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The Loop-Gas Approach to Bose-Einstein Condensation for Trapped Particles

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We examine Bose-Einstein condensation (BEC) for particles trapped in a harmonic potential by considering it as a transition in the length of permutation cycles that arise from wave-function symmetry. This "loop-gas" approach was originally developed by Feynman in his path-integral study of BEC for an homogeneous gas in a box. For the harmonic oscillator potential it is possible to treat the ideal gas exactly so that one can easily see how standard approximations become more accurate in the thermodynamic limit (TDL). One clearly sees that the condensate is made up of very long permutation loops whose length fluctuates ever more wildly as the number of particles increases. In the TDL, the WKB approximation, equivalent to the standard approach to BEC, becomes precise for the non-condensate; however, this approximation neglects completely the long cycles that make up the condensate. We examine the exact form for the density matrix for the system and show how it describes the condensate and behaves in the TDL.

I. INTRODUCTION

In recent years various groups have achieved Bose-Einstein condensation (BEC) in alkali gases. [1] The gases have been trapped magnetically in potentials accurately approximated by harmonic-oscillator wells. Because of these experiments there has been a deluge of theoretical papers on BEC in harmonic potentials, both for the ideal and the interacting gases. [2] However, even before the recent experimental achievements, there were a few theoretical considerations of bosons in harmonic potentials [3]$^-$ [6] including one by the author in this journal. [7] AJP has recently published two papers on BEC in trapped gases. [8], [9] One of the pleasant aspects of this system is the relative ease with which substantial theoretical advances can be made with this system, especially since the diluteness of the experimental gases often makes the ideal gas a fairly good approximation. The result has been some new insights into the nature of BEC.

BEC occurs most fundamentally because of the symmetry of the wave function. This property is necessary because bosons are identical particles, so that one cannot tell the difference between the arrangements, say, $(1,2)$ and $(2,1)$. This means that forms of the wave function that have the particles in differing permutation arrangements are equally likely. For example, for an ideal gas of just three particles in single-particle states ϕ_i might have, as one possible state,

$$\begin{aligned}\psi_{abc}(r_1,r_2,r_3) = \frac{1}{\sqrt{3!}}\,[&\phi_a(r_1)\phi_b(r_2)\phi_c(r_3) + \phi_a(r_2)\phi_b(r_1)\phi_c(r_3)\\ &+\phi_a(r_1)\phi_b(r_3)\phi_c(r_2) + \phi_a(r_3)\phi_b(r_2)\phi_c(r_1)\\ &+ \phi_a(r_2)\phi_b(r_3)\phi_c(r_1) + \phi_a(r_3)\phi_b(r_1)\phi_c(r_2)]\end{aligned} \tag{1}$$

Let us call the first term of this function the direct term; the next three are pair-exchange terms, with just two particles interchanged; the last two involve triple exchanges with $(1,2,3) \longrightarrow (2,3,1)$ or $(3,1,2)$. We might represent this by a triangle with lines connecting the particles that permute and, because of this picture, call this a permutation "cycle" or "loop." (A pair exchange is a special case of a loop although it looks like a line.) Any permutation of a set of particles can be broken down into a combination of loops and singlets (particles that are not exchanged, e.g., particle 3 in the second term above).

Feynman developed an approach to Bose systems when he adapted his path-integral view of quantum mechanics to statistical mechanics. [10] His work led to new understanding of superfluid helium and of the λ- transition. [10], [11] The path-integral approach involves the use of the configuration representation, $\rho(\mathbf{r_1},...,\mathbf{r_N};\mathbf{r'_1},...,\mathbf{r'_N})$, of the density matrix as a central entity, a form often particularly useful in providing physical insight. For example, the diagonal element gives the probability of finding the N particles at positions $\mathbf{r_1},...,\mathbf{r_N}$. In the case of bosons, the symmetry of the wave function requires that the many-body density matrix include the effects of all possible permutations of the N particles. Since the density matrix is bilinear in the wave functions possible for the system, it includes not only direct terms (first term squared in our three-particle example wave function), but also cross terms among various permutation arrangements. Such cross terms become important when the thermal de Broglie wavelength is longer than the separation between particles so that particle identity becomes a serious issue; that is, there is a substantial overlap between an arrangement and a permutation of that arrangement.

One might expect that small-scale (say, triple) exchange processes (as in the product of the first and fifth terms in the above wave function) could occur relatively easily when three particles chance to be near one another. What is not so clear is under what circumstances very large-scale (say, 50-particle) exchanges can occur as a unit. The occurrence of such grand "ring-around-the-rosy" exchange loops (the overlap of the direct and large-scale exchange terms in the wave function) is precisely what happens after the onset of BEC. This view is quite different from the usual one of an avalanche of particles falling into the lowest state – although that view is also valid. At BEC there is an "explosion" in the size of possible permutation-cycle events. Because their possibility is so clearly a result of particle identity – more evidently than the avalanche into the same state – an analysis of this point of view is a fruitful undertaking for the new intuition it provides. Finding this "loop-gas" relation between BEC and the growth of possible permutation cycles is the focus of this paper.

The equilibrium properties of a gas, including the onset of BEC, can be determined from the partition function, which is the sum or integral over the diagonal terms of the density matrix. Thus the partition function and quantities derived from it can show the effects of permutation loops. Although our result that BEC is accompanied by a large increase in the possible size of permutation loops is itself not so new; what we show is that considering the partition function for particles in a harmonic-oscillator potential allows a particularly clear demonstration of the interpretation in terms of permutation loops.

In his book, Feynman [10] gives two derivations of the partition function of the homogeneous boson ideal gas in a box with periodic boundary conditions. The first is standard (p.32 of his text); the second, arising from his interest in the density matrix approach, involves counting all possible permutation loops to compute the density matrix and then taking the trace to get the partition function (p.62). (This approach was developed earlier by Matsubara, [12] although this article is not referenced by Feynman.) The latter method accurately gives the partition function above the transition, but fails, in the homogeneous gas treated, to give all the insight for which one might hope, because an approximation that must be made to do the needed energy sums neglects the effects of the very long permutations. On the other hand, our exact treatment of the ideal gas in a harmonic potential is able to avoid this unfortunate approximation, include the condensate permutations, and thereby provide a rather useful bit of missing pedagogy concerning BEC.

Because we present an explicit computation of the density of the gas (from our calculation of the density matrix), we are able to demonstrate a curious feature of BEC in a trap. The density is, of course, largest at the center of the trap. As the temperature is lowered, BEC finally occurs when the density at the center reaches the *same* critical value that it has for a homogeneous gas with periodic boundary conditions. From the loop-gas point of view, one sees that, at this density and temperature, relatively short permutation loops suddenly join to make large loops involving macroscopic numbers of particles. In a box, these loops are spread out uniformly. However, in the trap, the density is critical near the center, so the macroscopic loops occur in that region. Of course, that feature corresponds precisely to the fact that the ground state of the oscillator, into which condensation is taking place, is more localized than any other state.

The density matrix itself provides several useful criteria for the occurrence of BEC, even when interactions are present. Certain integrals over the density matrix must be macroscopic (of order N), for example. [13] For a homogeneous fluid of particles in a box with periodic boundary conditions, the one-body reduced matrix, $\varrho_1(\mathbf{r},\mathbf{r}')$, which is the N-body matrix traced over all but the variables corresponding to a single particle, has the property [13]

$$\varrho_1(\mathbf{r},\mathbf{r}') \to \mathbf{n_0}/\mathbf{V} \quad \text{for} \quad |\mathbf{r}-\mathbf{r}'| \to \infty \tag{2}$$

where n_0 is the condensate number and V is the volume. This property has been useful in Monte Carlo simulations [14] of boson systems, e.g., superfluid ^{4}He, for finding n_0 theoretically. However, if the particles are in a trap, such as a harmonic well, then $\varrho_1(\mathbf{r},\mathbf{r}')$ will approach zero, simply because of the nature of the potential, when $|\mathbf{r}-\mathbf{r}'| \to \infty$, and other criteria must then be found. For actual experiments in a trap, the condensate is recognized by its sudden appearance as a compact cloud of particles that forms at the center of the trap.

By looking in detail at what is going on in configuration space and at permutation cycles, rather than by concentrating on the usual view of BEC as a collapse of many particles into the lowest state, one is able to arrive at quite different physical insights. Indeed such insights, first developed by Matsubara and Feynman, have had important applications in current research.

In recent years Ceperley and co-workers have developed a powerful numerical procedure, based on Feynman's path integral approach, known as Path-Integral Monte Carlo (PIMC). [15] The technique works well for dense systems such as superfluid helium, [15] and for interacting dilute gases as well. [16], [17], [18] The one-body density matrix limit above is no help for the trapped gases so that in recent PIMC simulations [16], [18] n_0 has been inferred by looking for the number of particles involved in long permutation cycles. These turn out, not coincidentally, to be localized near the center of the trap and, it is argued, constitute the condensate. In the ideal-gas analysis of this paper, such a useful connection between long permutation cycles and the localized condensate will arise in a simple analytic way

without the complications of the numerical simulations needed when interactions are present. (Although PIMC is somewhat related to the present paper, it is not a focus of this paper and its approach will not be investigated. For more information on it we refer the reader to the Ceperley review. [15])

In another recent related treatment [19] of the dilute Bose, all orders of permutation cycles are summed analytically, but while also including the effects of interactions in low order.

II. STANDARD TREATMENT

We first consider a standard textbook-type treatment of BEC in a harmonic well – even though no textbook actually covers this at present. The harmonic potential we use is written

$$U(\mathbf{r}) = \mathbf{\frac{1}{2}U_0}\left(\mathbf{\frac{r}{R}}\right)^{\mathbf{2}} \tag{3}$$

where r is the radial distance from the center of the potential, U_0 is the strength of the potential, and we have included a scale factor R that will become useful later. The energy levels are given in Cartesian coordinates as

$$E_{m_x,m_y,m_z} = \hbar\omega(m_x + m_y + m_z + \frac{3}{2}) \tag{4}$$

with $m_x, m_y, m_z = 0, 1, 2, 3, ...$ The angular frequency ω in this equation is related to the potential parameters by

$$\omega = \sqrt{\frac{U_0}{R^2 m}} \tag{5}$$

where m is the particle mass.

We find the properties of the BEC by writing the average particle number in the grand canonical ensemble

$$N = \sum_{m_x,m_y,m_z} \frac{1}{e^{\beta[\hbar\omega(m_x+m_y+m_z+\frac{3}{2})-\mu]} - 1} \tag{6}$$

where β is the inverse temperature, and μ the chemical potential.

The potential is macroscopic in size – all N particles fit in it, of course – but to take the thermodynamic limit (TDL) we need to increase the number N while at the same time keeping the average density constant. The way we do that here is to *weaken* the potential while increasing N. We now use the scale factor in Eq.(5); that is, we assume that $N/R^3 \sim N\omega^3$ is to be kept constant while we increase N. [20] Further discussion of the TDL that comes to the same conclusion is considered in Refs. 4, 7, 21, and 22. The last reference justifies this feature by showing that it is necessary in order to keep the free energy extensive. An equivalent result arises in our treatment below. We can define a characteristic temperature T_0 that remains constant in the TDL by writing

$$\hbar\omega = \hbar\sqrt{\frac{U_0}{R^2 m}} = \hbar\sqrt{\frac{U_0}{m}}\left(\frac{d}{N}\right)^{1/3} = \frac{kT_0}{N^{1/3}} \tag{7}$$

where $d = N/R^3$, k is the Boltzmann constant. From Eq.(7), we see that T_0 is given by

$$T_0 = \frac{\hbar}{k}\sqrt{\frac{U_0}{m}}d^{1/3} \tag{8}$$

From Eq.(7), we see that the harmonic oscillator states are very closely spaced for large N so that one would expect that it would be a good approximation to replace the sums in Eq.(6) by integrals. We write

$$\begin{aligned} N &= n_0 + \int_0^\infty dm_x \int_0^\infty dm_x \int_0^\infty dm_x \frac{1}{e^{\beta[\hbar\omega(m_x+m_y+m_z+\frac{3}{2})-\mu]} - 1} \\ &= n_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \int_0^\infty du \int_0^\infty dv \int_0^\infty dw \frac{1}{e^{u+v+w+\alpha} - 1} \end{aligned} \tag{9}$$

where we have let $u = \beta\hbar\omega m_x$, etc. and

$$\alpha = \frac{3}{2}\beta\hbar\omega - \beta\mu. \tag{10}$$

As usual in Bose systems the summand in Eq.(6) does not vary uniformly near $z = u + v + w = 0$ (it can peak very sharply there), and so the integral approximation miscounts n_0, which becomes macroscopic. Thus we have had to include it as a special term in Eq.(9). We next expand the integrand in the usual way and integrate over the three variables.

$$\begin{aligned} N &= n_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \int_0^\infty du \int_0^\infty dv \int_0^\infty dw e^{-(u+v+w+\alpha)} \frac{1}{1 - e^{-(u+v+w+\alpha)}} \\ &= n_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \int_0^\infty du \int_0^\infty dv \int_0^\infty dw \sum_{l=1}^\infty e^{-l(u+v+w+\alpha)} \\ &= n_0 + \left(\frac{kT}{\hbar\omega}\right)^3 \sum_{l=1}^\infty e^{-l\alpha} \left(\int_0^\infty du e^{-lu}\right)^3 = n_0 + \left(\frac{kT}{\hbar\omega}\right)^3 F_3(\alpha) \end{aligned} \tag{11}$$

where

$$F_3(\alpha) = \sum_{l=1}^\infty e^{-l\alpha} \frac{1}{l^3} \tag{12}$$

is one of the Bose integrals. [23]

If we use Eq.(7), we find

$$N = n_0 + N \left(\frac{T}{T_0}\right)^3 F_3(\alpha). \tag{13}$$

From this equation we see that our procedure for taking the TDL has led us to a properly extensive expression for the non-condensed particles. Any relation between ω and N other than $\omega^3 \sim 1/N$ would not lead to this result. For non-zero α , we can satisfy this equation with a negligible value of n_0. However, as T falls, the value of α needed to satisfy the equation approaches zero (becomes of order $1/N$) and F_3 reaches its maximum value of $\zeta(3)$, where $\zeta(n)$ is a Riemann zeta-function. Bose-Einstein condensation takes place at this point and we have

$$n_0 = N \left[1 - \left(\frac{T}{T_c}\right)^3\right] \qquad \text{for} \quad \mathrm{T} < \mathrm{T_c} \tag{14}$$

where $T_c = T_0 \zeta(3)^{-1/3}$ is the condensation temperature. In Fig. 1 we plot the condensate fraction n_0/N as a function of T as gotten from Eq.(14), and also from the exact expression Eq.(6) evaluated for finite $N = 1000$. [24]

Eq.(12) contains a sum over l. Just what is the physical significance of that sum? For the above derivation it resulted only from a mathematical trick invoked to do an integral, but in fact it has a fundamental meaning in terms of permutation loops as we will show in Sec. IV.

There is a considerably different looking derivation that has been used in the literature for this problem. [5], [6] It involves the WKB, or semiclassical, approximation for the density $n(\mathbf{p}, \mathbf{r})$ of particles having momentum $\mathbf{p}$ and position $\mathbf{r}$, which is

$$n(\mathbf{p}, \mathbf{r}) = \frac{\mathbf{1}}{\mathbf{h^3}} \frac{\mathbf{1}}{\mathbf{e}^{\beta[\mathbf{p^2/2m + U(r)} - \mu]} - \mathbf{1}} \tag{15}$$

The density of particles at position $\mathbf{r}$ is the integral of this over $\mathbf{p}$, which can be shown, by an expansion similar to that done above, to be

$$\begin{aligned} \rho(\mathbf{r}) &= \frac{1}{h^3} \int d\mathbf{p} \frac{\mathbf{1}}{\mathbf{e}^{\beta[\mathbf{p^2/2m + U(r)} - \mu]} - \mathbf{1}} \\ &= \left(\frac{2\pi mkT}{h^2}\right)^{3/2} \sum_{l=1}^\infty \frac{e^{l\beta\mu}}{l^{3/2}} e^{-\beta l U(\mathbf{r})} \end{aligned} \tag{16}$$

If we integrate this over $\mathbf{r}$ with the quadratic potential of Eq.(3), we will find just the second term on the right-hand side of Eq.(13). That is, the WKB approximation does not include the condensate, which must be added on specially as in our previous derivation.

We have given the standard approach to BEC for the trapped gas case. In the remaining sections we examine how we can get considerably more insight into BEC by looking at the process from the point of view of permutation loops; that is, we examine the so-called "loop gas." But first we consider an exact approach that avoids replacing sums by integrals.

III. AN EXACT APPROACH

When we replaced the sums by integrals above to get an answer that would be applicable in the thermodynamic limit, we lost the correct description of the condensate, which was added back in. In the case of the harmonically trapped gas, we can avoid this approximation by doing the sums exactly. In Eq.(6) we make the expansion of the integrand as done in Eq.(11):

$$N = \sum_{m_x,m_y,m_z} \sum_{l=1}^{\infty} e^{-l\beta\hbar\omega(m_x+m_y+m_z)-l\alpha} \tag{17}$$

Unlike the case of a free gas in a box where the energies go quadratically with the quantum numbers, the sums over m_x, m_y, and m_z can be done *exactly.* The result is

$$N = \sum_{l=1}^{\infty} \frac{e^{-\alpha l}}{(1-e^{-l\beta\hbar\omega})^3} \tag{18}$$

Such expressions have been obtained in the literature previously. [25]

To retrieve the approximations of Sec. I, we need to note that ω is of order $1/N^{1/3}$ so that, for l smaller than $N^{1/3}$, a very large number in the TDL, the argument of the exponential in the denominator is small. Expand in powers of it and keep only the first term of the expansion to find

$$N' = \sum_{l=1}^{\infty} \frac{e^{-\alpha l}}{(l\beta\hbar\omega)^3} = \left(\frac{kT}{\hbar\omega}\right)^3 F_3(\alpha) \tag{19}$$

This is identically the same expression found in the last section for the non-condensed gas. The condensate has been neglected because α is of order $1/N$ for $T < T_c$ as can be seen from the expression for n_0 :

$$n_0 = \frac{1}{e^{\alpha}-1} = \sum_{l=1}^{\infty} e^{-\alpha l} \cong \frac{1}{\alpha} \tag{20}$$

where the last approximation holds only below T_c. The size of α means that the l sum is significant to values up to order N. Since the approximation we used to get Eq.(19) was valid only for $l < N^{1/3}$, it is no surprise that we have made an error in deriving Eq.(19). We can see how this occurs in Fig. 2, which plots as a function of l, for finite $N = 1000$, the exact summand of Eq.(18), the approximate summand of Eq.(19), and the summand of n_0 of Eq.(20). (The last two summands do not quite add up to the exact total because of higher order terms neglected in Eq.(19). These would become smaller in the TDL.) The fact that the standard integration approximation neglects large l terms again draws attention to the question of the physical meaning of these terms. In the next section we show how the sum represents permutations cycles.

IV. LOOP GAS APPROACH

The "loop gas" view was first introduced by Matsubara [12] and then later by Feynman in connection with his path-integral method in statistical mechanics [10]; it has also been discussed by Elser [26], who seems to have invented the terminololgy "loop gas." These references all deal with the homogeneous system with periodic box boundaries. The term "loops" is used here as shorthand for "permutation cycles" or "exchange cycles." The reader will find that the derivation given here is more complicated than that of the last two sections, but the motivation is to achieve new physical insight into the relation between BEC and the growth of permutation cycles.

The boson N-body density matrix involves only symmetric states and is [10]

$$\rho_S(\mathbf{r_1},...\mathbf{r_N};\mathbf{r'_1},...,\mathbf{r'_N}) = \frac{\mathbf{1}}{\mathbf{N!}}\sum_{\mathbf{P}}\rho_{\mathbf{D}}(\mathbf{r_{P_1}},...\mathbf{r_{P_N}};\mathbf{r'_1},...,\mathbf{r'_N}) \tag{21}$$

where the sum is over all permutations and

$$\rho_D(\mathbf{r_1},...\mathbf{r_N};\mathbf{r'_1},...,\mathbf{r'_N}) = \sum_{\text{all states}} \mathbf{e}^{-\beta\mathbf{E_i}}\psi_{\mathbf{i}}(\mathbf{r_1},...,\mathbf{r_N})\psi^*_{\mathbf{i}}(\mathbf{r'_1},...,\mathbf{r'_N}) \tag{22}$$

is the density matrix for distinguishable particles. The partition function is the trace of this matrix or

$$Z = \frac{1}{N!}\sum_P \int d\mathbf{r_1}...\mathbf{dr_N}\langle\mathbf{r_{P_1}},...,\mathbf{r_{P_N}}|\mathbf{e}^{-\beta\mathbf{H}}|\mathbf{r_1},...,\mathbf{r_N}\rangle \tag{23}$$

where the variable $\mathbf{r_{Pj}}$ represents the coordinate of the particle interchanged with particle j in permutation P. The sum over permutations here is just the result of the possible cross terms between various permuted elements of the symmetrized wave functions caused by particle identity. By using the configuration representation of the density matrix, we are able to track how the symmetrization affects the results.

Any N-particle permutation breaks up into a number of smaller loop permutations. For example, for $N = 7$ we might have a 4-particle loop, a pair permutation (2-particle loop), and a single particle. In the 4-particle loop, we might have particle #1 interchanged with #2, #2 interchanged with #3, #3 interchanged with #4, and #4 with #1. Given a set of configurations containing all $C(q_1, q_2, ...)$ ways of having q_1 loops of length 1, q_2 loops of length 2, etc., we can write

$$Z_N = \frac{1}{N!}\sum_{\{q_1,q_2...\}} C(q_1, q_2, ...)\prod_l Z(l)^{q_l} \tag{24}$$

where the sum is over all combinations of permutation numbers such that

$$\sum_l q_l l = N, \tag{25}$$

and

$$Z(l) = \int d\mathbf{r_1}...\mathbf{dr_l}\langle\mathbf{r_{P_1}},...,\mathbf{r_{P_l}}|\mathbf{e}^{-\beta\mathbf{H}}|\mathbf{r_1},...,\mathbf{r_l}\rangle \tag{26}$$

corresponds to a unbroken permutation loop of l particles. Feynman [10] has given an argument to show that this quantity is

$$C(q_1, q_2, ...) = \frac{N!}{1^{q_1}2^{q_2}...q_1!q_2!...} \tag{27}$$

While the argument given by Feynman can be consulted, for completeness we rederive this result in the Appendix. Eq.(24), with the result Eq.(27), is quoted in a beautiful little paper on Bose and Fermi partition functions by D. I. Ford [27], as well as by Matsubara and Feynman.

To evaluate the most probable distribution of loops, we invoke the grand canonical ensemble and multiply Z_N by $e^{\beta\mu N}$ and sum over all particle N values. This trick removes the restriction of Eq.(25) and allows the individual sums on q_l to be done. The grand canonical partition function is

$$\begin{aligned}\mathcal{Z} &= \sum_N e^{\beta\mu N}Z_N = \prod_l\sum_{q_l}\frac{1}{q_l!}\left(\frac{Z(l)e^{\beta\mu l}}{l}\right)^{q_l} \\ &= \prod_l \exp\left\{\frac{Z(l)e^{\beta\mu l}}{l}\right\}\end{aligned} \tag{28}$$

What we want from this is the average particle number, $\langle N\rangle$, and the average number of particles, $\langle q_l\rangle$, in the permutation loop of length l. We use the standard relation

$$\langle N\rangle = \frac{\partial}{\partial\mu}kT\ln\mathcal{Z} = \sum_{\updownarrow}\mathcal{Z}(\updownarrow)]^{\beta\mu\updownarrow} \tag{29}$$

From this it is clear that the average value of the loop number q_l is

$$\langle q_l \rangle = \frac{Z(l)e^{\beta\mu l}}{l} \tag{30}$$

Because H is the Hamiltonian corresponding to an ideal gas, $Z(l)$ can be broken up into a product of single-particle densities. $Z(l)$ is most easily evaluated by making each single-particle operator $e^{-\beta H_i}$ diagonal by interposing complete sets of harmonic oscillator functions as follows:

$$\begin{aligned} Z(l) = \sum_{m_1,m_2,...} \int d\mathbf{r_1}...\mathbf{dr_l} \, \langle \mathbf{r_{P_1}}, ..., \mathbf{r_{P_l}} | \mathbf{m_1}, ..., \mathbf{m_l} \rangle \\ \times e^{-\beta(E_{m_1}+...+E_{m_l})} \, \langle m_1, ..., m_l | \mathbf{r_1}, ..., \mathbf{r_l} \rangle \end{aligned} \tag{31}$$

where we have included only one subscript m_i to represent all three quantum numbers for a single-particle state. The $\mathbf{r}$ integrations lead to factors like

$$\int d\mathbf{r_1} \, \langle \mathbf{m_{P_k}} | \mathbf{r_1} \rangle \, \langle \mathbf{r_1} | \mathbf{m_1} \rangle = \delta_{\mathbf{m_{P_k}},\mathbf{m_1}} \tag{32}$$

where P_k represents the particle number that moved into position $\mathbf{r_1}$ in the permutation. Since we have a ring exchange these δ-functions mean that *all* m_i become equal to one of them, call it m. The result is simply

$$Z(l) = \sum_m e^{-\beta l E_m} \tag{33}$$

which is a one-body partition function at inverse temperature βl. The sum, over the three quantum numbers represented by m is easily done:

$$Z(l) = \frac{e^{-3\beta l\hbar\omega/2}}{(1 - e^{-\beta l\hbar\omega})^3} \tag{34}$$

The numerator comes from the zero point energy in each E_m. Putting this result back into Eq.(29) (and dropping the averaging brackets), we find

$$N = \sum_l \frac{e^{-\alpha l}}{(1 - e^{-\beta l\hbar\omega})^3} \tag{35}$$

which, as expected, is precisely the same result as derived in Sec. III. However, this derivation has led to the very instructive result that the sum over l is a sum over *permutation loops*, which arise from the symmetrization of the wave function. Note also that in the homogenous gas in a box, one is unable to do the exact sum over states as we could in Eq.(33). In that case [10]· [12]· [26] one replaces the sum by an integral; the result is that the expression equivalent to Eq.(35) is approximate and neglects the condensate, which must once more be added in by hand. Eq.(35), on the other hand, is exact and *includes* the condensate.

Figure 2 illustrates the fact that the condensate is made up of large-scale permutation loops, a fact that is well-known, but has not been so well-illustrated previously. What has perhaps not been so clear previously is that loops of *all* sizes contribute nearly equally to the condensate. The average number of particles $p_l = \langle q_l \rangle \, l$ in a permutation loop is given by Eq.(30) as

$$p_l = \frac{e^{-\alpha l}}{(1 - e^{-lT_0/TN^{1/3}})^3} \tag{36}$$

where we have used Eq.(7). Because α is of order $1/N$ at $T < T_c$, the l sum extends to order N, but we know that the non-condensed particles are given by terms with $lT_0/TN^{1/3} \ll 1$, that is, for loops of size less than of order $N^{1/3}$. The terms for larger $l \gg N^{1/3}$ have $p_l \cong e^{-\alpha l}$, which is identical with the form given in the second last version of Eq.(20) for n_0. All these terms then contribute only to the condensate. Each such term in the condensate is crudely of order 1, but there are of order N such terms so they contribute a total number of particles on the order of N. The fact that permutation loops of length of order $l > N^{1/3}$ have only 1 particle in them on average means that the long permutation loops are forming and breaking with fluctuations in size that are extremely wild. [28]

V. DENSITY MATRIX

The density matrix is a very useful quantity allowing averages of any thermodynamic variable to be evaluated. The one-body reduced density, mentioned in Sec. I, is particularly useful in considerations of BEC as Penrose and Onsager [13] have shown. This quantity is defined by integrating the N-body density, Eq. (21) over all but one coordinate:

$$\varrho_1(\mathbf{r},\mathbf{r}') = \int \mathbf{dr_2...dr_N}\ \rho_{\mathbf{S}}(\mathbf{r},\mathbf{r_2...r_N};\mathbf{r}',\mathbf{r_2...r_N}) \tag{37}$$

The diagonal element $\varrho_1(\mathbf{r},\mathbf{r})$ is just the density of particles $\varrho(\mathbf{r})$ at position $\mathbf{r}$. It turns out, after a short derivation, that the one-body reduced density for the boson ideal gas has the rather simple, physically intuitive form

$$\varrho_1(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{m}} \mathbf{n_m}\psi_{\mathbf{m}}(\mathbf{r})\psi^*_{\mathbf{m}}(\mathbf{r}') \tag{38}$$

where

$$n_m = \frac{1}{e^{\beta(E_m-\mu)}-1} \tag{39}$$

is simply the occupation of the mth single-particle state as used in Eq.(6), and ψ_m is the corresponding single-particle state.

The density matrix $\varrho_1(\mathbf{r},\mathbf{r}')$ can be considered to be an operator with eigenvalues. In fact the spectral form of Eq.(38) shows that the eigenfunctions are the ψ_m and the eigenvalues are the n_m; it is straightforward to verify that $\int d\mathbf{r}'\varrho_{\mathbf{1}}(\mathbf{r},\mathbf{r}')\psi_{\mathbf{m}}(\mathbf{r}') = \mathbf{n_m}\psi_{\mathbf{m}}(\mathbf{r})$. The fact that $\varrho_1(\mathbf{r},\mathbf{r}')$ has a *large* eigenvalue, in this case n_0, leads to its usefulness as a criterion for BEC. Even when there are interactions, the large eigenvalue is the condensate number and the eigenfunction is the condensate "wave function," but note that the solution is no longer simply the ground-state of the oscillator potential. In the case of weakly interacting bosons, this condensate wave function is approximately the solution of the well-known Gross-Pitaevskii nonlinear Schrödinger equation. [2]

We can transform the density into a sum over permutation loops by expanding n_m in the now familiar way. We get

$$\varrho_1(\mathbf{r},\mathbf{r}') = \sum_{\mathbf{l=1}}^{\infty} \mathbf{e}^{\beta\mu\mathbf{l}} \left\{ \sum_{\mathbf{m}} \mathbf{e}^{-\mathbf{l}\beta\mathbf{E_m}}\psi_{\mathbf{m}}(\mathbf{r})\psi^*_{\mathbf{m}}(\mathbf{r}') \right\} \tag{40}$$

The quantity in curly brackets is simply the harmonic oscillator density matrix $d(\mathbf{r},\mathbf{r}')$ for a *single* free (distinguishable) particle, but at inverse temperature $l\beta$, rather than simply β. The value of this is well known, and is [10]

$$\begin{aligned} d_l(\mathbf{r},\mathbf{r}') = & \left(\frac{m\omega}{h\sinh(l\beta\hbar\omega)}\right)^{3/2} \\ & \times \prod_{i=x,y.z} \exp\left\{-\frac{m\omega}{2\hbar\sinh(l\beta\hbar\omega)}\left[(r_i^2+r_i'^2)\cosh(l\beta\hbar\omega)-2r_ir_i'^2\right]\right\} \end{aligned} \tag{41}$$

One can see, for example, that $d_l(\mathbf{r},\mathbf{0})$, and therefore $\varrho_1(\mathbf{r},\mathbf{0})$, goes to zero at large $\mathbf{r}$ in contrast to the homogeneous case of Eq.(2).

We are particularly interested in the particle density $\rho(\mathbf{r}) = \varrho_{\mathbf{1}}(\mathbf{r},\mathbf{r})$. With a bit of hyperbolic function manipulation, one finds this to be

$$\rho(\mathbf{r}) = \sum_{\mathbf{l=1}}^{\infty} \mathbf{e}^{\beta\mu\mathbf{l}} \left(\frac{\mathbf{m}\omega}{\mathbf{h}\sinh(\mathbf{l}\beta\hbar\omega)}\right)^{\mathbf{3/2}} \exp\left\{-\frac{\mathbf{m}\omega}{\hbar}\tanh\left(\frac{\mathbf{l}\beta\hbar\omega}{\mathbf{2}}\right)\mathbf{r^2}\right\} \tag{42}$$

One can integrate this $\rho(\mathbf{r})$ to verify the result of Eq.(18).

We have seen that the WKB approximation can be found by assuming that $l\beta\hbar\omega$ is small. If we do that here we find

$$\rho(\mathbf{r}) = \sum_{\mathbf{l=1}}^{\infty} \mathbf{e}^{\beta\mu\mathbf{l}} \left(\frac{\mathbf{2}\pi\mathbf{m}}{\mathbf{h^2 l}\beta}\right)^{\mathbf{3/2}} \exp\left\{-\frac{\mathbf{l}\beta\mathbf{m}\omega^{\mathbf{2}}}{\mathbf{2}}\mathbf{r^2}\right\} \tag{43}$$

This result agrees with Eq.(16) for the harmonic potential.

The largest value of the density occurs at the origin, of course, and we can ask what this value is at the BEC transition. For T above or equal to the transition temperature, the WKB approximation is valid in the TDL. Right at the transition the chemical potential vanishes (actually it is the quantity α of Eq.(10) that vanishes, but the WKB approximation neglects the zero-point energy, which is of order $1/N^{1/3}$.) We find that the critical density is

$$\rho_c(0) = \left(\frac{2\pi mkT_c}{h^2}\right)^{3/2} \sum_{l=1}^{\infty} \frac{1}{l^{3/2}} = \left(\frac{2\pi mkT_c}{h^2}\right)^{3/2} \zeta(3/2) \tag{44}$$

or

$$kT_c = \frac{2\pi\hbar^2}{m} \left(\frac{\rho_c(0)}{\zeta(3/2)}\right)^{2/3} \tag{45}$$

But this is precisely the transition temperature for an ideal gas in a *box* at *uniform* density $\rho_c(0)$! Thus the trapped gas, which has its BEC localized near the origin, has a condensate there under just the same conditions as the gas in a box. This interesting situation has been noted previously in the literature. [6], [19], [29].

In Fig. 3 we plot the full density as a function of position as well as the WKB approximation to it. One sees that the two are equal only for large r. In the case of $N = 1000$ at the temperature considered, the condensate number is about 456, so the non-condensed particle number is 544, despite the appearance in the plot that the condensate is much larger than the non-condensate. This feature is explained by the fact that there is a factor r^2 involved when one integrates this to find the total N value; this factor diminishes the interior points and emphasizes the wide wings.

Another way we can see that the high l permutation loops belong to the condensate is by considering the mean square radius of the individual permutation densities. This is

$$\sigma_l^2 = \frac{\int d\mathbf{r}\mathbf{r^2}\rho_\mathbf{l}(\mathbf{r})}{\int d\mathbf{r}\rho_\mathbf{l}(\mathbf{r})} \tag{46}$$

where ρ_l is the summand of Eq.(42). The result is

$$\sigma_l^2 = \frac{3}{2}\frac{\hbar}{m\omega}\frac{1}{\tanh l\beta\hbar\omega/2} \tag{47}$$

The WKB approximation for this is gotten by considering $l\beta\hbar\omega$ small, for which we find

$$\sigma_l^2(\mathrm{WKB}) = 3\frac{\hbar}{m\omega}\frac{1}{l\beta\hbar\omega} \tag{48}$$

This quantity drops off like $1/l$. The contribution from the condensate comes from large $l\beta\hbar\omega$ ($N^{1/3} < l \leq N$) and is

$$\sigma_l^2(\mathrm{condensate}) = \frac{3}{2}\frac{\hbar}{m\omega} \tag{49}$$

This is simply the mean square width of the ground-state of the harmonic oscillator. Figure 4 shows the plot of σ_l^2, $\sigma_l^2(\mathrm{WKB})$, and $\sigma_l^2(\mathrm{condensate})$ for $N = 1000$. We again see that, for $l > 40$ or so, that the permutation loops all refer to the condensate.

In recent path-integral Monte Carlo calculations [16], [18] for trapped gases, it was necessary to identify the condensate by use of the permutation cycles. Ref.16 assumed that the size of the largest cycle occurring was equivalent to the condensate number. [28] Ref.18, on the other hand, assumed that the condensate was made up of all particles for l greater than a value where σ_l^2 has become constant. However, we see that, for the latter approach, some of the particles having *small* permutation cycles also contribute to the condensate and must be counted.

VI. DISCUSSION

We have seen that it is possible and instructive to examine BEC via the permutation loop picture. Ideal gases trapped in a harmonic potential become particularly helpful in this regard because we can do many of the computations analytically and exactly. The very long permutation loops are characteristic of BEC and form when the thermal de Broglie wavelength becomes comparable to the average distance between particles. Under these conditions multi-particle exchange becomes possible and the coherence characteristic of BEC takes place with the particles exhibiting the strong symptoms of indistinguishability.

The best known characteristic of BEC is the presence of a macroscopic fraction of the particles in the lowest state. For the ideal gas, in a harmonic trap at absolute zero, those particles would be in the oscillator ground-state. From the point of view of permutations, this situation is equivalent to all possible lengths of permutation cycles being equally likely (up to length N, which is taken to infinity in the TDL). As the temperature is raised, but still below the condensation temperature, the shorter loops become increasingly prevalent. Shorter loops occur when particle indistinguishability is less a factor and corresponds to particles being spread out over excited oscillator states. Finally, above the transition temperature, no state has a macroscopic occupation of particles and most permutation cycles are short; very long ones are rare.

BEC and the λ-transition in liquid helium have been compared with a polymer transition, [15] with long chain polymers forming below the transition temperature. In fact there is a transition in sulphur [30] in which the opposite effect occurs: above the transition there are very long chains of sulphur atoms, while below the transition only eight-atom rings form; the isomorphism involves $\beta \to kT$. Interestingly the specific heat of sulphur has a "λ-transition."

The reduced single-particle density matrix has the lowest state as an eigenfunction with the condensate number as eigenvalue. For the ideal gas demonstrating this is a straightforward matter with its connection to long permutation loops made evident in the density. However, the property carries over into the interacting gas as well. Finding the eigenfunction of the one-particle density is one of the most important theoretical problems in the interacting fluid, with the solution representing the condensate wave function and the "order parameter" of the state. The solution of the Gross-Pitaevskii equation is a standard approximation to this wave function. In the case of real harmonically trapped gases, which actually do interact, this equation seems to represent the experimental situation fairly accurately. [2]

The PIMC approach was invented by Feynman and has been exploited in a wide range of fields, including the description of polymers. [31] One of its most successful applications has been to bosons and liquid ^{4}He by Ceperley and co-workers. [15] The approach considers in detail the particle positions in space, using the expression Eq.(21) as its basis, and takes the formation of permutation loop "polymers" as one of its most important features. The interested reader should consult the review of Ceperley. [15]

APPENDIX

In this Appendix we derive the expression Eq.(27) for the number of ways of forming q_1 permutation loops of length 1, q_2 of length 2, ...q_l of length l, etc. Suppose we consider an 9-particle system having two 3-particle loops [(1$\to$ 2 $\to$ 3 $\to$ 1) and (4$\to$ 5 $\to$ 6 $\to$ 4)], a 2-particle loop [(7$\to$ 8 $\to$ 7)], and a singlet [(9)]. We can mix up these particles to get other non-equivalent 3-, 2-, and 1-loops. We want to count ways we can do this. For example, suppose we replace 1 by 4 and 4 by 1, giving (4$\to$ 2 $\to$ 3 $\to$ 1), (1$\to$ 5 $\to$ 6 $\to$ 1), (7 $\to$ 8 $\to$ 7), and (9). This is a new arrangement. There are 5! different ways of mixing the particles to get new permutations arrangements, but not all of them are distinct. For example if we replace 2 by 1, 3 by 2, and 1 by 3, we get the permutation loop (3$\to$ 1 $\to$ 2 $\to$ 3), which is just the same as the original arrangement, with the loop rotated one click, which makes no real change. In a loop of length l there are l such loop rotations that don't count for new arrangements. Another way of replacing particles that does *not* lead to new arrangements is by interchanging all the particles in one 3-loop of the same length by those of the other 3-loop. There are 2! such interchanges of loops possible in our special case. Thus the total number of possible distinct arrangements in our 9-particle case is $9!/3^2 2!$. For the N-particle case we easily generalize to find that the number of distinct arrangements for the N particle case is

$$C(q_1, q_2, ...) = \frac{N!}{1^{q_1} 2^{q_2} ... q_1! q_2! ...} \tag{50}$$

where $N!$ is the total number of ways of rearranging N particles, l^{q_l} is the number of ways of "rotating" the q_l permutations loops of length l, none of which produces a new arrangement, and $q_l!$ is the number of ways of interchanging whole loops of the same length, which also does not produce a new arrangement. The expression of Eq.(50) is known as "Cauchy's formula." [32]

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FIGURE CAPTIONS

Figure 1. Condensate fraction versus T/T_0. The condensation transition temperature is $T_0/\zeta(3)^{1/3} = 0.94T_0$. The solid line is the thermodynamic limit case given by Eq.(14). The dotted line is the exact solution for N =1000.

Figure 2. Summands of various expressions of Sec. III for N versus summation index l. Here we have $N = 1000$ and $T/T_0 = 0.7$. The solid line is the summand of the exact expression Eq.(18); the dashed line represents the WKB summand of Eq.(19); and the dotted line is the summand of the condensate in Eq.(20). The maximum value of the exact case at $l = 1$ is 423. Since the index l corresponds to permutation loops, that means there are 423 singlets; the condensate (the dotted line) includes all the large l values (the long permutation loops) as well as some of the small loops and corresponds to a total of 456 particles; the remaining small, non-condensate loops contribute 121 particles. Note that the summands of Eq.(19) and Eq.(20) do not quite add up to the exact result, because of the higher order neglected terms in the WKB expression.

Figure 3. Density as a function of r. The solid line is the exact density, the dashed line is the WKB approximation, which represents the non-condensed particles, and the dotted line is the condensate density, derived using the first term in sum of Eq.(38). $T/T_0 = 0.8$ here. Density is in units of $(m\omega/\hbar)^{3/2}$ and position in units of $(\hbar/m\omega)^{1/2}$.

Figure 4. Mean square width (in units of $(\hbar/m\omega)$) for particles in permutation loop l versus l. The solid line is the exact result, the dashed line is the WKB approximation to the mean-square width, representing the non-condensed particles, and the dotted line is the condensate width (3/2).

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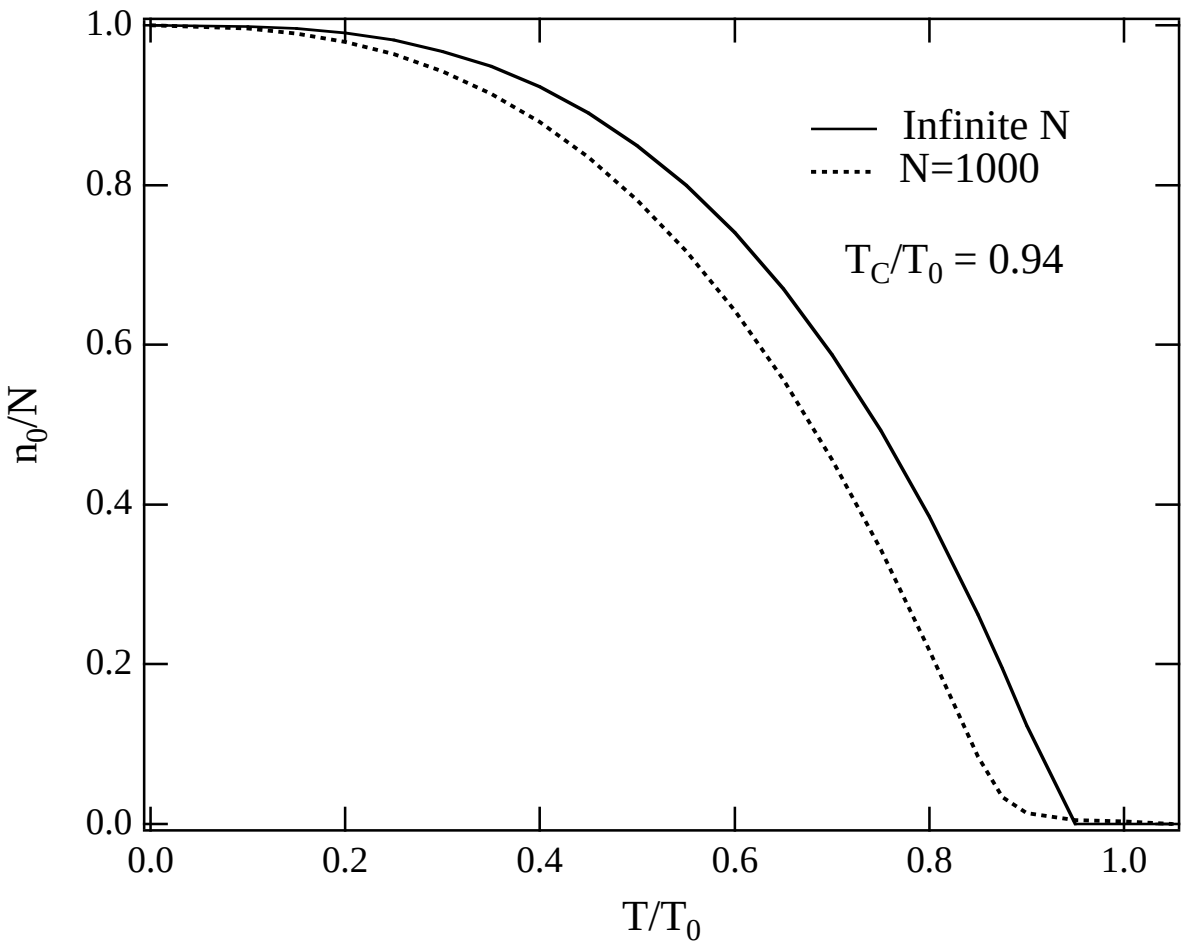
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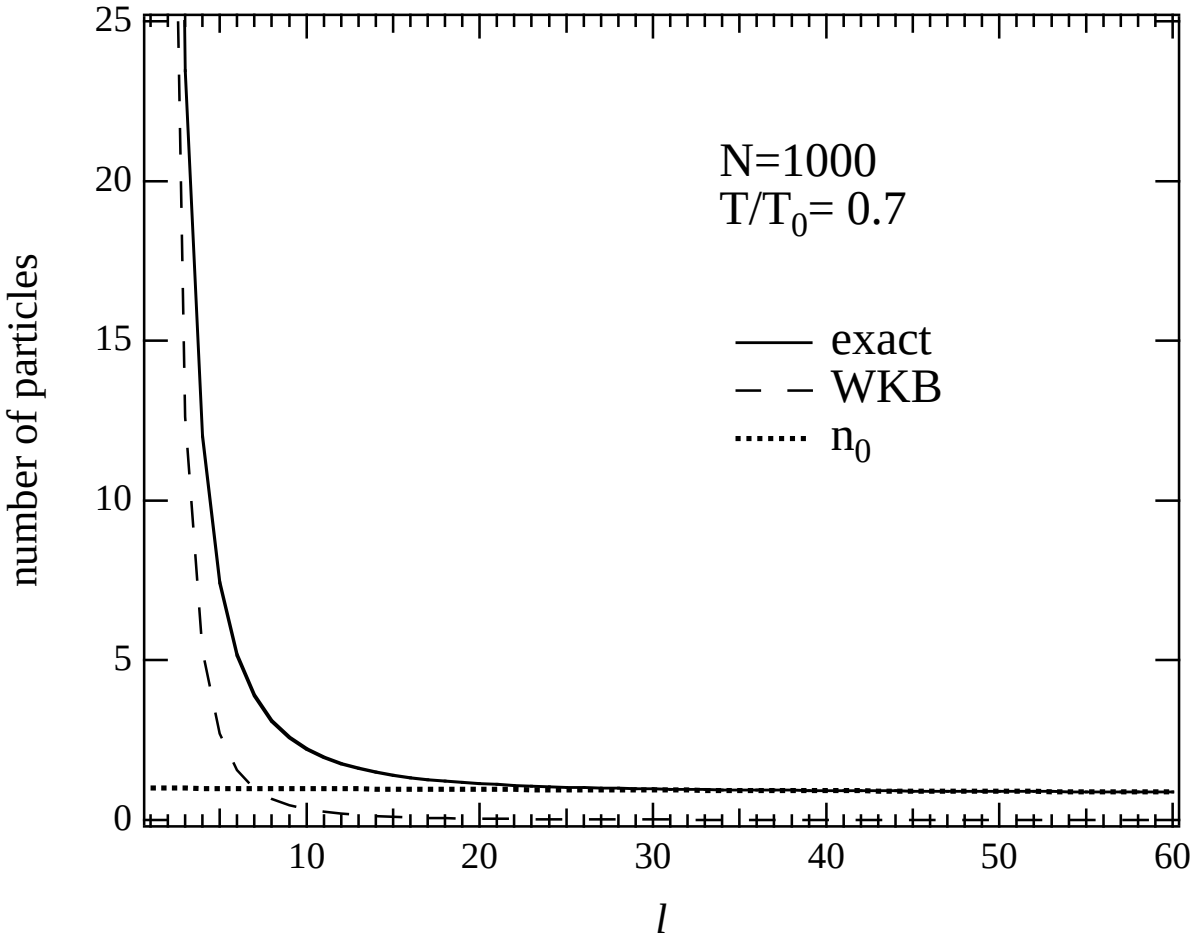
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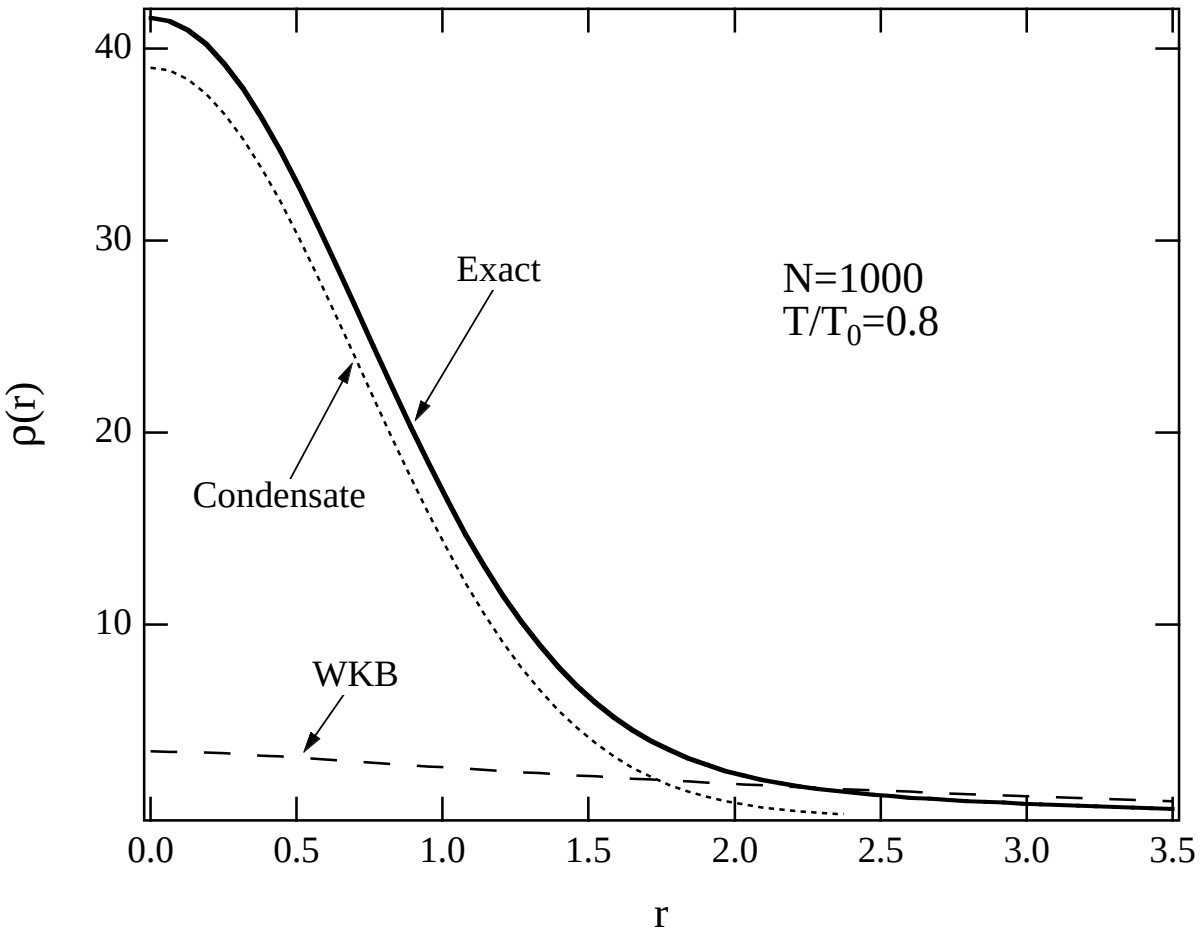
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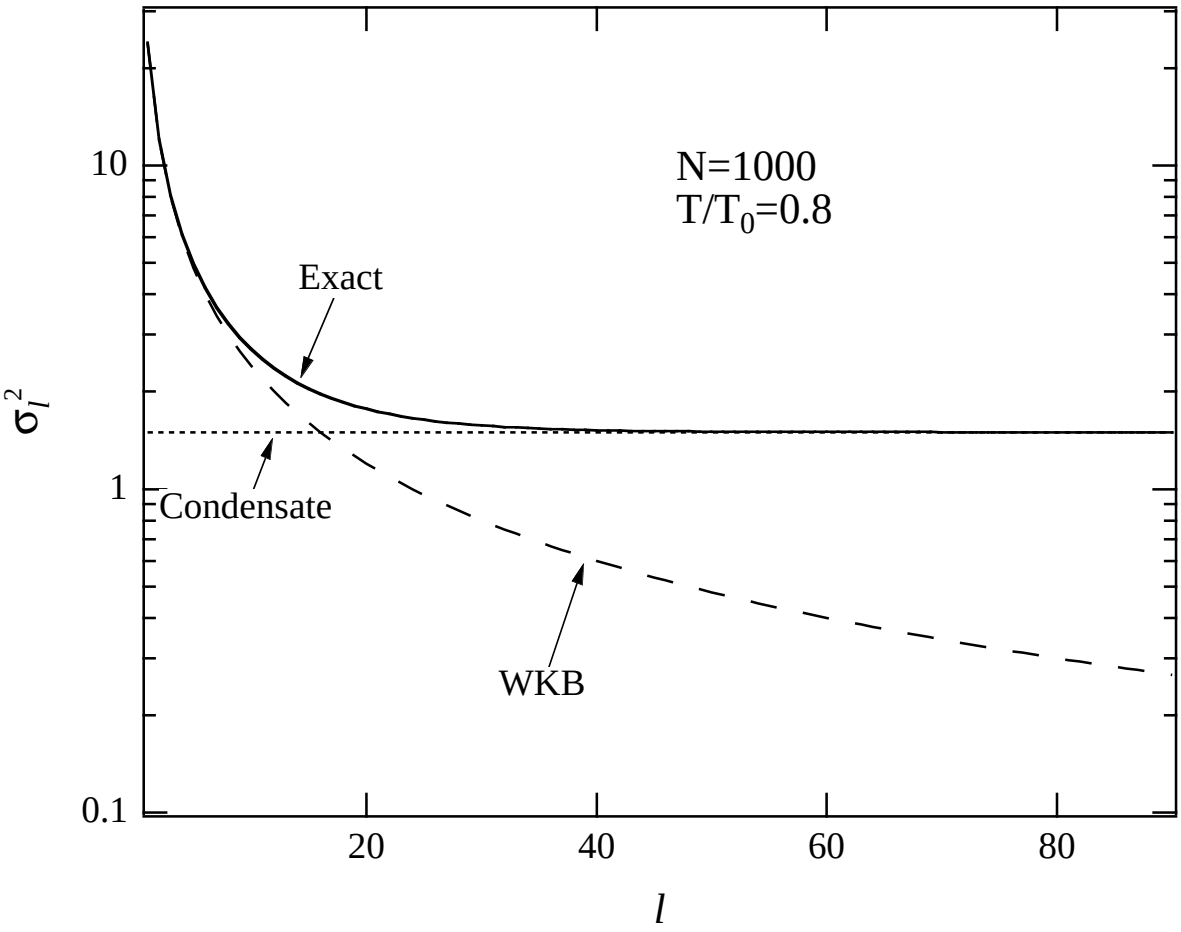
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