Bose-Einstein condensation in one-dimensional power-law traps: A path-integral Monte Carlo simulation

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Bose-Einstein condensation is known to occur in one-dimensional power-law potentials $V(x)\propto|x|^{\eta}$ as a true phase transition for $\eta<2$, but only if there are no interactions between the particles. We show, via a path-integral quantum Monte Carlo scheme, that for both $\eta<2$ and $\eta=2$ the spatial distribution of finite numbers of hard-core bosons suddenly becomes bimodal below a certain temperature, with a central condensate of particles distributed according to the lowest single-particle eigenstate. At still lower temperatures, the hard-core interactions cause the single-particle ground state to become a poor description for the interacting gas. If $\eta<2$, the energy per particle undergoes a sudden decrease near the same temperature at which the bimodal distribution appears. It is found that this drop in energy disappears if the range of the interaction potential is sufficiently large. [S1050-2947(98)09308-1]

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Recent observations of Bose-Einstein condensation (BEC) [1–3] in gases of magnetically trapped ultracold alkali-metal atoms [4–7] have opened up exciting new prospects for studying the quantum statistics of bosonic systems. Prominent among current goals is the construction of extremely anisotropic trapping configurations in order to determine whether a condensate can be produced in less than three dimensions, a possibility that was initially ruled out by Hohenberg's theorem [8], which states that BEC cannot occur in ideal one-dimensional (1D) or two-dimensional systems. Widom [9] later pointed out that this theorem only applies to homogeneous systems, and proved that BEC phase transitions occur in a 2D rotating gas and a 1D gas in the presence of a gravitational field. Further examples include an attractive δ-impurity system in any number of dimensions [10], a general 2D power-law trap, and a 1D power-law trap more confining than parabolic [11].

The potential wells that trap the atoms in experiments are, to a good approximation, harmonic oscillator potentials. It has been pointed out that lowering the number of dimensions D of a harmonic oscillator increases the transition temperature as $T_c\sim N^{1/D}$ and is therefore favorable for BEC [12]. In any case, the absence of a true phase transition has been proved for parabolically confined ideal bosons in one dimension [13,14]. There is only a pseudotransition, characterized by a sudden rise in the ground-state occupancy, which occurs at a temperature that goes to zero as $1/\ln N$ in the thermodynamic limit [15]. This effect has nevertheless been referred to as Bose-Einstein condensation [12] and is assigned a transition temperature T_c, determined by $N=\tau_c\ln(2\tau_c)$ where $\tau_c=k_BT_c/\hbar\omega$.

Bose-Einstein condensation does occur meanwhile in a 1D power-law potential $V(x)\propto|x|^{\eta}$ if $\eta<2$ [11]. That is, there is a true phase transition in that case. In general, BEC in the thermodynamic limit is only possible in 1D and 2D systems if the density can increase without bound somewhere in the system. Since this divergence is prevented in an interacting gas, there can be no BEC phase transition for nonideal bosons in one dimension [15–17]. In a 2D harmonic oscillator, a transition to a superfluid state in the thermodynamic limit has been proposed [17], and a similar phase may also be present in some 1D potentials.

Experiments are carried out with finite numbers of particles so questions of density divergence never arise in realistic situations, and since an interacting Bose gas can exhibit essentially ideal behavior as long as the range of the interaction potential is small compared with the average distance between particles, the observation of Bose-Einstein condensation (at least as a pseudotransition) in 1D systems may well be feasible in the laboratory.

In this article we report simulations of finite numbers of ideal and weakly interacting (hard-core) bosons in 1D power-law traps. We are particularly interested in the experimental implications of our results, which are limited to a few hundred atoms. Meanwhile, the thermodynamic limit of a trapped nonideal Bose gas in 1D is an interesting problem which also deserves attention, but which is not considered here. In fact, the interacting systems we study here are directly relevant to a possible future experimental setup. In a real trap, atomic motion could be restricted to a single spatial dimension since the freezing out of motion in two dimensions can be ensured by making the length scale of the confinement potential much smaller in those dimensions. The system that we actually simulate is strictly 1D with the power-law confinement given by $V(x)=V_0(|x|/L)^{\eta}$ with $V_0,L=1$.

Path-integral Monte Carlo (PIMC) methods represent the most powerful approach for studying the finite-temperature properties of many-body systems in the quantum regime. PIMC schemes have recently been used to simulate BEC for hard-core bosons in three dimensions [18,19]. In this article we will apply the PIMC method for bosonic systems [20,21], specifically following the formulation of Ref. [21]. PIMC is based on the fact that the partition function $\mathcal{Z}=\mathrm{Tr}\,\rho$ of a many-body system can be written in the form of a path integral [22] if the density operator $\rho=e^{-\beta(H_0+H_1)}$ is decomposed according to the Trotter formula

$$e^{-\beta(H_0+H_1)}=\lim_{M\to\infty}(e^{-\beta H_0/M}e^{-\beta H_1/M})^M, \tag{1}$$

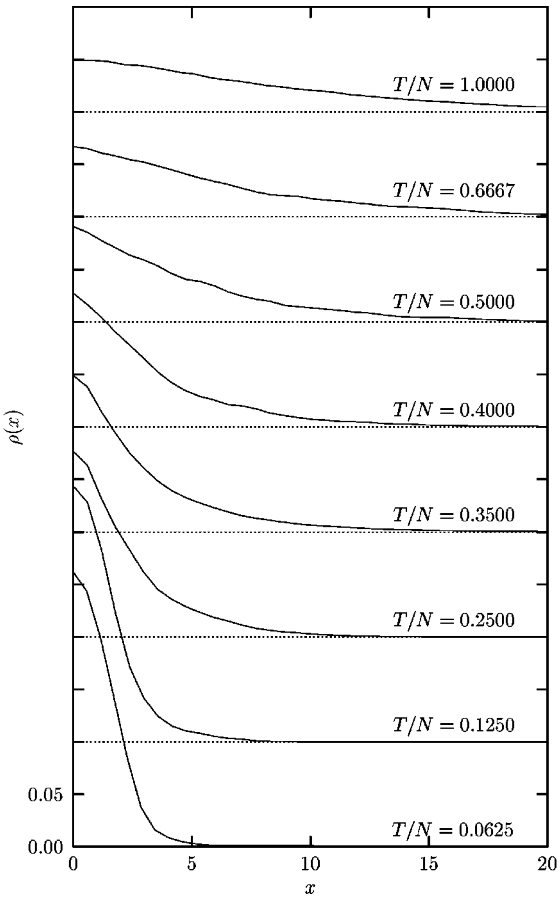

FIG. 1. The spatial atomic density $\rho(x)$ of 50 atoms in a trap with $\eta=1.5$ and hard-core radius $a=10^{-3}$ at different temperatures. For clarity, all but the lowest curve have been offset vertically at equal intervals of 0.1; a dotted line is used to indicate the zero point of each curve.

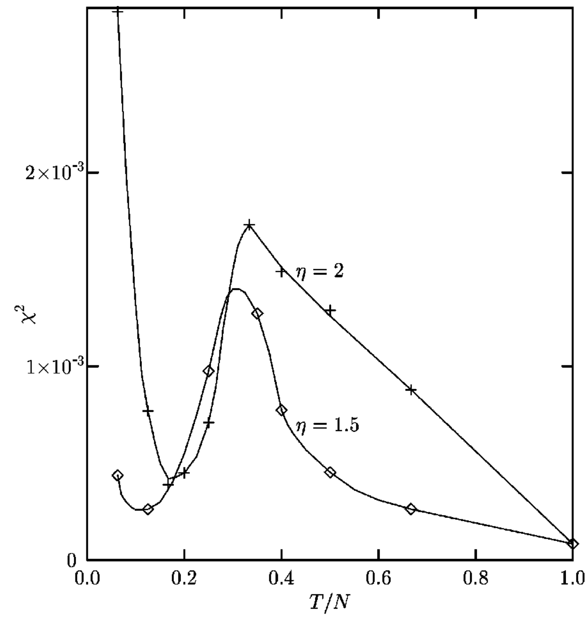

FIG. 2. The goodness of fit χ^2 for fits of $\rho(x)$ to the single-particle ground state for both $\eta=1.5$ (diamonds) and $\eta=2$ (crosses). Lines connecting data points provide a visual guide only. The peaks shows that the distributions become bimodal due to the onset of BEC. The effect of the hard-core interactions causes χ^2 to increase again at low temperature.

where $H_0=-(\hbar^2/2m)\sum_i^N \nabla_i^2$ and $H_1=V(\mathbf{r}_1,\mathbf{r}_2,\ldots,\mathbf{r}_N)$ are, respectively, the kinetic and potential energy operators of the system, $\beta=1/k_BT$ is the inverse of the temperature T, and k_B is the Boltzmann constant. For convenience, we use $\hbar=m=1$. For bosons, a sum over permutations of all the particles is necessary in order to symmetrize the density matrix [20,21]. In practice this means that the Monte Carlo simulation consists of permutation moves as well as coordinate moves.

The inclusion of a hard-core interaction potential, with core radius a, is straightforward for a 1D system. We have designed an efficient algorithm based on a system of cells, each of length $2a$. N-particle configurations that consist of one or more multiply occupied cells are immediately rejected. Otherwise the only interatomic separations that are computed are those between atoms that occupy adjacent cells.

In all our simulations, great care is taken to ensure that the results are convergent with respect to the Trotter number M as well as the number of Monte Carlo iterations. Since no approximations remain, we can be confident that our results are correct within the statistical errors. For the potentials studied here, around 10^6 Monte Carlo sweeps, including about 10^5 warm-up sweeps, are required with larger η generally requiring slightly fewer iterations.

The technique used to compute the spatial atomic density $\rho(x)$ is straightforward: A system of small boxes is set up along the x axis. After each complete Monte Carlo sweep over all particles, the coordinates of each atom are binned in the appropriate box. The number of counts in each box leads directly to $\rho(x)$. The size of the boxes must be chosen with care. If they are too small, then the number of counts per box will be small and the statistics poor. On the other hand, the exact result for $\rho(x)$ can only be obtained in the limit of infinitesimally small box size. In the present work we have used a small box size so that it was necessary to carry out a large number of Monte Carlo sweeps in order to reduce the statistical noise to a reasonable level. Consequently, the results presented here are limited to calculations for samples of 50 atoms.

In cases where BEC occurs a bimodal atomic distribution appears below the transition temperature—a broad distribution due to the uncondensed portion and a narrow distribution due to the condensate (or pseudocondensate). Even for an ideal Bose gas, this does not necessarily confirm the existence of a phase transition. The sudden appearance of a bimodal distribution is, however, directly related to an abrupt increase in the fraction, N_0/N, of particles occupying the single-particle ground state. For a finite number of ideal bosons, we know that such an abrupt increase occurs for both $\eta=2$ where there is a pseudotransition and for $\eta<2$ for which a true phase transition occurs. Neither system can have a BEC phase transition if the bosons are interacting.

Figure 1 shows the evolution of the atomic density $\rho(x)$ with decreasing temperature for $\eta=1.5$ with $N=50$ and $a=10^{-3}$. A central peak emerges and gradually grows as the system is cooled. In order to interpret this result, we have fit the data to a function of the form of the probability density, $\psi_{0,\eta}^2(x)$, for a single particle in the ground state of the same

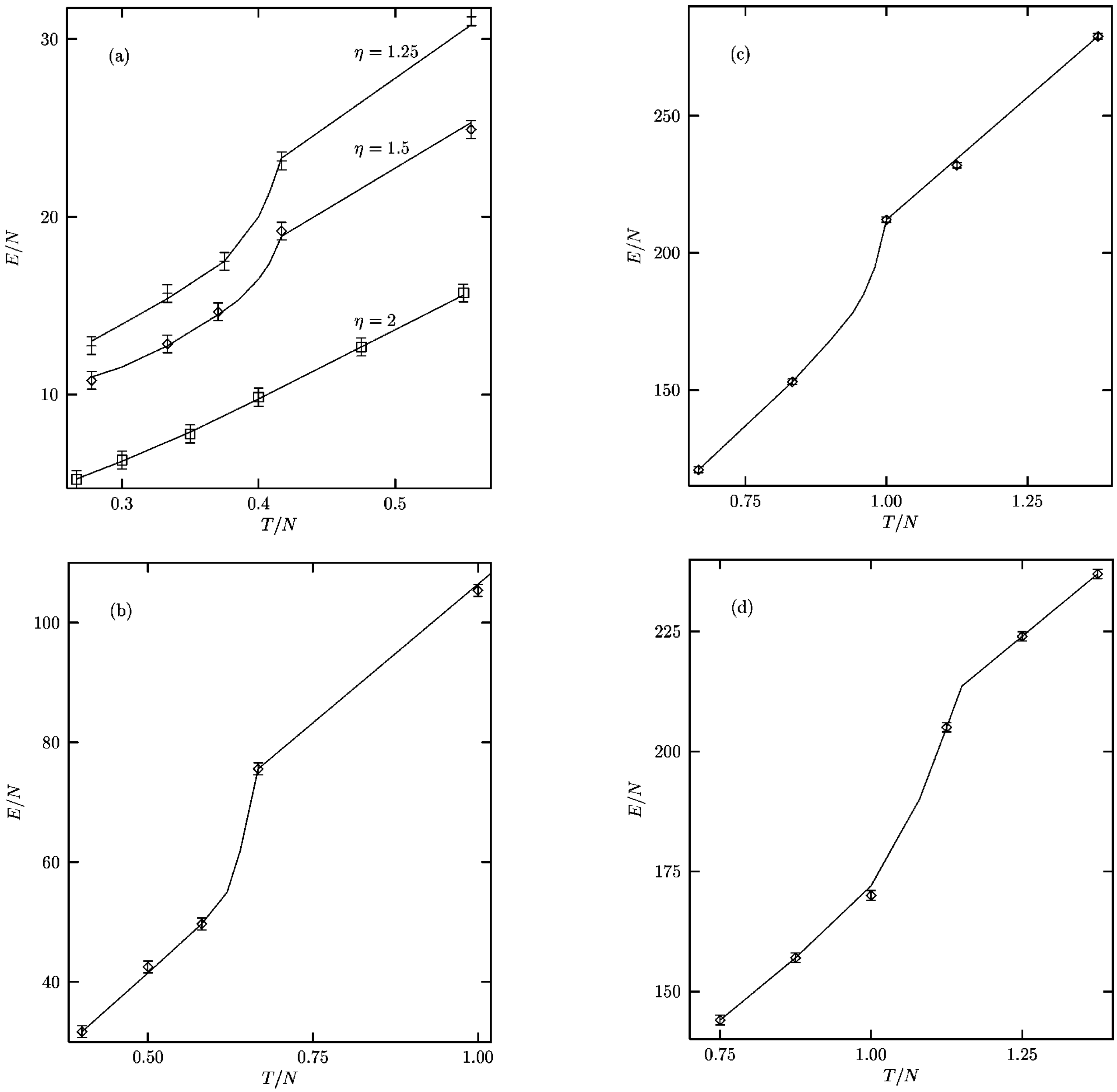

FIG. 3. The energy per atom of (a) 50, (b) 100, (c) 200, and (d) 400 hard-core bosons with $a = 10^{-3}$. (a) includes results for η=1.25 (crosses), 1.5 (diamonds), and 2 (boxes), while (b), (c), and (d) include only η=1.5. Lines connecting data points provide a visual guide only. A change in the slope of the curve is an indication of Bose-Einstein condensation for η=1.25 and 1.5.

potential, and thus obtained the goodness of fit, χ^2 [23]. In Fig. 2 we plot χ^2 for η=1.5 and η=2. For η=1.5, χ^2 increases steeply at $T/N \simeq 0.4$ and reaches a local maximum at $T/N \simeq 0.35$. For η=2, χ^2 increases more gradually and peaks at around the same temperature (note that for 50 ideal bosons with η=2, $T_c/N = 0.418$). The hump in χ^2 is associated with the emergence of a central condensate of atoms, which occurs at $T/N \simeq 0.4$ for η=1.5, as shown in Fig. 1. When the condensate forms, χ^2 first of all increases because the atomic distribution becomes bimodal. As the temperature is decreased further below $T = T_c$, the condensate fraction N_0/N begins to approach unity, so that χ^2 becomes very small. In an ideal Bose gas, N_0/N continues to increase until $N_0/N = 1$ (and $\chi^2 = 0$) at $T = 0$.

As the system is cooled, the atom density in the center of the trap increases, and it becomes progressively more difficult for the hard-core Bose gas to mimic the ideal Bose gas. In particular, if the sum of the hard-core diameters $2Na$ is sufficiently large on the length scale of $\psi_{0,\eta}(x)$, then it will become impossible for all of the atoms to be distributed according to $\psi_{0,\eta}(x)$. In that case, the low-temperature condensate would broaden with respect to the ideal case and the probability density would eventually become very different from $\psi^2_{0,\eta}(x)$ (so that χ^2 would increase) as T is lowered. In fact, we find that in the present case, the length scale of $\psi_{0,\eta}(x)$ is only about a factor of 10 greater than $2Na$, so it is not surprising that χ^2 increases in the region $T/N < 0.2$ for both η=1.5 and η=2 (at a slightly higher temperature). In fact, comparison of $\rho(x)$ for η=1.5 and η=2 shows that the density in the central region of the trap is always greater for η=2, which explains why this increase in χ^2 is at higher T in that case.

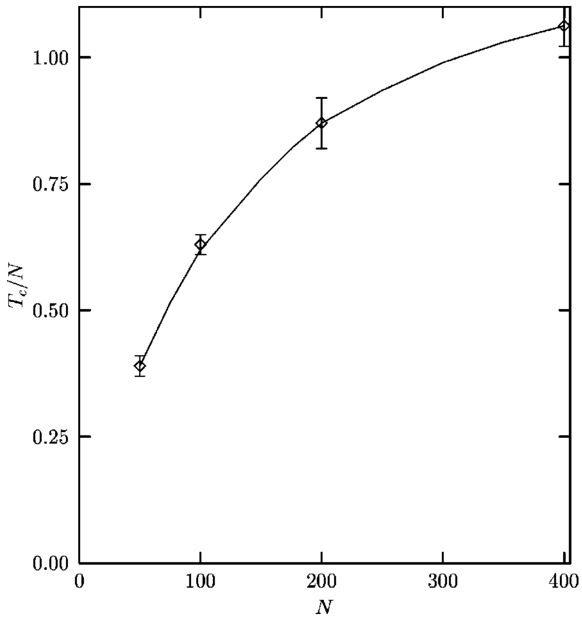

FIG. 4. The N dependence of the transition temperature with $\eta=1.5$ and $a=10^{-3}$. The line connecting data points provides a visual guide only. For large N it appears that T_c scales roughly with N.

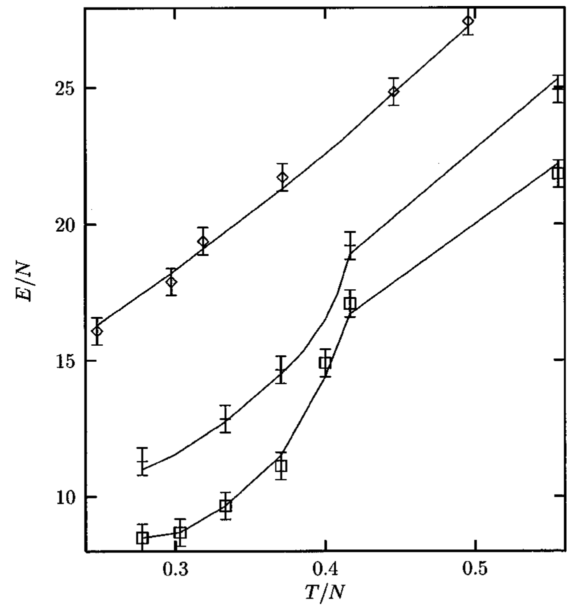

FIG. 5. The average energy per particle for $N=50$ with $\eta=1.5$ and $a=10^{-2}$ (diamonds), $a=10^{-3}$ (crosses), and $a=10^{-4}$ (boxes). Lines connecting data points provide a visual guide only. BEC is found to occur at roughly the same temperature for $a=10^{-3},10^{-4}$.

As we have stated, condensation of an ideal Bose gas in one dimension occurs as a true phase transition in potentials more confining than parabolic. Such a transition would be accompanied by an abrupt change in the slope of the energy-temperature curve near $T=T_c$. If the interactions in a real Bose gas are sufficiently weak then such an effect should still be observed. The energy per particle, E/N, of up to 400 atoms, displayed in Fig. 3, varies smoothly above or below a certain temperature (which we take to be the pseudotransition temperature T_c), whereas at that temperature it drops sharply. This behavior is qualitatively similar to what we expect to see for ideal bosons. The energy curve for $N=50$ with $\eta=1.5$, shown in the middle of Fig. 3(a), changes slope at a temperature just above the peak in χ^2, corresponding to the peak in Fig. 2. As in the ideal gas, it is only for $\eta=2$ that there is no drop in energy near T_c, as shown in Fig. 3(a). Furthermore, we find that the drop in energy increases as η is decreased. In fact, we find that the change in the slope of the energy curve also occurs for higher $\eta<2$, but as η increases the drop in energy eventually becomes comparable with our error estimation.

In Fig. 4 we plot the pseudotransition temperature T_c, extracted from our energy data for $\eta=1.5$. For large N, the dependence of T_c upon N is different from the 3D case where $T_c \propto N^{1/3}$ for ideal [12,14] or weakly interacting [4,18] bosons in a harmonic oscillator. Here it appears that T_c scales roughly with N for large N. On the other hand, we do not make the claim that the relation between T_c and N shown in Fig. 4 can be directly extrapolated to higher N. Since the density of atoms in the condensate increases with N, the interparticle repulsions would presumably eventually smear out the pseudotransition. The observation of condensation for progressively higher N would therefore require progressively smaller a.

We have computed the energy E of up to 400 weakly interacting hard-core bosons in 1D power-law traps. We chose the hard-core radius $a=10^{-3}$ because that is likely to be close to the experimental value. We have repeated some of those simulations for various a. In Fig. 5 we plot the average energy per particle for $N=50$ with $\eta=1.5$ and $a=10^{-2},10^{-3},10^{-4}$. The difference between the regimes of strongly and weakly interacting hard-core bosons is striking. The average energy in the strongly-interacting case ($a=10^{-2}$) varies smoothly with temperature over the whole range. Because the hard-core radius is not small on the scale of the average distance between particles in the center of the trap, condensation is prevented. For smaller a (10^{-3} or 10^{-4}), the average energy exhibits a change of slope which occurs at approximately the same temperature in both cases, while the energy drop increases with decreasing a. We have also carried out similar simulations for $\eta=1.25$, 1.75, and found equivalent behavior. In those cases, there is no observed drop in energy for $a=10^{-2}$, while the value of T_c in each case has no observed difference for $a=10^{-3}$ and $a=10^{-4}$. For 50 atoms in a 1D power-law trap of unit length L, $a\simeq 10^{-3}$ is required to observe BEC. Because the average distance between particles varies as $1/N$, smaller a ought to be required for larger N.

The results presented here should be very interesting from the experimental point of view. We have provided simulation results for interacting bosons confined in one dimension. Our results are reliable insofar as the PIMC method we have used does not contain any significant approximations. We have calculated anomalous behavior in the energy and spatial distribution for weakly interacting bosons in one dimension. Despite the absence of a BEC phase transition in the thermodynamic limit of nonideal bosons, it seems likely that these phenomena are due to BEC of finite numbers of interacting atoms. The distinction that exists between the regimes $\eta<2$ and $\eta=2$ for an ideal gas is observed in the interacting gas. It is only for $\eta<2$ that BEC is revealed by a drop in the energy, while the appearance of a bimodal distribution is also more abrupt. In other words, power-law traps more confining than harmonic offer by far the more promising situation for observing BEC in the laboratory. The energies we have calculated could be directly compared with future experimental measurements following a procedure similar to that in Ref. [7]. Likewise, calculation of the appropriate χ^2's is straightforward [6] given the velocity distribution of the atom cloud. The possibility of obtaining sufficiently anisotropic trapping conditions is discussed in Ref. [12], although only harmonic confinement is considered.

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[1] S. N. Bose, Z. Phys. **26**, 178 (1924).

[2] A. Einstein, Sitzungsber. K. Preuss. Akad. Wiss., Phys. Math. K1. No. 22, 261 (1924); No. 1, 3 (1925).

[3] For a recent account, see articles in *Bose-Einstein Condensation*, ed. by A. Griffin, D. W. Snoke, and S. Stringari (Cambridge University Press, Cambridge, England, 1995).

[4] M. H. Anderson, J. R. Ensher, M. R. Matthews, C. E. Wiemann, and E. A. Cornell, Science **269**, 198 (1995).

[5] C. C. Bradley, C. A. Sackett, J. J. Tollet, and R. G. Hulet, Phys. Rev. Lett. **75**, 1787 (1995).

[6] K. B. Davies, M.-O. Mewes, M. R. Andrews, N. J. van Druten, D. S. Durfee, D. M. Kurn, and W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995).

[7] J. R. Ensher, D. S. Jin, M. R. Matthews, C. E. Wiemann, and E. A. Cornell, Phys. Rev. Lett. **77**, 4984 (1996).

[8] P. C. Hohenberg, Phys. Rev. **158**, 383 (1967).

[9] A. Widom, Phys. Rev. **176**, 254 (1968).

[10] L. C. Ioriatti, Jr., S. G. Rosa, Jr., and O. Hipólito, Am. J. Phys. **44**, 744 (1976).

[11] V. Bagnato and D. Kleppner, Phys. Rev. A **44**, 7439 (1991).

[12] W. Ketterle and N. J. van Druten, Phys. Rev. A **54**, 656 (1996).

[13] S. R. de Groot, G. J. Hooyman, and C. A. ten Seldam, Proc. R. Soc. London, Ser. A **203**, 266 (1950).

[14] F. Brosens, J. T. Devreese, and L. F. Lemmens, Solid State Commun. **100**, 123 (1996).

[15] W. J. Mullin, J. Low Temp. Phys. **106**, 615 (1997).

[16] W. J. Mullin, Report No. cond-mat/9709077, where $D=1$ is a straightforward extension.

[17] S. I. Shevchenko, Zh. Eksp. Teor. Fiz. **100**, 1824 (1991) [Sov. Phys. JETP **73**, 1009 (1991)].

[18] W. Krauth, Phys. Rev. Lett. **77**, 3695 (1996).

[19] P. Grüter, D. Ceperley, and F. Laloë, Phys. Rev. Lett. **79**, 3549 (1997).

[20] E. L. Pollock and D. M. Ceperley, Phys. Rev. B **30**, 2555 (1984).

[21] M. Takahashi and M. Imada, J. Phys. Soc. Jpn. **53**, 963 (1984).

[22] R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[23] See, for example, J. R. Taylor, *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements* (University Science Books, Sausalito, California, 1997).