(n_i|N,K)W(N,K) = u^{n_i} v^{in_i} C(n_i)[(1-uv^i)]^{g_i} \sum_N \sum_K u^N v^K W(N,K), \tag{69}$$

replacing $R(u,v)$ by its defining sum on the right-hand side.

Consider now the single-particle ground state, for which the energy vanishes and the degeneracy is one. Hence

$$\sum_N \sum_K u^N v^K Pr(n_0|N,K)W(N,K) = u^{n_0}[(1-u)] \sum_N \sum_K u^N v^K W(N,K). \tag{70}$$

Comparing equal powers of u and v, we immediately obtain

$$\mathrm{Pr}(n_0|N,K) = [W(N-n_0,K) - W(N-n_0-1,K)]/W(N,K). \tag{71}$$

An expression analogous to Eqs. (65) and (71) has been derived in Ref. [10] by a different line of reasoning.

Probability distributions of n_0 for the three ensembles are shown in Fig. 3. The GCE distribution, $\mathrm{Pr}(n_0|u,v)$, decreases with n_0 and thus below T_c, has a radically different form from the other two. Below T_c, the MCE distribution, $\mathrm{Pr}(n_0|N,K)$, is narrower than the CE distribution, $\mathrm{Pr}(n_0|N,v)$, because of the additional constraint. Also, the most probable values of n_0 [peak values of $\mathrm{Pr}(n_0)$] differ between the CE and MCE. For T sufficiently low, both $\mathrm{Pr}(n_0|N,K)$ and $\mathrm{Pr}(n_0|N,v)$ approach distributions peaked at $n_0 \approx N$. On the other hand, above T_c, all three distributions have nearly the same shape. These conclusions do not depend on $\langle N \rangle$.

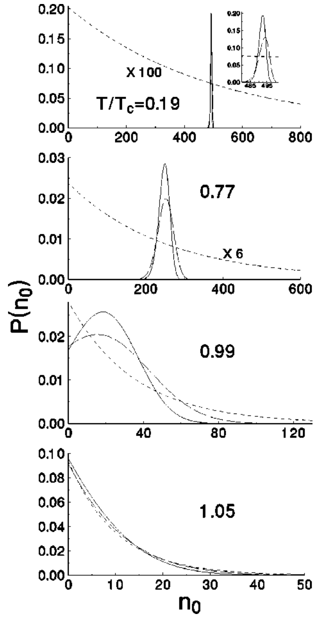

FIG. 3. Probability distributions for the ground-state occupation number, $\mathrm{Pr}(n_0)$ for $N=500$ atoms, for several values of T for the three ensembles. Below T_c, the shape of the GCE distribution differs drastically from that of the CE and MCE. The MCE distribution exhibits a slightly narrower Gaussian than the CE. Above T_c, the three distributions have a similar shape.

Given the probability distribution we now compute averages for the ground and first excited state occupation numbers. An elementary computation yields

$$\langle n_0 \rangle_{N,K} = \sum_{i=1}^{N-1} W(i,K)/W(N,K). \tag{72}$$

Also for the first excited state, a reasonably simple expression results:

$$\langle n_1 \rangle_{N,K} = \frac{3}{W(N,K)} \sum_{j=1}^{N} W(N-j,K-j). \tag{73}$$

More complicated expressions can be found for $\langle n_k \rangle_{N,K}$, for $k>1$.

From Eq. (72), we obtain the *recursion relation*

$$\begin{aligned}\langle n_0 \rangle_{N,K} &= [W(N-1,K)/W(N,K)] \\ &\quad \times \left[1 + \sum_{i=1}^{N-2} W(i,K)/W(N-1,K) \right] \\ &= e^{\alpha(N,K)} \big[1 + \langle n_0 \rangle_{N-1,K} \big],\end{aligned} \tag{74}$$

by shifting N into $N-1$ to specify $\langle n_0 \rangle_{N-1,K}$, and observing that by definition $[W(N-1)/W(N)] = e^{S(N-1,K)/k - S(N,K)/k} = e^{\alpha(N,K)}$, where $\alpha = \mu/T$.

If N is large compared to unity this results in the *approximation*

$$\langle n_0 \rangle_{N,K} \approx 1/(e^{-\alpha(N,K)} - 1). \tag{75}$$

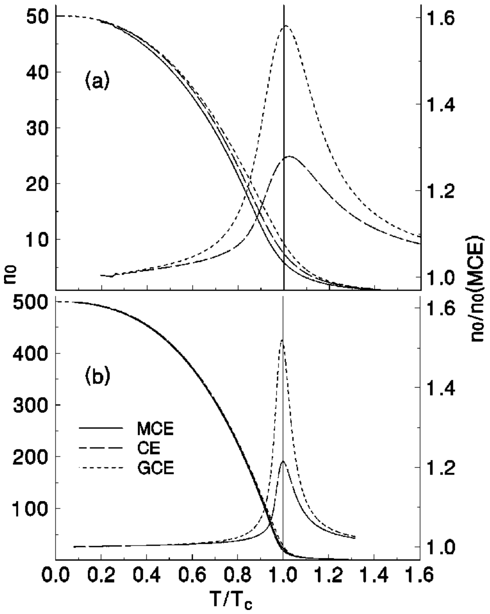

FIG. 4. Values for $\langle n_0\rangle$ vs T for (a) 50 and (b) 500 atoms, for the three ensembles (left axis). The curves peaking near T_c are the ratios of the GCE and CE results to the MCE results (right axis).

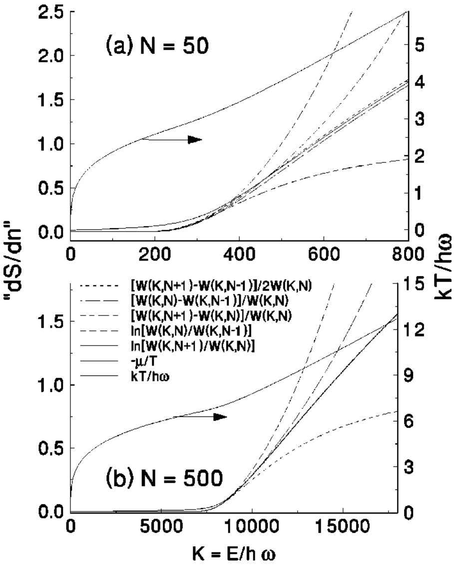

FIG. 5. Various possible discretizations for computing $-\mu/T = \partial S/\partial N$ for the MCE, as compared with the GCE value (solid line). (a) 50; (b) 500 atoms, showing the convergence with N.

This is the same as the GCE expression provided we can replace the grand canonical averages, $\langle N\rangle$ and $\langle K\rangle$, with N and K. Thus the microcanonical result differs in *two* ways from the grand canonical one; the averages are replaced with actual values of N and K, *and* the recursion relation is approximated.

A more direct comparison between Eq. (74) and Eq. (75) is obtained by repeated application of the recursion relation, which yields

$$\begin{aligned}\langle n_0\rangle_{N,K} = {} & e^{\alpha(N,K)} + e^{[\alpha(N,K)+\alpha(N-1,K)]} \\ & + e^{[\alpha(N,K)+\alpha(N-1,K)+\alpha(N-2,K)]} + \cdots \\ & + e^{[\alpha(N,K)+\cdots+a(1,K)]}, \end{aligned} \tag{76}$$

with N terms altogether on the right-hand side. This may be compared with an expansion of the denominator of the approximate result:

$$\langle n_0\rangle_{N,K} = e^{\alpha(N,K)} + e^{2\alpha(N,K)} + e^{3\alpha(N,K)} + \cdots . \tag{77}$$

In fact, the MCE average, $\langle n_0\rangle_{N,K}$, is quite close to the equivalent GCE average, except for T near T_c for small N. Figure 4 shows $\langle n_0\rangle$ values for all three ensembles, for $N=50$ and 500. (For the MCE, T is obtained from Eq. (27), $(\partial S/\partial E)_N = 1/T$, where $S = k\ln[W(N,E)]$.) As is well known [21,8,14], the effect of the BEC transition for finite N is not abrupt. For $N=50$ and 500, Fig. 4 shows that the relative extent of the transition region decreases as N increases. We also plot in Fig. 4 (right-hand scale) the ratio between the GCE and the MCE values for $\langle n_0\rangle$ and the ratio between the CE and the MCE values. Both of these ratios exhibit a maximum near T_c, and these maxima decrease slowly as N increases. However, the width of the ratio curves does diminish sharply with increasing N.

C. Chemical potential and fugacity

1. Mean values of μ/T and μ

There are significant differences in the meaning and role of the chemical potential μ in the three different ensembles. These differences are often ignored because it is usually assumed, in the homogeneous situation, that the sample as well as the bath is to be taken to the thermodynamical limit of large N, with N/V finite. A small number of atoms in a harmonic trap cannot be considered to be at the thermodynamical limit, and these differences become appreciable.

Before comparing results for the different ensembles, we discuss discretization procedures, a topic raised at the end of Sec. III A. For example, for the microcanonical ensemble, the partial differential expression in Eq. (27) for $-\mu/T$ can be interpreted as $[1/W(N,K)][W(N+1,K)-W(N,K)]$ or other similar expressions, or as $S(N,K)-S(N-1,K) = \ln[W(N,K)] - \ln[W(N-1,K)] = \ln[W(N,K)/W(N-1,K)]$, or similarly. We compare results with these different forms in Fig. 5. Especially for $T > T_c$, the $\Delta W/W$ forms differ widely from the $\Delta\ln W$ forms, and the differences do not diminish rapidly as N increases, as seen by comparing Figs. 5(a) and 5(b). In this figure, the solid line gives the value of $-(\mu/T)_{\rm GCE}$ for which $\langle N\rangle$ equals the given N in the grand canonical sum, Eq. (52). It is seen that the two Δ ln W forms narrowly bracket $-(\mu/T)_{\rm GCE}$, with the differences decreasing approximately as $1/N$. So this indicates a clear preference for this form. Below T_c, $-(\mu/T)_{\rm GCE}$ exhibits deviations proportional to $1/N$ from every one of these discretizations. For the quantity $1/T = \partial S/\partial E$, the differences are relatively smaller, and largest as $T \to 0$.

A comparison of the values for μ obtained as above for the three ensembles is one measure of the degree to which these three approaches lead to a consistent thermodynamics. Figure 6 shows such a comparison. For the GCE, $\mu_{\rm bath} = \langle \mu_{\rm system}\rangle_{\beta,N}$, which is the value of μ for which the sum in Eq. (52) equals the given N exactly. For the CE,

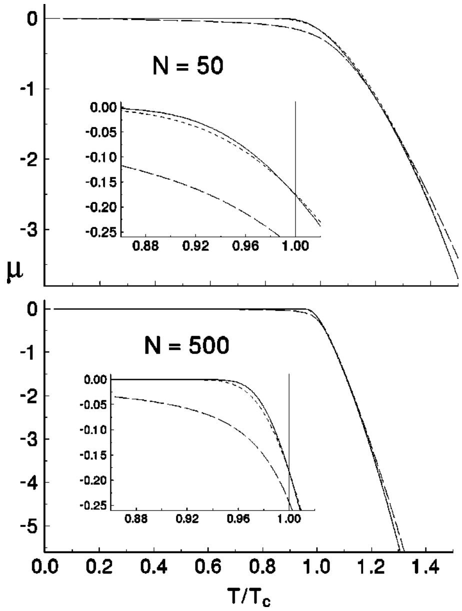

FIG. 6. Values of the chemical potential for the three ensembles for (a) 50 and (b) 500 atoms. Solid lines: MCE; short dashed lines: CE; long dashed lines: GCE.

$$\mu_{\text{system}}=\frac{\partial F}{\partial N}=-T\frac{\partial \ln[Z(N,v)]}{\partial N}, \tag{78}$$

where F is the free energy, and for the MCE (making the discrete form explicit), $\mu=\ln[W(N,K)/W(N-1,K)]/\ln[W(N,K)/W(N,K-1)]$. There are indeed differences for small N, especially for $T<T_c$. An obvious example occurs for T near zero. For the MCE for $K\leqslant N$ the number of configurations, W, is independent of N, hence from the second Eq. (27) $\mu=0$ exactly, whereas this is not true for the GCE. Note also that the large discrepancies near T_c diminish with N.

Also from Fig. 6, it is evident that in no ensemble is $\mu=0$ (or $u=1$) at $T=T_c$, although this condition is most nearly satisfied for the MCE and for larger values of N.

Although values for μ for given N and T for the different ensembles do not agree, if one considers the fugacity, $u=\exp(\mu\beta)$, rather than μ, the appropriate *average* of the MCE quantity agrees exactly with the GCE quantity provided that specific conventions are adopted for the partial derivatives. If the second of Eqs. (27) is interpreted as

$$\left(-\frac{\mu}{T}\right)_{\text{MCE}}=S(N,K)-S(N-1,K)=\ln\left(\frac{W(N,K)}{W(N-1,K)}\right). \tag{79}$$

Then the GCE average does indeed equal the fugacity exactly:

$$\begin{aligned}\left\langle e^{(\mu/T)(\text{MCE})}\right\rangle_{u,v} &=\frac{1}{R(u,v)}\sum_{N'=0}^{\infty}\sum_{K'=0}^{\infty}\left(\frac{W(N'-1,K')}{W(N',K')}\right)u^{N'}v^{K'}W(N',K')\\ &=\frac{u}{R(u,v)}\sum_{N'=0}^{\infty}\sum_{K'=0}^{\infty}W(N',K)u^{N'}v^{K'}=u,\end{aligned} \tag{80}$$

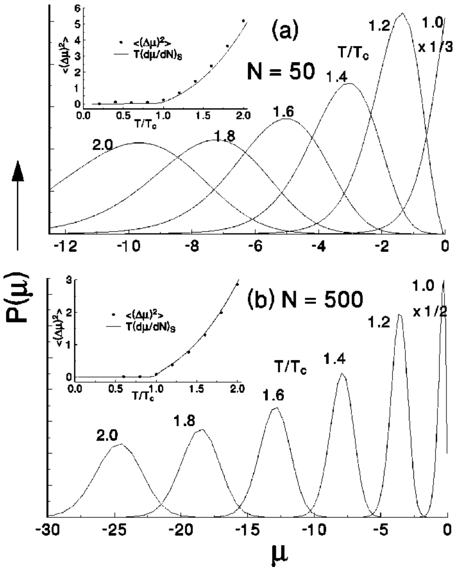

FIG. 7. For the GCE, μ_{bath} is fixed, but there is a probability distribution over μ_{system} as shown in these curves for several values of T/T_c, for (a) 50 and (b) 500 atoms. The insets show the variance $\langle(\Delta\mu)^2\rangle$ as compared with $T(d\mu/dN)_S$.

where the second equality follows because $W(-1,K)\equiv 0$. The form of the derivative used here is consistent with the discussion above concerning Fig. 5. Equation (80) suggests that the fugacity, u, rather than μ, is the fundamental parameter.

2. Fluctuations of μ

As stated in Sec. III A, for the microcanonical ensemble, N and K (or E) are fixed parameters, and therefore the chemical potential, obtained from Eq. (27) with $S=k\ \ln[W(N,K)]$, is also a sharply defined quantity. For the *canonical* ensemble, N is given and therefore again μ is fixed, and may be determined from Eq. (78). For the GCE, the system is considered to be in thermal equilibrium with a heat bath and particle reservoir for which $T=T_{\text{bath}}$ and $\mu=\mu_{\text{bath}}$ and (or equivalently, the given variables are $v\equiv v_{\text{bath}}$ and $u\equiv u_{\text{bath}}$). We will discuss the probability distribution of μ_{system}, consider $\langle(\Delta\mu_{\text{system}})^2\rangle$, and make comparisons with the estimates for a Gaussian distribution in Sec. III A.

The probability distribution of μ_{system} may be obtained from Eq. (6). For given u and v or T_{bath} and μ_{bath}, for each pair of (discrete) values N and K, with probability $P(N,K)=u^Nv^KW(N,K)/R(u,v)$, we have $\mu_{\text{system}}(N,K)/T=-\ln[W(N,K)/W(N-1,K)]$ [in accord with Eq. (79)] and therefore $P[\mu_{\text{system}}(N,K)]=P(N,K)$. We compute $P[\mu_{\text{system}}(N,K)]$ over the relevant range of N and K values, and sum the probabilities within each bin $n\Delta\mu<\mu<(n+1)\Delta\mu$.

Examples of $P(\mu_{\text{system}}|u,v)$ are shown in Fig. 7. Above T_c, there is a nearly Gaussian distribution over μ_{system} with a peak close to μ_{bath}. However, below T_c, the long tail in $P(N|u,v)$ as shown in Fig. 2 implies that a large fraction of the atom distribution will be associated with a very small value of $|\mu_{\text{system}}|$. Hence there is a peak in $P(\mu_{\text{system}}|u,v)$ at $\mu_{\text{system}}=0$, or, more precisely, in the bin $\Delta\mu_{\text{system}}<\mu_{\text{system}}\leqslant 0$. The shape of this peak will depend on the bin size

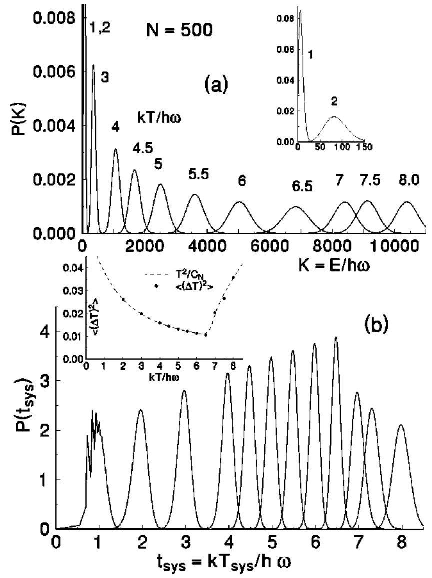

FIG. 8. For the CE, $T_{\rm bath}$ is specified, but there is a distribution over E values of the system (top). In view of this distribution, there is a corresponding distribution over $T_{\rm system}$ values (bottom). The results are for 500 atoms, for which $kT_c/\hbar\omega = 6.7805$. The individual distributions in the bottom plot correspond to the temperatures indicated above. The irregular $P(T_{\rm system})$ distribution for $T = \hbar\omega/k$ arises because of odd-even asymmetry in K. The inset shows a comparison of $\langle(\Delta T)^2\rangle$ as compared with the analytic expression T^2/C_N.

$\Delta\mu_{\rm system}$ used in computing $P(\mu_{\rm system}|u,v)$.

In Sec. III B [Eq. (50)], we obtained the result that the variance $\langle(\Delta\mu)^2\rangle = T(\partial\mu/\partial N)_S$. We have numerically computed this partial derivative by obtaining $\mu_{\rm bath}(E,N) = \mu_{\rm system}(E,N)$ to satisfy $\langle N\rangle = N$ in Eq. (52), and $S(E,N) = \int_0^E (dE'/T)_N + \ln(N) + 1/2N + \cdots)$, where the terms in N are constructed to ensure that $\partial S/\partial N = \mu/T$ as $T\to 0$. We have found that with this construction of $S(E,N)$, the desired condition $\mu_{\rm bath}/T = \mu_{\rm system}/T = -\partial S/\partial N$, is obtained to a high degree of accuracy. The fitted variances from the $P(\mu_{\rm system}|u,v)$ agree well but not exactly with the analytic expression, as shown in the inset of Fig. 7.

D. Energy and temperature

In the grand canonical ensemble, for given bath parameters u and v, or $\mu_{\rm bath}$ and $T_{\rm bath}$, there is a distribution over N and K, given by

$$P(N,K|u,v) = u^N v^K W(N,K)/R(u,v). \tag{81}$$

Since K, like N, is a non-negative quantity, the distributions exhibit similar non-Gaussian behavior when the probability of $K=0$ or $N=0$ becomes significant.

For the canonical ensemble *(N* fixed), $T_{\rm bath}$ is given and K fluctuates. The probability distribution for K is given by

$$P(K|N,v) = v^K W(N,K)/Z(N,v). \tag{82}$$

Examples are shown in Fig. 8(a). For each value of K, $T_{\rm system}$ is determined from the first Eq. (27), so there is also a distribution over $T_{\rm system}$, shown in Fig. 8(b). When the distributions are essentially Gaussian, the widths deduced from them agree well with the expression $\langle(\Delta T)^2\rangle = T^2/C_N$ given above [Eqs. (31) and (45)], as shown in Fig. 8(b) (inset). Note that the fluctuation in $T_{\rm system}$ is *minimum* at $T = T_c$.

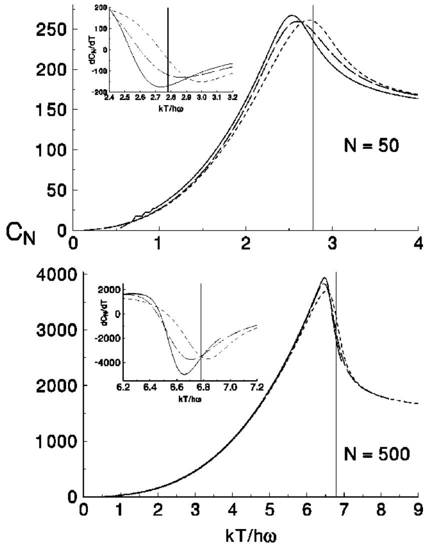

FIG. 9. The specific heat, $C_N = d\langle E\rangle/dT$ for (a) 50 and (b) 500 atoms. The insets show dC_N/dT. The minimum in the slope provides a possible definition for T_c that is close to Eq. (54) but may be extended to interacting atoms.

Analogous to Eq. (81) for the fugacity, the grand canonical average of the microcanonical $v = \exp(-\beta)$ [where T is obtained from the first of Eqs. (27)] equals the grand canonical bath parameter, v. If one defines the partial derivative as in Eq. (79),

$$-\left(\frac{1}{T}\right)_{\rm MCE} = -\ln\left(\frac{W(N,K)}{W(N,K-1)}\right), \tag{83}$$

then the GCE average is

$$\langle v_{\rm MCE}\rangle_{u,v} = \frac{1}{R(u,v)}\sum_{N'=0}^{\infty}\sum_{K'=0}^{\infty} W(N',K'-1)u^{N'}v^{K'} = v. \tag{84}$$

Hence the average of the MCE variable v is the GCE bath parameter, while this is not precisely true for β or T. This suggests that v is a more fundamental parameter than T or β. Unlike the fugacity, v traditionally has no name but perhaps could be called the ‘‘thermicity’’ or ‘‘hotness.’’

V. SPECIFIC HEAT

For trapped atoms, N rather than volume or pressure is to be considered constant. Thus for the specific heat, one has $C_N = (dE/dT)_{N={\rm const}}$ for the MCE, or $C_N = (d\langle E\rangle/dT)_{N={\rm const}}$ for the CE, or $(d\langle E\rangle/dT)_{\langle N\rangle={\rm const}}$ the GCE. Figure 9 shows the results, again for $\langle N\rangle = 50$ and 500, for the three ensembles considered here. The differences between the peak position for the different ensembles show that the different assumed conditions—whether there is a heat bath, and whether there is exchange of particles as well as energy with it—do make a difference in the value of C_N, especially the point at which C_N reaches its maximum. The peak in C_N

sharpens as N increases and the differences between the three ensembles diminish.

Possible definitions for T_c

A precise value for the BEC critical temperature, T_c, offers one way to characterize a Bose system. For example, there have been several recent discussions [22–25] regarding the change in T_c between ideal and real Bose gases. In recent quantum Monte Carlo calculations [25] for a box potential, T_c was identified as the point at which $N^{1/3}\rho_s/\rho(T)$ is independent of N, where ρ_s/ρ is the superfluid fraction. This definition, based on the divergence of the correlation length in such a homogeneous though finite system, may not be easy to apply to Bose atoms in a harmonic potential. Also, for finite N, the smooth n_0 versus T curve (Fig. 4) does not provide an unambiguous, precise definition for T_c. Furthermore, as pointed out above, the definition of T_c in Refs. [14] and [21] [Eq. (54) above] is based on the fictitious assumptions that the fugacity is exactly unity and that n_0 is exactly zero at T_c, and that the GCE expressions apply to trapped atoms. In any case, this definition is difficult to extend to the case of interacting atoms. In Ref. [24], the critical temperature for atoms in a harmonic trap is taken to be the temperature at which the density at the origin is equal to the free-space critical density, $\rho_c^{\text{fs}}=2.612/\lambda_T^3$ [3], where λ_T is the thermal de Broglie wavelength. We have found that at T_c as defined in Eq. (54), the density at the center of an isotropic harmonic trap is typically more than twice ρ_c^{fs}, so this definition leads to a higher critical temperature than Eq. (54). (Alternatively, one could consider the *average* density within the range of the classical turning points for an atom with $E=kT_c$.)

For Bose atoms in a harmonic trap, the specific heat presents a less ambiguous definition of T_c that may be applied to interacting atoms as well as to an ideal gas. The peak in the specific heat function provides one natural benchmark. The plots in Fig. 9, however, indicate that the peak in $C_N(T)$ tends to occur where ≈10% of the atoms are in the ground state, hence does not correspond with the onset of finite ground state occupation as one expects, and occurs at a temperature significantly lower than T_c as defined in Eq. (54). The minimum of dC_N/dT offers an alternative benchmark point that corresponds to the discontinuity in the $C_N(T)$ function at infinite N. For an ideal Bose gase, the exact recursion relation methods discussed in Sec. II are suited for calculations in the region of T_c, but the large values for $W(N,K)$ limit the MCE methods to 500 or 1000 atoms, and to five times that number for $Z(N,v)$ and the CE. Figure 10 shows T_c values from Eq. (54) in comparison with results from the three ensembles deduced from the most negative slope and the peak of the $C_N(T)$ function. The inset shows that the difference between these two points for the GCE results remains nearly constant for N up to 10^6 atoms, and that the point at which $C_N(T)$ has the most negative slope is close to the value given by Eq. (54). When the point of most negative slope of $C_N(T)$ is used to obtain a value for T_c from the CE results, $kT_c/\hbar\omega$ is about 0.1 less than for the GCE for $500<N<5000$.

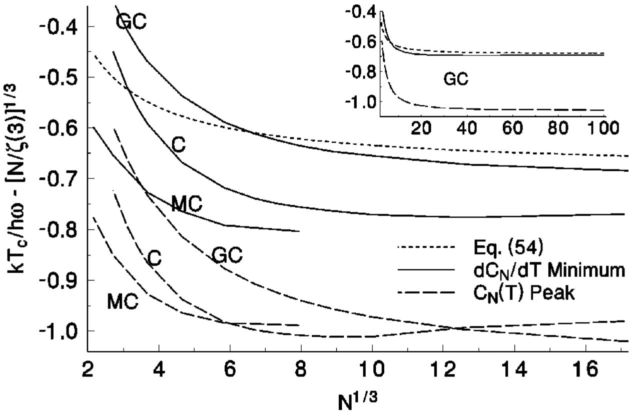

FIG. 10. Variation of the critical temperature with atomic number for the three ensembles. The plotted curves are for $kT_c/\hbar\omega-[N/\zeta(3)]^{1/3}$ vs $N^{1/3}$. The short-dashed line represents Eq. (54). The long-dashed lines represent the minimum of $dC_N(T)/dT$ for the three ensembles, and the solid lines represent the peak of $C_N(T)$. GCE, CE, and MCE results are denoted by GC, C, and MC, respectively. Note that the MCE results extend only to $N=500$, CE results to $N=5000$. The inset extends the GCE results up to $N=10^6$.

VI. CONCLUSION

For ideal Bose atoms in a harmonic potential, we have obtained recursion relations linking the distributions for different dimensions and also we have used previously derived recursion relations for the canonical and microcanonical partition functions. From these we have studied the statistical mechanics and in particular the fluctuations of various parameters for small atom numbers. The three most commonly used ensembles have quite distinct statistical properties. For the GCE, the number of particles in the system fluctuates, and correspondingly, the system chemical potential or fugacity will fluctuate although the bath values are fixed. For the CE as well as for the GCE, the bath temperature is given, but the total energy of the system fluctuates and thus the temperature of the system will fluctuate about the bath value. For the GCE, we have obtained estimates of the fluctuations of intensive variables, T and μ, as well as extensive variables N and E. Although previous discussions have focused primarily on the ground-state occupation number, n_0, the statistical fluctuations of all of these quantities are of interest in characterizing the different ensembles.

However, estimates of variances do not tell the full story because the probability distributions are often non-Gaussian below T_c. For the GCE with $T\ll T_c$, the probability distribution of total atomic number, N, and ground-state occupation number, n_0, are close to a simple exponential decrease, rather than a Gaussian distribution, and the probability distribution of the chemical potential also decreases from a peak value at $\mu=0$. For the CE and MCE, the n_0 distributions are more nearly Gaussian. As recently reported elsewhere [12,11], the fluctuation of n_0 is less with the microcanonical ensemble than with the canonical ensemble, and much less with the canonical ensemble than with the grand canonical ensemble. It is pertinent here to note Politzer's conclusion [7] that fluctuations of n_0 in the GCE are much reduced when atom-atom interactions are present. The effect of atom-atom interactions on other conclusions here is clearly an important issue but outside the scope of the present study.

The specific heat function, $C_N(T)$, provides a useful comparison between the different ensembles and a test of the rate of convergence of the results with N or $\langle N\rangle$. We propose that the point of most negative slope of $C_N(T)$ provides an unambiguous definition for T_c that is close to values from the recently proposed definition [14,21] [Eq. (54) above] for an ideal Bose gas, and extendable to interacting atoms.

Fractional variances or fluctuations typically decrease with N, and so become less important for large numbers of atoms. Nevertheless, results from this study do highlight the conclusion that the GCE, though most commonly used for modeling and computations, is actually inconsistent with the experimental conditions in which there is no equilibration of matter or energy with a heat bath. Thus one of our goals has been to develop methods for using the microcanonical ensemble. For small numbers of atoms ($N \leqslant 500$ here, possibly up to 1000 atoms) it is possible to obtain explicit results and study the statistical properties of the microcanonical and canonical as well as the grand canonical ensembles.

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