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Bose-Einstein Condensation, Fluctuations, and Recurrence Relations in Statistical Mechanics

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Abstract

We calculate certain features of Bose-Einstein condensation in the ideal gas by using recurrence relations for the partition function. The grand canonical ensemble gives inaccurate results for certain properties of the condensate that are accurately provided by the canonical ensemble. Calculations in the latter can be made tractable for finite systems by means of the recurrence relations. The ideal one-dimensional harmonic Bose gas provides a particularly simple and pedagogically useful model for which detailed results are easily derived. An analysis of the Bose system via permutation cycles yields insight into the physical meaning of the recurrence relations.

I. INTRODUCTION

The achievement of Bose-Einstein condensation (BEC) in alkali gases[1] was a remarkable feat in atomic and low-temperature physics. The gases are most often trapped magnetically in potentials accurately approximated by harmonic oscillator wells. The result has been a deluge of theoretical papers on BEC in harmonic potentials, both for ideal and interacting gases.[2] Experimentally, the gases are sufficiently dilute and weakly interacting that the ideal gas is a good first approximation for their description, making the subject more accessible to students even in their first statistical-physics course.

A basic problem with the standard presentation of BEC is that the grand canonical ensemble misrepresents several physical quatities when a condensate is present. For example, grand canonical ensemble calculations greatly overestimate the fluctuations of the condensate number. Although, because of their isolation, the most realistic description of the experimentally condensed gases is via the microcanonical ensemble, the canonical ensemble gives equally accurate results. In the latter the system of interest is in contact with a heat bath but the particle number is kept fixed, which is crucial.

Calculations using the canonical ensemble are avoided in most elementary treatments of BEC because of mathematical complications. The grand canonical ensemble removes these complications by putting the system in contact with a particle bath. Unfortunately, when there is a condensate, the de Broglie wavelength can be larger than the system size, making the distinction between system and bath meaningless and leading to the fluctuation inaccuracy mentioned. Moreover, the trapped Bose systems of current interest consist of relatively few particles. There exist simple methods using recurrence relations that have been exploited often in recent work to treat finite systems in the canonical ensemble; however, these relations are not well known outside the research literature. It is these techniques that we want to discuss here.

Because the experimental trapped systems are finite, they are not equivalent to systems in the thermodynamic limit. The trapped systems have a nonuniform distribution established by the external harmonic potential. The true thermodynamic limit in these systems would require that as the particle number N is increased, we also would decrease the frequency ω of the potential in such a way that the maximum density—proportional to $\omega^d N$, where d is the spatial dimension of the system—remains constant.[3,4] Although this limit is not physically

realized and finite systems have no real phase transitions, the experimental transformation of the system into its lowest state is still rather sudden. Nevertheless, the existence of a mathematically sharp phase transition is not crucial to the description of real systems. What is important is the appearance of a "condensation," by which we mean the rapid accumulation of a substantial fraction of the N particles into the ground state (without big fluctuations about this average) when the temperature falls below a certain finite value. We will show that even a finite one-dimensional ideal Bose gas in a harmonic potential has this property.

The choice of the canonical ensemble and the use of the recurrence relations are particularly suitable for the study of finite systems. Thus a simple model with physical properties amenable to calculation is available to be exploited for pedagogical or other purposes.

In Sec. II we will review the standard grand canonical ensemble treatment of the one-dimensional (1D) harmonic ideal Bose gas and identify a temperature below which there is a substantial accumulation of particles in the ground state. We will also identify the physically unrealistic fluctuations in the ground-state occupation that appear in the grand canonical ensemble description. In Sec. III we will show how the 1D Bose gas can be treated by developing a recurrence relation for the partition function. More general recurrence relations for the average number of particles in a single-particle state and for the partition function are developed in Sec. IV. Armed with these tools, we compare canonical ensemble calculations with their grand canonical ensemble equivalents. For a finite system there are only small differences in the mean values; however, there are large differences in the root-mean-square fluctuations. In Sec. V we look at the condensation problem from a quite different point of view, namely that of permutation cycles à la Feynman.[5] Such a view gives a physical explanation to several mathematical formulations found in the previous sections and especially to the partition function recurrence relation. From this point of view we also see that the grand canonical ensemble misrepresents the condensate, while the canonical ensemble treats it accurately. We find the somewhat surprising result that the condensate is made up of equally probable permutation cycles of all lengths up to the condensate number.

II. GRAND CANONICAL TREATMENT

We first consider a grand canonical ensemble treatment of BEC in a one-dimensional (1D) harmonic well. Although our approach is typical of most statistical physics textbooks, we know of only one such book that actually covers this particular example.[6] The harmonic potential leads to equally spaced single-particle energy levels given by

$$\epsilon_p = p\Delta, \tag{1}$$

with p a nonnegative integer. The zero-point energy, omitted in Eq. (1), can be restored to any physical quantity at the end of the calculation. The constant Δ is related to the harmonic angular frequency ω by $\Delta = \hbar\omega$.

In the grand canonical ensemble[7] the average number of particles N is given by the relation

$$N = \sum_p \frac{1}{e^{\beta(\epsilon_p - \mu)} - 1}, \tag{2}$$

where $\beta = 1/k_B T$ and μ is the chemical potential. In Bose problems the denominator is often expanded in powers of $e^{-\beta(\epsilon_p - \mu)}$ to yield

$$N = \sum_{l=1}^{\infty} e^{l\beta\mu} \sum_{p=0}^{\infty} e^{-\beta l p \Delta} = \sum_{l=1}^{\infty} e^{l\beta\mu} Z_1(\beta l), \tag{3}$$

where

$$Z_1(\beta l) = \frac{1}{1 - e^{-\beta l \Delta}} \tag{4}$$

is the one-body partition function at the effective inverse temperature βl. In Sec. V we will see that the sum over l in Eq. (3) represents a sum over permutation cycles.

For the very weak potentials used to trap N particles experimentally, the harmonic oscillator states are very closely spaced ($\hbar\omega \ll k_B T$). Thus to a good approximation we can replace the sum over p in Eq. (3) by an integral. (Alternatively, we could directly replace the sum in Eq. (2) by an integral to arrive at the same result.) Because $\int dp\, e^{-\beta l p \Delta} = (\beta l \Delta)^{-1}$, we find

$$N \approx N' = \frac{1}{\beta\Delta} \sum_{l=1}^{\infty} e^{l\beta\mu} \frac{1}{l} = -\frac{k_B T}{\Delta} \ln(1 - e^{\beta\mu}). \tag{5}$$

The sum in Eq. (5) is one of the Bose integrals,[8] which in this case can be evaluated analytically. Of course, changing the sum to an integral is valid only if the summand is a smooth function of p; we then lose the contribution of the lowest state when it becomes

occupied with order N particles. Hence N' in Eq. (5) is just the contribution of the excited states, and we obtain the total number N by including the ground-state population:

$$N = n_0 + N', \tag{6}$$

where

$$n_0 = (e^{-\beta\mu} - 1)^{-1}. \tag{7}$$

We want to identify a Bose-Einstein "transition temperature," that is, one below which there will be a sizable fraction of the N particles in the ground state. From Eq. (7) this requirement implies that $-\beta\mu = (\gamma N)^{-1} \ll 1$, where γ is a number of order unity. If we invert Eq. (5), we obtain

$$1 - e^{-\beta N'\Delta} = e^{\beta\mu} \approx 1 + \beta\mu, \tag{8}$$

so that $\beta N'\Delta \approx \ln \gamma N$. Because N' is of order N at the transition, we find that the condensate will be large for temperatures below T_0 defined by[3,9]

$$T_0 = \frac{N\Delta}{k_B \ln N}. \tag{9}$$

We can show[3] that the density of the system is proportional to $N\Delta$, so that, in the thermodynamic limit, we keep the numerator $N\Delta$ constant while letting $N \to \infty$, $\Delta \to 0$. Then the characteristic temperature will go to zero as $1/\ln N$, which is small only for extremely large N. In actual 1D experiments,[10,11] where N is about 10^4, the logarithm reduces this characteristic temperature only by a factor of order ten compared to $N\Delta/k_B$, an experimentally accessible value. Nevertheless, we say that there is a "quasi-condensation" rather than a real one. For a two-dimensional (2D) ideal gas we find that an actual phase transition occurs; however, in accord with the Hohenberg theorem,[3] this transition disappears if there are particle-particle interactions. On the other hand, some authors have claimed that the 1D and 2D finite interacting systems at sufficiently low temperature have a *true* condensation, because the coherence length becomes larger than the finite condensate size.[12,13] (Moreover, in 2D we expect a true phase transition of the Kosterlitz-Thouless variety[14] at a temperature of order $\Delta\sqrt{N}$.)

It is straightforward to solve Eq. (3) numerically for the chemical potential μ and compute the exact condensate number Eq. (7) for some given average N value. In Fig. 1 we show the occupation of the first two energy levels for $N = 500$. We see that T_0 provides a fairly good estimate of the quasi-condensation temperature.

Many textbooks compute particle-number fluctuations in the grand canonical ensemble.[7] The grand partition function for any ideal Bose gas with states ϵ_p each occupied by n_p particles is[7]

$$\mathcal{Z} = \sum_N Z_N \, e^{\beta\mu N} = \prod_p \sum_{n_p=0}^{\infty} e^{-\beta(\epsilon_p-\mu)n_p} = \prod_p \frac{1}{1-e^{-\beta(\epsilon_p-\mu)}}. \tag{10}$$

where Z_N is the canonical partition function of an N-particle system. The average square deviation of the occupation number n_p is

$$\overline{\Delta n_p^2} \equiv \overline{(n_p - \overline{n}_p)^2} = (k_B T)^2 \frac{\partial^2 \ln \mathcal{Z}}{\partial \epsilon_p^2} = \overline{n}_p + \overline{n}_p^2. \tag{11}$$

With no condensate we have $\overline{n}_p \ll 1$ for all except a negligible number of excited states, so $\overline{\Delta N^2} = \sum_p \overline{\Delta n_p^2} \approx \sum_p \overline{n}_p = N$, and we have a normal distribution with

$$\frac{\sqrt{\overline{\Delta N^2}}}{N} = O(N^{-1/2}). \tag{12}$$

However, with a condensate of order N, we have

$$\frac{\sqrt{\overline{\Delta n_0^2}}}{N} = O(1), \tag{13}$$

that is, the fluctuations of the condensate are as large as the condensate itself—a manifestly unphysical result. This problem is not new,[15,16] but has received a large amount of recent attention,[17,18,19,20,21,22,23,24,25,26,27] including the invention of a new "fourth" ensemble—the so-called "Maxwell demon" ensemble—to take care of it.[21]

There are various explanations of what goes wrong with the grand canonical ensemble. Grossmann and Holthaus[17] state that "[T]he relative mean square fluctuations of the ground state population, and thus the relative fluctuations of the total particle number, approach unity: as a result of particle exchange with the reservoir, the uncertainty of the number of particles becomes comparable with $\langle N \rangle$ itself. This fluctuation catastrophe is related to the divergency of the quantum coherence length λ_T for $T \to 0$. When λ_T vastly exceeds the length scale characterizing the system under consideration, a rigid distinction between 'system' and 'reservoir' is no longer practical." The difficulty also can be stated in more mathematical terms. The grand canonical ensemble often is shown to be equivalent to the canonical ensemble by using the method of steepest descents,[28] which evaluates the canonical partition function by an approximation to a complex integral of the grand canonical partition function. Wilkens and Weiss[23] state that "The most common procedure is to evaluate the contour integral in a stationary phase approximation. In leading order one recovers

the grand-canonical formulation. However, below T_c, fluctuations are badly represented in this approach. The reason is that, for large N, the saddle point is located within a distance $O(1/N)$ from the branch point while the Gaussian approximation for the fluctuations assumes a much larger range of validity $O(1/N^{1/2})$."

We will not pursue the cause of this difficulty further, but will avoid it by using the canonical ensemble.

III. ONE-DIMENSIONAL BOSE GAS BY THE CANONICAL ENSEMBLE

We next examine the 1D ideal Bose gas by using the canonical ensemble. There is a simple recurrence relation for the partition function of this model. As we will see in Sec. IV, there are more general recurrence relations by which other problems (for example, the 3D ideal Bose gas) can be treated. The connection between the two formulations turns out to be a special case of a famous theorem in number theory as we demonstrate in Sec. IV.

If we let $z = e^{\beta\mu}$, the grand partition function of Eq. (10) can be written as

$$\mathcal{Z} = \sum_N Z_N z^N = \sum_N \sum_{\{n\}}{}' z^N e^{-\beta\Delta \sum_p p n_p}, \tag{14}$$

where the prime in the sum over $\{n\}$ implies a sum over all $n_0, n_1, n_2, \ldots = 0, 1, 2, \ldots$ such that $\sum_p n_p = N$. If we define $x = e^{-\beta\Delta}$, the last exponential in Eq. (14) can be written as x^M with $M = E/\Delta = \sum_p p\, n_p$ and $\mathcal{Z}$ becomes

$$\mathcal{Z} = \sum_N \sum_{\{n\}}{}' x^M z^N = \sum_N \sum_M c_N(M)\, x^M z^N, \tag{15}$$

where $c_N(M)$ is the degeneracy factor for the energy state M of N particles.

In the 1D oscillator problem, this degeneracy factor $c_N(M)$ has a very interesting mathematical property.[19,29,30,31,32] It is just the number of ways that one can partition the integer M into N or less integers. For example, $M = 4$ can be partitioned in 5 ways: $1+1+1+1$, 1+1+2, 1+3, 2+2, and 4, which is equivalent to the number of ways that four Bose particles can be put in equally spaced states 0, 1, 2, 3, 4 to have 4 units of energy. Euler, Gauss, Hardy, Ramanujan, and many other famous mathematicians have contributed theorems on partitions.[33]

We do not need an explicit expression for $c_N(M)$. We can identify the canonical partition

function in Eq. (15) as

$$Z_N = \sum_M c_N(M)\, x^M. \tag{16}$$

We also have from Eq. (10) that

$$\mathcal{Z}(z) = \prod_p \frac{1}{1 - zx^p} = \frac{1}{1-z}\frac{1}{1-zx}\frac{1}{1-zx^2}\cdots \tag{17}$$

We next replace z in $\mathcal{Z}(z)$ by xz so that

$$\mathcal{Z}(xz) = \frac{1}{1-zx}\frac{1}{1-zx^2}\cdots = (1-z)\mathcal{Z}(z), \tag{18}$$

or

$$\sum_N \sum_M c_N(M)\, x^{M+N} z^N = (1-z) \sum_N \sum_M c_N(M)\, x^M z^N. \tag{19}$$

We equate equal powers of z to obtain

$$\sum_M c_N(M)\, x^{M+N} = \sum_M c_N(M)\, x^M - \sum_M c_{N-1}(M)\, x^M \tag{20}$$

so that

$$x^M Z_N = Z_N - Z_{N-1}, \tag{21}$$

and

$$Z_N = \frac{1}{1-x^N}\, Z_{N-1}. \tag{22}$$

This recurrence relation is trivial to solve explictly. We obtain

$$Z_N = \prod_{k=1}^{N} \frac{1}{1-x^k} = \prod_{k=1}^{N} Z_1(\beta k). \tag{23}$$

Many derivations and uses of this result are found in the current research literature.[17,18,22,23,34,35,36] although the result itself has been around for many years.[6,29,30,31,37] The above derivation is from Ref. 30. Equation (23) is applicable to the 1D harmonic Bose gas. However, in a recent article, Schönhammer[38] showed that an almost identical relation holds for the 1D ideal harmonic *Fermi* gas. His derivation can easily be adapted to work for bosons. The Fermi partition function differs only in having a factor $e^{-\beta E_0}$, where $E_0 = N(N-1)\Delta/2$ is the Fermi zero-point energy. This result means that the internal energies, given by $-\partial \ln Z_N/\partial\beta$, differ only by E_0 and that the two systems have identical heat capacities[29,32] given by

$$C = \frac{dE}{dT} = k_B \sum_{k=1}^{N} \frac{(\beta k\Delta)^2 e^{\beta k\Delta}}{(e^{\beta k\Delta}-1)^2}. \tag{24}$$

As shown in Fig. 2, this quantity is linear in T at low temperatures (that is, for $\Delta \ll k_B T \ll T_0$) and approaches Nk_B at $T \gg T_0$. The relation between fermions and bosons for this system was first pointed out in Ref. 29.

There is a curious aside to this relation between Bose and Fermi partition functions.[6,39,40,41,42] The 1D harmonic gas has a constant density of states, which leads to the equality of the heat capacities. Consider instead *free* particles in 2D where the single-particle states are $\epsilon_p = p^2/2m$ and the density of states is a constant because $p\,dp = m\,d\epsilon$. One can show by using standard grand canonical ensemble techniques that the 2D free Fermi and Bose gases have identical heat capacities. This result is rather remarkable considering the considerable difference between the Fermi and Bose derivations of C. Moreover, the 2D Fermi/Bose heat capacity is fit extremely well by Eq. (24).

IV. MORE RECURRENCE RELATIONS

It is possible to go beyond the 1D harmonic case and derive canonical recurrence relations valid for any ideal gas. We first derive relations for the distribution functions following a method due to Schmidt,[43] who showed how the standard Fermi and Bose distribution functions in the grand canonical ensemble could be obtained by this means. We have

$$\overline{n}_p(N)\, Z_N = \sum_{\{n\}} n_p e^{-\beta \sum_k \epsilon_k n_k} \delta_{N,\Sigma_i n_i}, \tag{25}$$

where the Kronecker delta restricts the sum to N particles. Let $n_p = n'_p + 1$ and $n'_k = n_k$ for $k \neq p$. Then

$$\overline{n}_p(N) Z_N = \sum_{\{n'\}} (n'_p + 1) e^{-\beta(\sum_k \epsilon_k n'_k + \epsilon_p)} \delta_{N-1,\Sigma_i n'_i}. \tag{26}$$

The term corresponding to $n'_p = -1$ does not contribute and the right side involves standard partition function sums corresponding to $N-1$ particles. We have

$$\overline{n}_p(N)\, Z_N = \left[\overline{n}_p(N-1) Z_{N-1} + Z_{N-1}\right] e^{-\beta\epsilon_p}, \tag{27}$$

or

$$\overline{n}_p(N) = e^{-\beta\epsilon_p} \frac{Z_{N-1}}{Z_N} \left[1 + \overline{n}_p(N-1)\right], \tag{28}$$

which is Schmidt's recurrence relation.[43] Equation (28) appeared much earlier in the literature.[31,44,45,46] These derivations assume that $\overline{n}_p(N-1) \approx \overline{n}_p(N)$ and use the relation $Z_N = e^{\beta F_N}$, where F_N is the Helmholtz free energy and $F_N - F_{N-1} \approx \partial F_N/\partial N = \mu$, to

find

$$\overline{n}_p(N) = \frac{1}{e^{\beta\epsilon_p} Z_N/Z_{N-1} - 1} = \frac{1}{e^{\beta(\epsilon_p - \mu)} - 1}. \tag{29}$$

We end up with a canonical derivation of the standard grand canonical ensemble distribution function for bosons. An analogous derivation is valid for fermions.[43,47]

Unfortunately, the assumption that $\overline{n}_p(N-1) \approx \overline{n}_p(N)$ leads back to the same fluctuation inaccuracies inherent in the grand canonical ensemble. But we need not make this assumption; Eq. (28) has a direct solution. By using the obvious starting values, $\overline{n}_p(0) = 0$ and $Z_0 = 1$, we can prove by induction[46] that

$$\overline{n}_p(N) = \sum_{l=1}^{N} e^{\beta\epsilon_p l} \frac{Z_{N-l}}{Z_N}. \tag{30}$$

To use this relation, we need the partition functions involved. If we sum the relation over all p, we get

$$N = \sum_p \overline{n}_p(N) = \sum_{l=1}^{N} \left[\sum_p e^{\beta\epsilon_p l} \right] \frac{Z_{N-l}}{Z_N}. \tag{31}$$

The quantity in square brackets is just the one-body canonical partition function at the effective inverse temperature βl, and a recurrence relation for Z_N results:

$$Z_N = \frac{1}{N} \sum_{l=1}^{N} Z_1(\beta l) Z_{N-l}. \tag{32}$$

This relation was apparently first derived by Landsberg,[46] but appears many times in the current research literature.[22,23,34,36,48,49,50,51,52,53,54,55] It was derived in this journal by Ford,[56] although he made no application of it. Ford showed that such a result stems from the relation of Fermi and Bose partition functions to symmetric polynomials. Recently Schmidt and Schnack[57] extended this idea.

The use of Eqs. (28) and (32) allows us to determine the canonical distribution functions for the finite 1D harmonic Bose system. (We could as easily find the properties of the finite 3D harmonic Bose gas.) We start the recurrence in Eq. (32) with $Z_0 = 1$ and find every $Z_L, L \leq N$. These values are then put into (28), starting with $\overline{n}_p(0) = 0$ to find each distribution function $n_p(L), L \leq N$, in sequence. The results are shown in Fig. 3. There is a small disagreement between the results for the canonical ensemble and the grand canonical ensemble for $N = 500$, but these become smaller for larger N. The real difference between the two ensembles arises in the fluctuations.

We can, in the same way, develop a recurrence relation for the mean square distribution. We find

$$\overline{n_p^2}(N) = e^{-\beta\epsilon_p}\frac{Z_{N-1}}{Z_N}\left[1+\overline{n}_p(N-1)+\overline{n}_p(N-1)^2\right]. \tag{33}$$

With this relation and Eq. (28) we obtain the root-mean-square fluctuation in the ground-state distribution function for the canonical ensemble, which can be compared to the same result for the grand canonical ensemble as given by Eq. (11). The results are shown in Fig. 4. As expected, we see that the grand canonical ensemble result goes to the total number of particles as T becomes small, while that of the canonical ensemble goes to zero after peaking near the quasi-transition temperature T_0.

We can sharpen the distinction concerning fluctuations by deriving the probablility $P_0(n)$ of finding n particles in the state with $\epsilon_0 = 0$. For the 1D harmonic gas in the canonical ensemble this quantity is given by

$$\begin{aligned} P_0(n) &= \frac{1}{Z_N}\sum_{n_0,n_1,\ldots} e^{-\beta\Delta(n_1+2n_2+3n_3+\cdots)}\delta_{n,n_0}\delta_{N,\Sigma_{i=0}n_i} \\ &= \frac{1}{Z_N}\sum_{n_1,n_2,\ldots} e^{-\beta\Delta(n_2+2n_3+3n_4+\cdots)}e^{-\beta\Delta(n_1+n_2+n_3+\cdots)}\delta_{N-n,\Sigma_{i=1}n_i}. \end{aligned} \tag{34}$$

The series in the second exponential on the right can be replaced by $N-n$ and extracted from the sum; the remaining factor becomes a partition function for $N-n$ particles or

$$P_0(n) = e^{-\beta\Delta(N-n)}\frac{Z_{N-n}}{Z_N}. \qquad \text{(Canonical ensemble)} \tag{35}$$

The equivalent quantity can be derived for the grand canonical ensemble. We find

$$P_0(n) = (1-e^{\beta\mu})e^{n\beta\mu}. \qquad \text{(Grand canonical ensemble)} \tag{36}$$

The two $P_0(n)$ functions are plotted in Fig. 5 for $T = 0.12T_0$. We see that the canonical ensemble value is sharply peaked around the average value while the grand canonical ensemble function is incorrectly wide and monotonic.

If we include interactions, the fluctuations in the grand canonical ensemble are tempered to a more physically reasonable value.[20] However, we would still prefer to be able to treat the ideal gas correctly for its conceptual and pedagogical importance and because experimentalists can now reduce the effective interactions to near zero by use of Feshbach resonances.[2]

One might argue that the microcanonical ensemble, in which the system of interest is isolated, is more nearly equivalent to the actual experimental conditions of Ref. 1 than the canonical ensemble. However, it can be shown by use of the recurrence relations for the microcanonical ensemble[22,23] that the microcanonical and canonical ensembles give almost identical results.

V. PERMUTATION CYCLES

The sums in Eqs. (3) and (32) have a physical interpretation as sums over permutation cycles. This view of BEC was first developed by Matsubara[58] and Feynman,[5] and was recently discussed in this journal by one of us.[59] Here we examine permutation cycles in the context of recurrence relations. The boson N-body wave function is symmetric and the density matrix can be written in terms of symmetrical permutations of particles.[5] The partition function is the trace of the density matrix and involves a sum over all permutations,

$$Z_N = \frac{1}{N!}\sum_{\mathrm{P}} \int d\mathbf{r}_1 \ldots d\mathbf{r}_N \langle \mathbf{r}_{P1}, \ldots, \mathbf{r}_{PN} | e^{-\beta H} | \mathbf{r}_1, \ldots, \mathbf{r}_N \rangle, \tag{37}$$

where the variable $\mathbf{r}_{P_j}$ represents the coordinate of the particle interchanged with particle j in permutation P.

Any N-particle permutation can be broken up into smaller permutation cycles.[5,59] For example, for $N = 7$ we might have a 3-particle permutation cycle $1 \to 2 \to 3 \to 1$ plus a 4-particle cycle $4 \to 5 \to 6 \to 7 \to 4$. The corresponding matrix element in Eq. (37) breaks up into a product of cycle terms:

$$\begin{aligned} \langle 3125674 | e^{-\beta H} | 1234567 \rangle &= \langle 312 | e^{-\beta H_3} | 123 \rangle \langle 5674 | e^{-\beta H_4} | 4567 \rangle \\ &= \sum_p e^{-3\beta\epsilon_p} \sum_m e^{-4\beta\epsilon_m} = Z_1(3\beta) Z_1(4\beta), \end{aligned} \tag{38}$$

where, for example, $H_3 = h_1 + h_2 + h_3$ with each h_i being a one-body Hamiltonian. We have reduced the cycle matrix elements to one-body partition functions at an effective temperature. The details of this derivation are given in Ref. 59. Every term in the sum of Eq. (37) can be reduced in this way to a product of permutation cycles represented by products of one-body partition functions. A single configuration will consist of q_1 loops of length 1, q_2 loops of length 2, etc., and may be arranged in $C(q_1, q_2, \ldots)$ different ways. Thus we can

write

$$Z_N = \frac{1}{N!} \sum_{\{q_1,q_2,\ldots\}}{}' C(q_1, q_2, \ldots) \prod_l Z_1(\beta l)^{q_l}, \tag{39}$$

where the prime on the sum implies that it is over all combinations of permutation cycles such that

$$\sum_l q_l l = N. \tag{40}$$

Feynman[5] has given an argument (repeated in Ref. 59) to show that

$$C(q_1, q_2, \ldots) = \frac{N!}{1^{q_1} 2^{q_2} \ldots q_1!\, q_2! \ldots}. \tag{41}$$

Again there is a connection to the theory of numbers. The sum in Eq. (39) is over the number of ways of partitioning the integer N into smaller integers. An example of $C(q_1, q_2, \ldots)$ is the breaking of particles 1, 2, $\ldots$, 5 into a 2-cycle and a 3-cycle, that is, partitioning 5 into $2 + 3$. With five particles there are several ways of doing this: We can take particles 1 and 2 in the 2-cycle with 3, 4, and 5 in the 3-cycle, or take particles 1 and 3 in the 2-cycle with the remaining particles in the 3-cycle, etc. In all there are $C = 5!/(2^1 3^1 1! 1!) = 20$ distinct ways of doing this, as the reader can verify.

For the case of the 1D harmonic Bose gas, we can combine Eqs. (4), (23), and (39) to find an interesting relation:

$$Z_N = \prod_{k=1}^{N} Z_1(\beta k) = \sum_{\{q_1,q_2,\ldots\}}{}' \frac{1}{1^{q_1} 2^{q_2} \ldots q_1!\, q_2! \ldots} \prod_l Z_1(\beta l)^{q_l} \tag{42}$$

or

$$\frac{1}{(1-x)(1-x^2)\cdots(1-x^N)} = \sum_{\text{partitions of } N} \frac{1}{1^{q_1} 2^{q_2} \ldots q_1!\, q_2! \ldots} \frac{1}{(1-x)^{q_1}(1-x^2)^{q_2}\cdots}. \tag{43}$$

Equation (43) is known as Cayley's decomposition in the theory of partitions of numbers.[33] A simple special case is $1/(1-x)(1-x^2) = \frac{1}{2}\left[1/(1-x)^2 + 1/(1-x^2)\right]$.

The right-hand side of Eq. (42) is, in fact, the solution of the recurrence relation (32). This solution tells us how to interpret the recurrence relation itself. The sum in Eq. (32) is a sum over permutation cycles: We can generate the N-body partition function for the Bose system by adding a particle either as a singlet ($Z_1(\beta)$) with the other $N-1$ particles grouped independently (Z_{N-1}), or as part of a pair-exchange cycle ($Z_1(2\beta)$) with the other $N-2$ particles in all their possible combinations (Z_{N-2}), or as part of a triple cycle, and so

on, with each configuration having equal probablity $1/N$. (The work of Laloë et al.[60,61] on interacting gases is closely related to this approach.)

A further useful quantity is the average number $\overline{p}_l = \overline{q}_l l$ of particles involved in permutation cycles of length l. This number is found by using Eq. (32):

$$N = \sum_l \overline{p}_l = \sum_l Z_1(\beta l) \frac{Z_{N-l}}{Z_N}, \tag{44}$$

which tells us that

$$\overline{p}_l = Z_1(\beta l) \frac{Z_{N-l}}{Z_N}. \tag{45}$$

We can easily plot $\overline{p}_l$, but before we do, it is useful to separate out the contributions to $\overline{p}_l$ from the condensate and the excited states. From Eq. (30) we have

$$\overline{n}_0 = \sum_l \frac{Z_{N-l}}{Z_N}, \tag{46}$$

so that $\overline{p}_l^{(0)} = Z_{N-l}/Z_N$ is the contribution of the condensate to the average particle number in the permutation cycle of length l. However, this quantity is essentially unity until l is of order N. On the other hand, for small l in the one-dimensional oscillator, $Z_1(\beta l) \approx 1/(\beta l \Delta)$ in Eq. (45) (cf. Eq. (5)), which is the contribution of the non-condensate to the permutation cycles. Figure 6 shows $\overline{p}_l$ vs. l for the canonical ensemble. Notice the rapid drop-off of $\overline{p}_l$ for small l, corresponding to the non-condensate. However, for low temperatures (that is, when there is a large condensate) $\overline{p}_l \approx \overline{p}_l^{(0)} \approx 1$ out to a value equal to the condensate number $\overline{n}_0$, where $\overline{p}_l$ must drop off to satisfy Eq. (46). We might have guessed before the calculation that the condensate consists only of very long permutation cycles of approximately $\overline{n}_0$ particles. Now we see that this is not true; the condensate particles have equal probability of being in singles, pair cycles, triple cycles, and so on out to an $\overline{n}_0$-cycle.

The dotted line in Fig. 6 is the grand canonical ensemble estimate of $\overline{p}_l$. We find this estimate from Eq. (3), which we can show[59] also to be a sum over permutation cycles. Thus

$$\overline{p}_l = e^{l\beta\mu} Z_1(\beta l). \qquad \text{(Grand canonical ensemble)} \tag{47}$$

We also have

$$n_0 = \frac{1}{e^{-\beta\mu} - 1} = \sum_{l=1}^{\infty} e^{\beta\mu l}. \qquad \text{(Grand canonical ensemble)} \tag{48}$$

The summand $e^{\beta\mu l}$ is the condensate contribution to $\overline{p}_l$ in the grand canonical ensemble. The dotted line in the plot shows that the grand canonical ensemble does not do a very good job of representing the true nature of condensate permutation cycles in the Bose gas.

Because the condensate contribution to $\overline{p}_l$ must drop off at $\overline{n}_0$, we could estimate $\overline{n}_0$ by finding the value of l for which $\overline{p}_l \approx 0.5$. For the lowest temperature $0.12T_0$ in Fig. 6 this estimate gives $\overline{n}_0 = 472$, whereas the exact result is 471. This approach also allows us to estimate $\overline{n}_0$ in path-integral Monte Carlo simulations involving trapped interacting particles, where no standard estimators of $\overline{n}_0$ exist.[62,63,64]

The picture we have then of the condensate is that it does indeed fluctuate wildly, *not* in overall particle number as would be suspected from the grand canonical ensemble, but rather in how it breaks into permutation cycles, with its particles having an equal probability of being in cycles of all sizes up to the condensate number itself.

VI. DISCUSSION

Our goals in this paper have been multiple: (a) Illustrate the inadequacies of the grand canonical ensemble in its depiction of fluctuations in a Bose-condensed system. (b) Show how the canonical ensemble can do a much better job in describing a condensed system. (c) Find recurrence relations that allow simple treatments of finite ideal Bose systems. (d) Study a simple model system, the 1D harmonically trapped ideal Bose gas, which illustrates all of the important elements of BEC in a finite system and has its own particularly simple recurrence relation. (e) Delve deeper into the intricacies of BEC to find the physical meaning of the recurrence relations by looking at permutation cycles. (f) Illustrate the close relation between Bose and Fermi systems for cases where the density of states is constant.

All our work here involves non-interacting Bose systems. Although real gases have non-negligible physical effects due to interactions, many of the ideas we have developed carry over to the interacting regime.[49,50,53,60,61,62,63,64] Although it is probably not possible to develop recurrence relations for interacting systems,[65] the idea of the condensate involving all sizes of permutation cycles, the usefulness of even a 1D model of a Bose gas, and the close relation between the 1D Bose and Fermi gases, are ideas that are still expected to hold for interacting systems.

An important feature of the present paper is that the 1D model is so simple that instructors can use it in elementary courses in statistical physics without sacrificing much important physics. The computer programs needed to carry out the recurrence relations are simple and can be coded by the students themselves. There are thought to be few models where

the canonical ensemble is soluble, but we have seen here that any ideal system where the single-particle energies are known is actually tractable. Usually one does not care so much about using the canonical ensemble because the grand canonical ensemble makes the math easier. However, we have seen that for the case of BEC the grand canonical ensemble is not always accurate and the canonical ensemble becomes not only accessible but necessary.

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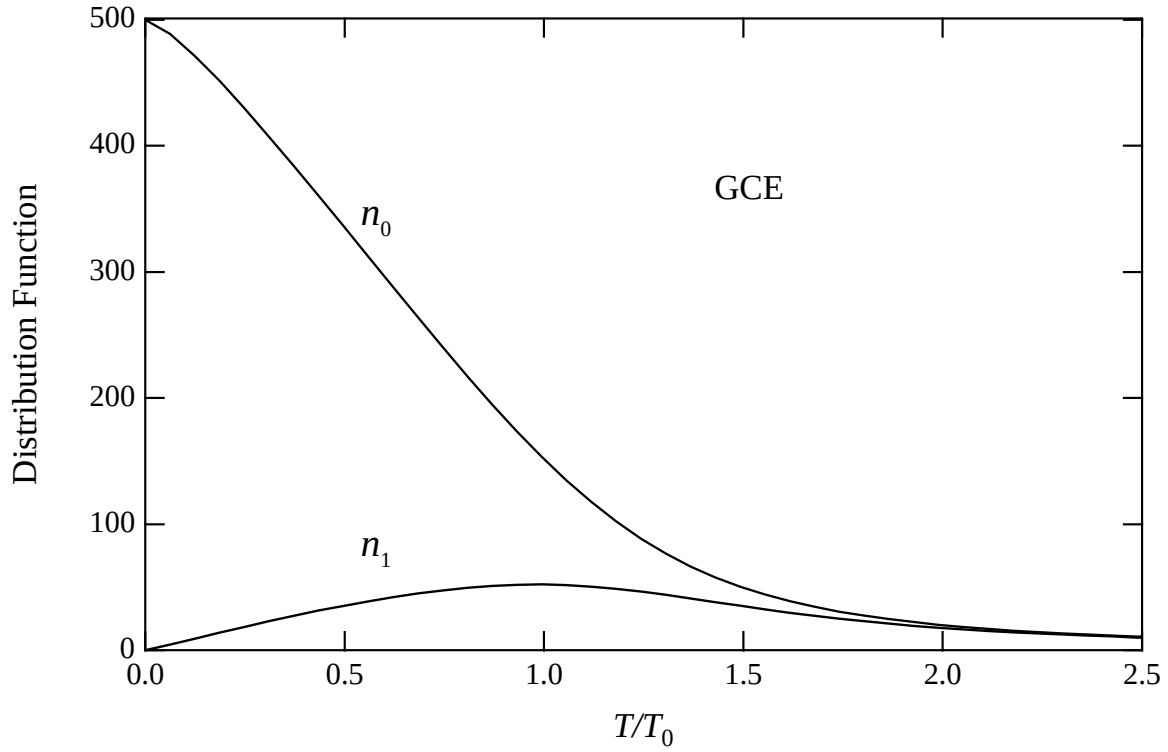
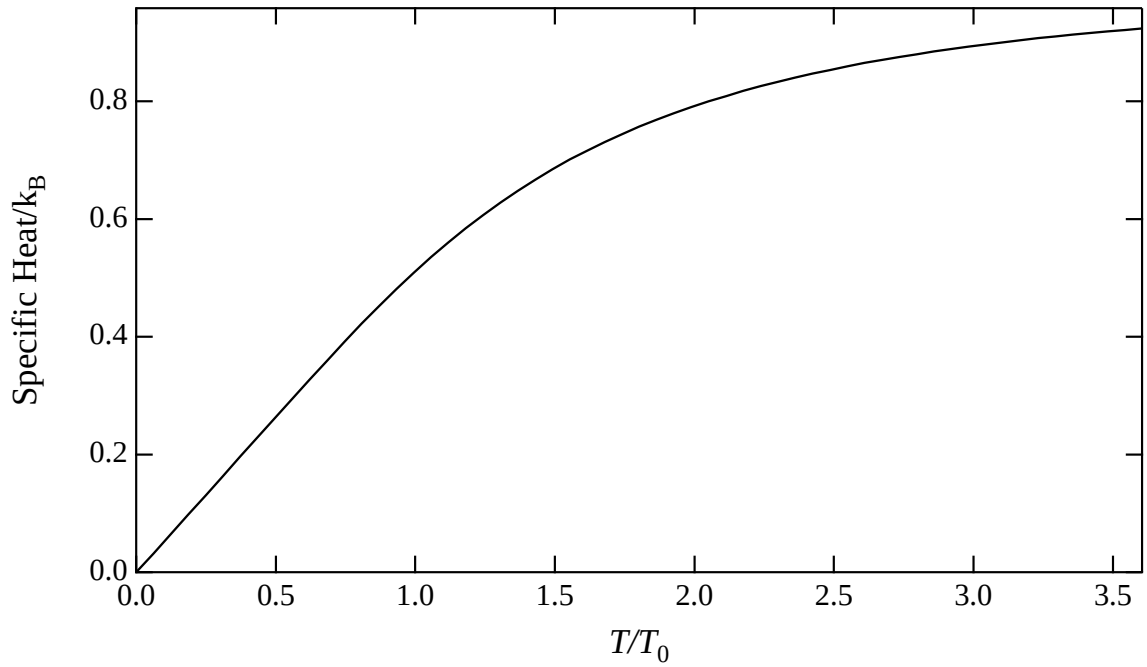


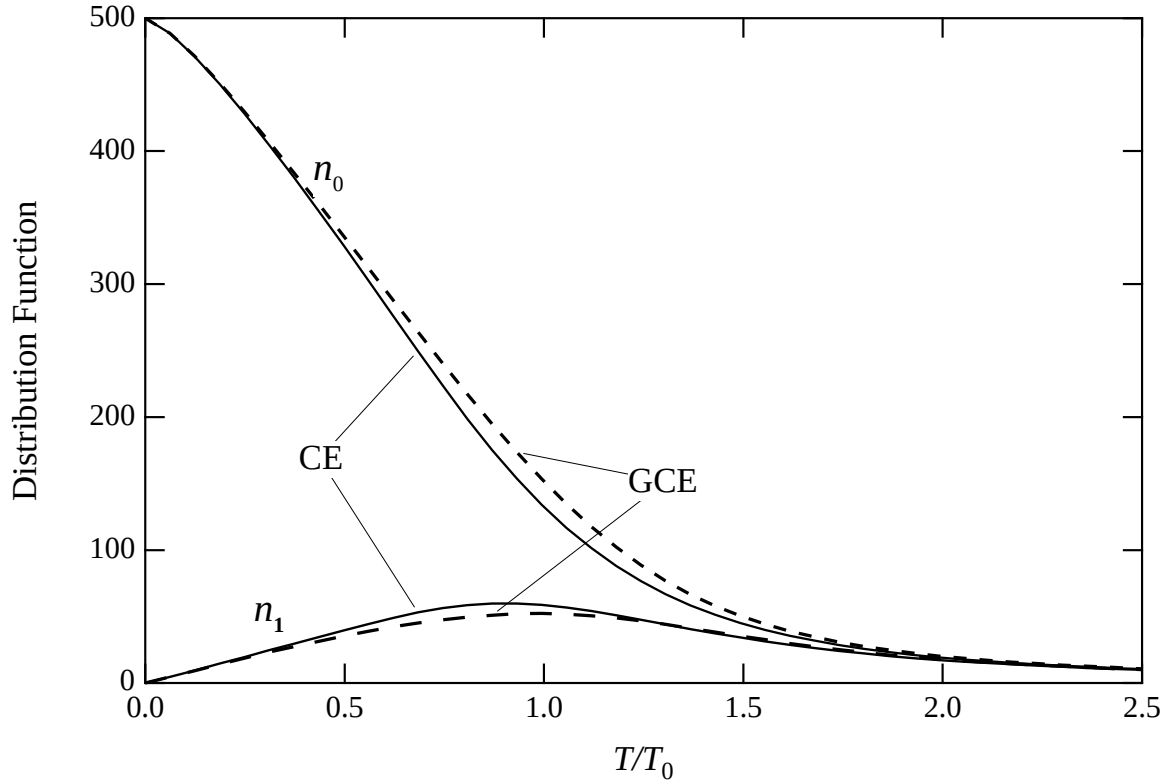
Mullin Fig. 1

FIG. 1: Grand canonical ensemble calculation of the number of particles in the two lowest states versus T/T_0 for the 1D harmonic Bose gas. The results shown for all the figures are for $N = 500$.



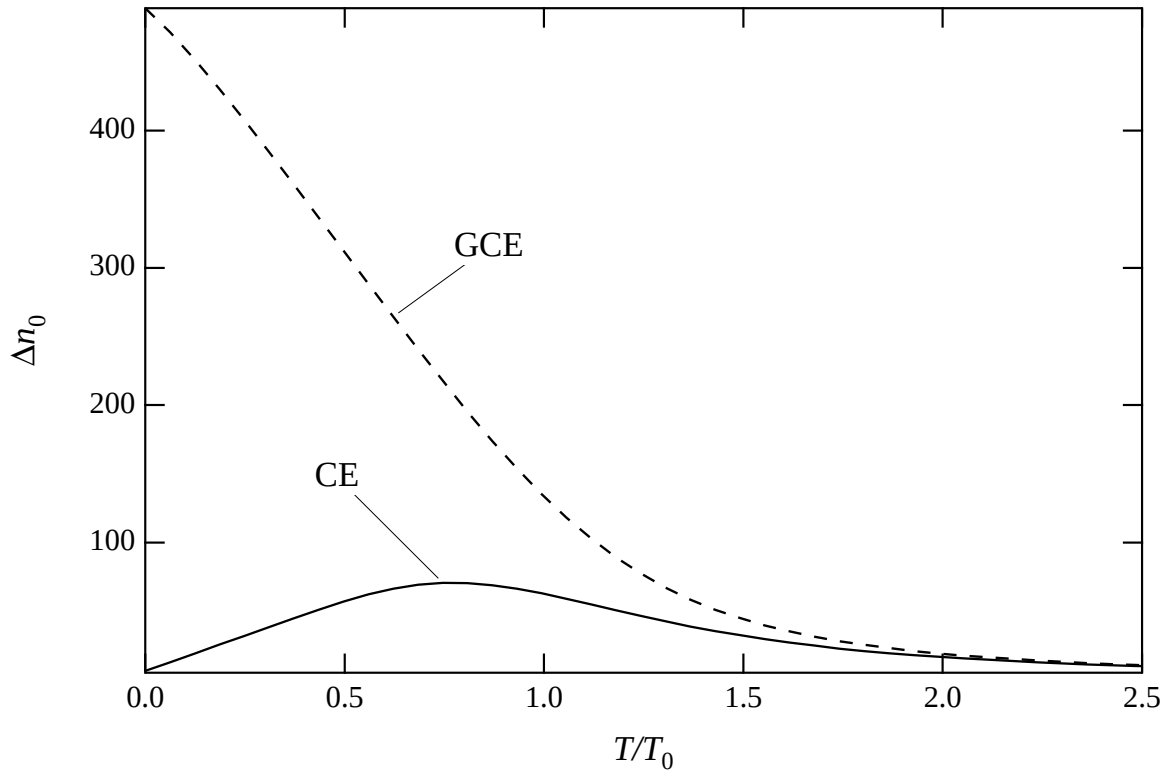
Mullin Fig. 2

FIG. 2: Heat capacity per particle (in units of k_B) for the 1D ideal harmonic Bose gas. This quantity is identical to the same quantity for a 1D ideal harmonic Fermi gas.[38]



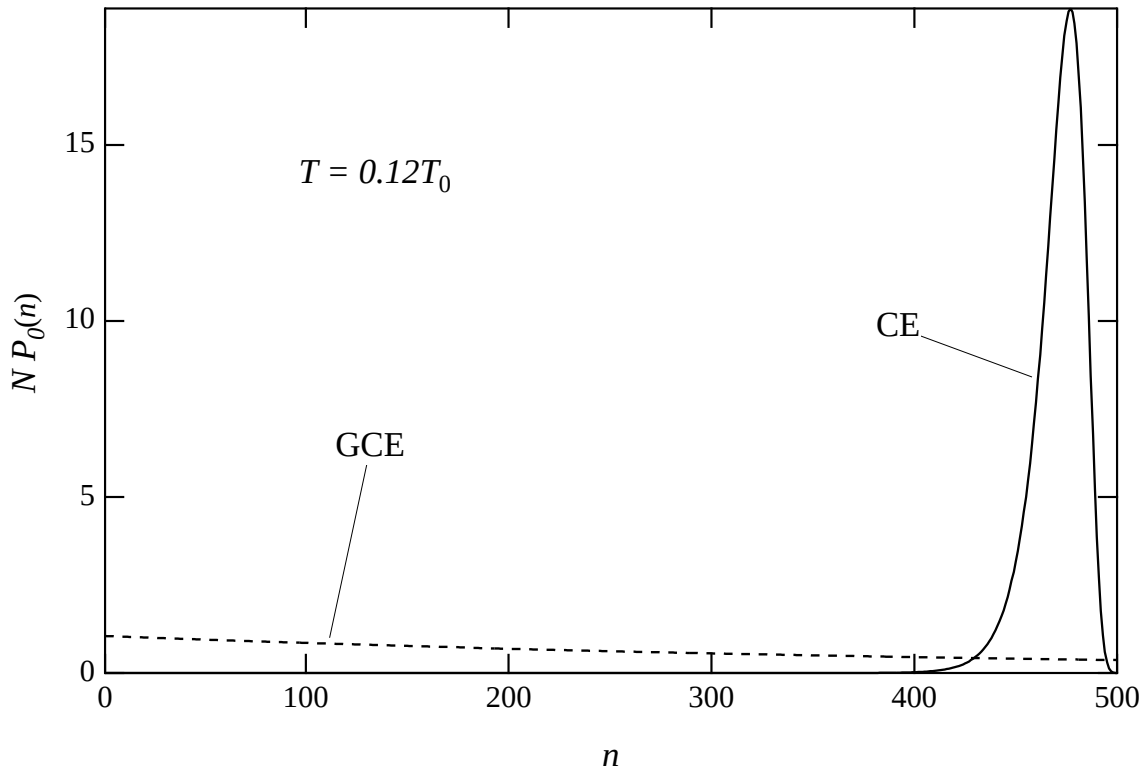
Mullin Fig. 3

FIG. 3: Comparison of the grand canonical ensemble and canonical ensemble calculations of the number of particles in the two lowest states versus T/T_0 for the 1D harmonic Bose gas.



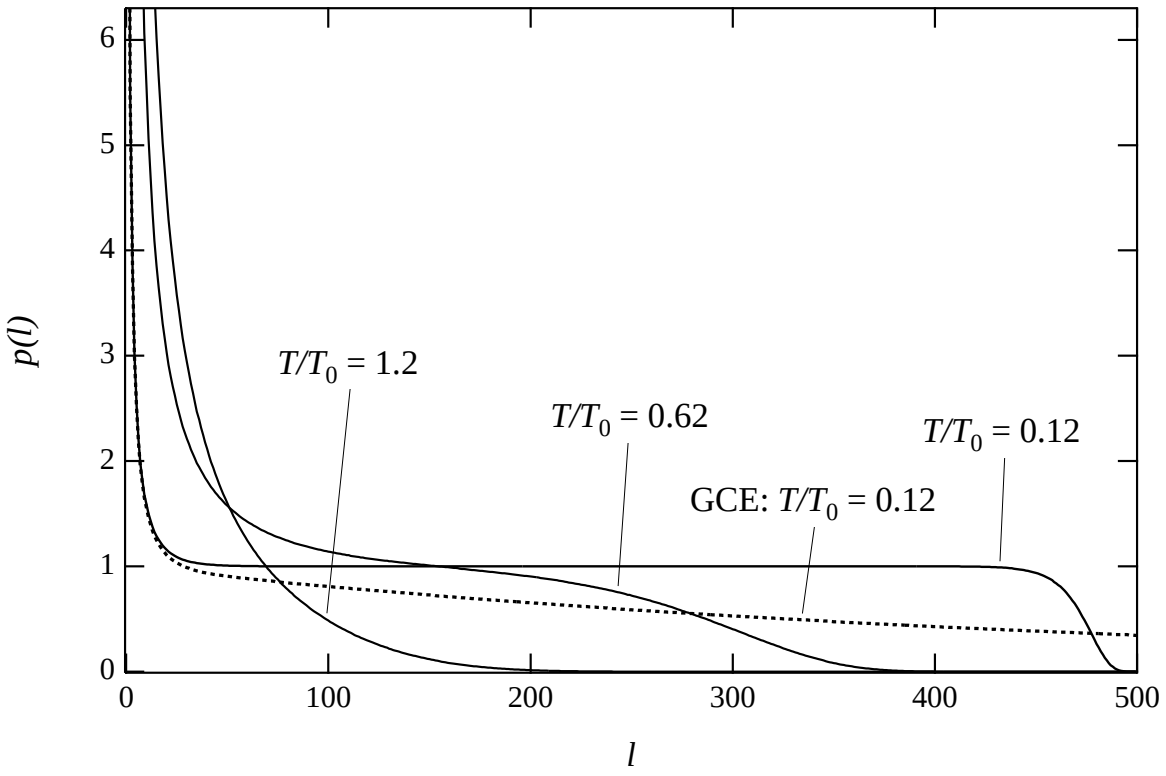
Mullin Fig. 4

FIG. 4: Root-mean-square fluctuation of the number of particles in the ground state of the 1D harmonic Bose gas for the grand canonical and canonical ensembles. The fluctuations in the condensate in the grand canonical ensemble become as large as the occupation itself, which is unphysical. The canonical ensemble result is more reasonable.



Mullin Fig. 5

FIG. 5: The probability of finding n particles in the ground state versus n for the 1D harmonic Bose gas at $T = 0.12T_0$ for both the canonical ensemble (solid line) and grand canonical ensemble (dotted line). The result for the grand canonical ensemble is unphysical.



Mullin Fig. 6

FIG. 6: The number of particles in permutation cycles of length l versus l for the canonical ensemble (solid lines) at various temperatures for the 1D harmonic Bose gas. Also shown by the dotted line is the same quantity at the lowest temperature for the grand canonical ensemble.