

Quantum Monte Carlo Calculations for a large number of bosons in a harmonic trap

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In this paper, I present a precise Quantum Monte Carlo calculation at finite temperature for a very large number (many thousands) of bosons in a harmonic trap, which may be anisotropic. The calculation applies directly to the recent experiments of Bose-Einstein condensation of atomic vapors in magnetic traps. I show that the critical temperature of the system decreases with the interaction. I also present profiles for the overall density and the one of condensed particles, and obtain excellent agreement with solutions of the Gross-Pitaevskii equation.

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The achievement of Bose-Einstein condensation (BEC) in dilute atomic vapors of ^{87}Rb [1] and ^{23}Na [2] has created extraordinary experimental and theoretical activity. The experiments pose fundamental theoretical questions, ranging from a clear understanding of the dynamics of BEC in a finite sample [3] to the behavior under time-dependent perturbations.

Besides these tantalizing and very controversial questions about the dynamics of the quantum coherence, there are many questions about the *statics* (thermodynamics) of the BE-condensate in a harmonic trap. In this paper, I show that we can obtain the static properties from Path-Integral Quantum Monte Carlo (QMC) calculations which suffer from no systematic uncertainties other than the choice of the interatomic (pseudo-)potential. I will present results for 10000 particles in isotropic and anisotropic traps around the BEC transition point, *i.e.* at the temperatures and particle number of current experimental interest.

The hamiltonian of the system is given by

$$H = \sum_{i=1}^N p_i^2/2m + \sum_{i,j} V(r_{ij}) + \frac{m}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (1)$$

where V is the interatomic potential [4]. This potential has many bound states, which, in the experiment, are inaccessible due to the kinematics of two-particle collisions. In thermodynamic calculations, as the one presented here, it is necessary to work with a pseudo-potential. I simply adopt a hard-core term of radius a_0 - as others have done before. More refined choices can easily be implemented.

The physical parameters - and the units - are as in ref. [5]: we consider two harmonic traps (isotropic and anisotropic), and units in which all frequencies are equal to 1 in the isotropic case, and $\omega_x = \omega_y = 1$, $\omega_z = \sqrt{8}$ in the anisotropic case. The anisotropy seems to be close to the experimental situation. The value a_0 for the hard-core radius is taken to be $a_0 = 0.0043$ in the above units [5].

To situate the computations of the interacting case, it is useful to remember the basic result for non-interacting bosons (in our isotropic potential, and with the above units) [6] [7]: for large N , the transition temperature T_c scales as $T_c \sim \tilde{T}_c N^{1/3}$ with $\tilde{T}_c \sim 0.94$. For $N = 10.000$ particles this gives $\beta_c \sim 0.05$. Let us mention in passing that at this value of N there are no more detectable differences between the canonical and the grand-canonical formalism [8].

The partition function Z , the trace over the density matrix, satisfies the usual convolution equation:

$$Z = \frac{1}{N!} \sum_P \int dR \rho(R, R^P, \beta) = \frac{1}{N!} \sum_P \int \dots \int dR dR_2 \dots dR_M \rho(R, R_2, \tau) \dots \rho(R_M, R^P, \tau) \quad (2)$$

Here $\tau = \beta/M$; R is the $3N$ -dimensional vector of the particle coordinates $R = (r_1, r_2, \dots, r_N)$, and R^P denotes the vector with permuted particle labels: $R^P = (r_{P(1)}, r_{P(2)}, \dots, r_{P(N)})$.

In the limit $M \rightarrow \infty$, the exact convolution equation eq. (2) reduces to the Feynman-Kac formula (*cf* [10]), as a consequence of the Trotter break-up $\exp[\tau(H_1 + H_2)] \sim \exp[\tau H_1] \exp[\tau H_2]$ for $\tau \rightarrow 0$.

However, it is the basic technical lesson of past QMC work [11] [12] that eq. (2) should only be taken to intermediate temperatures τ such that the approximation of the complete density matrix $\rho(R, R', \tau)$ by a product of pair terms becomes accurate

$$\rho(R, R', \tau) \simeq \prod_i \rho_1(r_i, r'_i, \tau) \prod_{i < j} \frac{\rho_2(r_i, r_j, r'_i, r'_j, \tau)}{\rho_1(r_i, r'_i, \tau) \rho_1(r_j, r'_j, \tau)} \quad (3)$$

The one-particle density matrices $\rho_1(r_i, r'_i, \tau)$ in eq. (3) describe a particle in the harmonic potential: an exact solution is known (*cf.*, *e.g.* [10]), and can easily be sampled. This product of one-particle density matrices is used as *a priori* probability density in the sense of ref. [12]. A very efficient method is used to generate a sequence of configurations, and to sample permutations. The second part in eq. (3) is equal to 1 for $V = 0$. It plays the role of a correction term due to two-body interaction. The Metropolis algorithm is used to incorporate this term, and to generate configurations which are distributed according to eq. (2).

To obtain the correction factor we need the two-particle density matrix. Fortunately, for the special case of the harmonic potential, the two-particle hamiltonian - and therefore the density matrix - decouples into a center-of-mass term (which is unaffected by the interaction) and a term describing the relative motion. The latter is given by:

$$H_{rel} = p^2/2\mu + V(r) + \frac{\mu}{2}(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2) \quad (4)$$

where $\mu = m/2$ is the reduced mass.

The eigenfunctions of the pure hard-sphere potential (eq. (4) without the terms in ω) can be obtained exactly ([13]). Adding an isotropic trap potential, the same may still be possible. However, since I am interested in treating the general *anisotropic* trap, I have obtained the relative-motion density matrix from the exact solution of the hard-core potential density matrix ρ_{hc} , into which I incorporate the harmonic term *via* the Trotter break-up.

$$\rho_{2,rel}(r, r', \tau) \simeq X(r) \times \rho_{hc}(r, r') \times X(r') \quad (5)$$

with $X(r) = \exp[-\tau\mu(\omega_x^2 x^2 + \omega_y^2 y^2 + \omega_z^2 z^2)/4]$. The τ finally retained in the simulation has to be chosen to accommodate both eq. (3) and eq. (5). Extensive tests have convinced me that for the density attained, a value of $\tau = 0.01$ is appropriate. This value is about 6 *orders of magnitude* larger than the one which would have to be used with the simple Trotter break-up.

For the value of $\tau = 0.01$ which was found sufficient, we can explicitly compute the effective *range* of the interaction, beyond which the correction factor in eq. (3) is practically one. This range turns out to be about 0.2. It is evident that one may introduce a 3-dimensional grid, with the grid size larger than the interaction range. At any time, particles are assigned to boxes formed by the grid. In evaluating the pair density matrix eq. (3), an efficient algorithm can be set up to compute the correction term only for close-by pairs. As a result, the program behaves gracefully as N is increased, and the actual limit of the calculation is rather given by the memory requirements than by CPU considerations.

The program has been checked very carefully. In the non-interacting case, I am able to reproduce all the exactly known results. For an isotropic trap, and in the absence of

interactions, *e. g.* I have reproduced the analytically known results for the condensate fraction N_0/N , which is plotted in fig. 1. I also plot the same quantity with interactions: the condensate fraction clearly decreases with respect to the noninteracting case. From this I conclude that T_c decreases. Notice that the interaction influences the condensate fraction much more than the finite-size effects for the non-interacting gas, which are also shown.

On the left side of fig. 2, I show the corresponding density profiles $\rho(x) = \int \int dydz \rho(x, y, z)$ of the particles. The center density increases sharply as T is lowered. This is the hallmark of real-space BEC in the confining potential.

We pause for a moment to discuss BEC in the path-integral framework: below T_c , particles have a finite probability to belong to extended permutation cycles of length l . Notice that in the confined geometry the off-diagonal one-particle density matrix at large separations trivially vanishes, instead of going to a value proportional to N_0 (as in the translational invariant system). In the present simulation, I instead obtain the number of condensed particles from the permutations of the system: the maximum length of l which has non-zero probability is equal to N_0 . For non-interacting particles in the limit $T \rightarrow 0$, the probability to belong to extended permutation cycles is independent of l (having all particles in the condensate does therefore not mean that they are all on the same cycle). At any temperature, noninteracting bosons which are on the different permutation cycles are statistically independent [12] - a property which is used in the QMC code to generate the *a priori* probability. The spatial distribution of particles in a cycle of length l is given by the diagonal density matrix at temperature $l\beta$ [10]:

$$\rho(x, x, l\beta) \sim \exp(-m\omega x^2 \tanh \frac{\omega}{2}\beta l) \quad (6)$$

Since $\beta_c \sim 1/N^{1/3}$, the particles on long cycles with $l \gg N^{1/3}$ (especially $l \sim N$) are distributed according to the lowest single-particle state $\Psi_0^2(x) \sim \exp(-m\omega x^2)$.

As we introduce interactions, we have to give up the concept of condensation into the lowest single-particle state. However, we preserve the two other essential features: below the transition, long permutation appear, and particles on long permutation cycles are distributed identically: they populate the macroscopic quantum state. We can thus gain access at the distribution of the condensed particles by computing the density profiles as before, but restricted to particles on cycles longer than some value l_{min} . I have verified explicitly that for $l_{min} \gtrsim 20$ the density profile does not depend on this parameter, *i. e.* that the condensation concerns the ground state. The density profiles for the condensed particles is given on the right side of fig. (2); the distributions are normalized to 1 at any temperature. As we expect, the distribution of condensed particles is broader at low temperature, where the many particles in the condensate strongly repel each other.

Can we obtain a more quantitative description of the condensate at finite temperature? To answer the question, I have computed the solution of the isotropic Gross-Pitaevskii (G-P) equation [14] [15] for the same value of a_0 as is used in the QMC-calculation, and for the number of particles corresponding approximately to the condensate fraction, as obtained from fig. 1. The results [16] are plotted together with $\rho(x)$ for the condensed particles on the right side of fig. 2. The agreement is truly remarkable for all the three curves, especially since there are no adjustable parameters. Even the number of condensed particles has been simply taken from fig. 1, without trying to optimize the fit. It can thus be said that, to a very high precision, the condensed particles are described by the G-P wavefunction.

The numerical results presented in fig. 2 suggest the following quantitatively correct picture for the Bose-Einstein condensation in a trap at finite temperature: below the (interaction-dependent) T_c , $N_0(T)$ particles are condensed. To a very high precision, these particles are distributed according to the appropriate G-P wavefunction. The non-condensed particles are distributed as in the free case and are very much spread out. There is very little mutual interaction between condensed and non-condensed particles: on the one hand, the non-condensed particles are very dilute in the central region of the trap, where most of the particles present are “condensed”, on the other hand the G-P wavefunction disturbs the non-condensed particles only on a small portion of their support.

The above picture allows us to understand the competition of energy gain and entropy destruction which underlies the condensation into the macroscopic wavefunction. The balance of entropy is the same for the non-interacting and interacting case, since the non-condensed part is undisturbed by the interaction, and the condensed one has zero entropy. The energy of the G-P wavefunction is of course much higher than in the absence of interactions. Condensation is therefore less favored, and we understand that the critical temperature must decrease with the interaction, as shown in fig. 1. It will be very simple to perform a one-parameter (in N_0) variational minimization of the free energy which describes the non-condensed particles as free, and which uses the energy of the G-P wavefunction.

Rather than to proceed in this direction, I finally present some results for the anisotropic trap, which is the case of direct interest to experiments. In fig. 3, I present density plots for this case at different temperatures, and compare to the solution of the anisotropic G-P wavefunction with $N = 10000$ [5]. As before, there is very close agreement between the two calculations. The calculation also confirms that, in the limit of zero temperature, the number of condensed particles, N_0 , seems to be extremely close to N . This agrees with recent work in which the interaction of the G-P groundstate with non-condensed particles was studied in the Bogolubov approximation [17]. I have performed the same calculation as in fig. 1 for the isotropic case (the noninteracting curve is easily computed, even for finite N [9]), and the results are analogous. For example, at $\beta = 0.06$, the noninteracting gas in the anisotropic trap has $N_0/N = 0.76$, but I only find a value of 0.6 for the interacting case.

Even though the main impetus in this paper has been on the dependence of the critical temperature on the interaction, and on the comparison of the condensate wave function with the Gross-Pitaevskii formalism, it should be evident that the QMC calculation goes much beyond these results. We can obtain complete information on inter-particle correlation, compute the complete thermodynamics of the system, *etc.* In particular, it is possible [18] to obtain the nonclassical moment of inertia which has attracted some attention lately [19], and which will be of experimental relevance as soon as rotating traps will become available. If the above picture is correct, this moment (which basically follows the normal part of the gas) should depend on the interaction only through N_0 .

I would also like to draw the reader’s attention to the fact that the very efficient algorithm is of general usefulness for the study of weakly interacting bosons. Other possible applications are bosons in 3 dimensions without confining potential, but particularly in 2 dimensions, where the effect of a small interaction will be even more important than in the case treated here, since the non-interacting gas has no phase transition at all. To stimulate work in this area, as well as to facilitate direct comparison with experiences on trapped bosons, I will make available the FORTRAN code used in the present investigation.

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Figure Captions

1. Ratio of condensed particles N_0/N vs reduced temperature $\tilde{T} = TN^{1/3}$ in an isotropic trap with $\omega = 1$ for the noninteracting case in the thermodynamic limit ($N \rightarrow \infty$, full line) and for $N = 10000$ (dashed line), as well as for 10000 interacting particles with $a_0 = 0.0043$. The number of condensed particles decreases with the interaction.
2. Density profile vs x for temperatures $\beta = 0.06(\tilde{T} = 0.78)$, $\beta = 0.07(\tilde{T} = 0.66)$, $\beta = 0.12(\tilde{T} = 0.39)$ (left side, from below). On the right side is plotted the density profile of the “condensed” particles for the same temperatures (from *above*, the curves are normalized to one). These density profiles are in excellent agreement with the Gross-Pitaevskii solutions for the N_0 obtained from fig. 1 (dotted lines). The values used are $N_0 = 2000$ for $\beta = 0.06$ (upper) $N_0 = 4000$ for $\beta = 0.07$ (middle) $N_0 = 8000$ for $\beta = 0.12$ (lower).
3. Density profile vs x for an anisotropic trap with $N = 10000$. As in fig. 2, we plot the total density on the left, and the normalized density of condensed particles on the right. The temperatures are $\beta = 0.06$ (dotted line), and $\beta = 0.16$ (full line). The dashed curve is the Gross-Pitaevskii solution for $N = 10000$.