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Quantum-Monte-Carlo Calculations for Bosons in a Two-Dimensional Harmonic Trap

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Path-Integral-Monte-Carlo simulation has been used to calculate the properties of a two-dimensional (2D) interacting Bose system. The bosons interact with hard-core potentials and are confined to a harmonic trap. Results for the density profiles, the condensate fraction, and the superfluid density are presented. By comparing with the ideal gas we easily observe the effects of finite size and the depletion of the condensate because of interactions. The system is known to have no phase transition to a Bose-Einstein condensation in 2D, but the finite system shows that a significant fraction of the particles are in the lowest state at low temperatures.

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1. INTRODUCTION

Recent experiments on alkali atoms cooled by laser methods and evaporation in a magnetic trap have allowed the observation of Bose-Einstein condensation (BEC) in a harmonic potential formed by an external magnetic field. By varying the trapping field so that it is very narrow in one dimension, it is possible to separate the single-particle states in the oscillator potential into well-defined bands. By occupying only states in the lowest band one has an effective two-dimensional system. In contrast to such a quasi-2D system, the system considered here is genuinely two dimensional.

In this paper we will investigate the behaviour of harmonic Bose systems in 2D using the very powerful finite-temperature Path-Integral Monte Carlo (PIMC) simulation technique.[1] The PIMC technique is in principle capable of describing systems of arbitrary interaction strength and density

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and allows one to study the static properties of the condensed gases. The only fundamental uncertainty arises from the choice of the interaction potential. Here a hard-core potential appropriate for the s-wave scattering length of ^{87}Rb was chosen. In this case the hard-core parameter is $a_0 = 0.0043$ in the dimensionless units of Ref. 2. The analogous three dimensional case has been studied previously.[3]

The Hamiltonian for the system under consideration is

$$H = \sum_{i=1}^{N} \frac{p_i^2}{2m} + \sum_{i,j} V(r_i - r_j) + \frac{m}{2} \sum_{i=1}^{N} (\omega_x^2 r_{i,x} + \omega_y^2 r_{i,y}). \qquad (1)$$

The density matrix for N Bose particles at inverse temperature $\beta = 1/k_b T$ can be written as a convolution with M intermediate density matrices or "time slices" at inverse temperature $\tau = \beta/M$. Then the probability density for finding a many-particle configuration $\mathbf{R} = (r_1, \cdots, r_N)$ is

$$\rho(\mathbf{R}, \mathbf{R}; \beta) = \frac{1}{N!} \sum_{\mathcal{P}} \int \cdots \int \rho(\mathbf{R}, \mathbf{R}_1; \tau) \times$$

$$\times \rho(\mathbf{R}_1, \mathbf{R}_2; \tau) \cdots \rho(\mathbf{R}_{M-1}, \mathbf{R}^{\mathcal{P}}; \tau) d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_{M-1}$$

where $\mathbf{R}^{\mathcal{P}}$ denotes a vector with permuted particle labels. The Metropolis algorithm is used to sample from this distribution. With larger M or correspondingly larger temperatures for each time slice, the intermediate density matrices approach the classical limit which leads to the *primitive approximation*. In order to make the computation for many particles feasible, M can be reduced by several orders of magnitude by calculating the density matrix ρ_2 for the interaction involving just two particles and approximating each time slice by[1]

$$\rho(\mathbf{R}, \mathbf{R}'; \tau) = \prod_{i=1}^{N} \rho_1(r_i, r_i'; \tau) \prod_{i<j} \frac{\rho_2(r_i, r_j; r_i', r_j'; \tau)}{\rho_1(r_i, r_i'; \tau)\rho_1(r_j, r_j'; \tau)}. \qquad (2)$$

As long as only two particles interact, this is equivalent to using the primitive approximation.

To calculate ρ_2, we note that in the harmonic potential the Hamiltonian for two particles decouples into a center of mass and a relative motion term with the latter given by

$$H_{rel} = \underbrace{\frac{p^2}{2\mu} + V(r)}_{H_{HC}} + \frac{\mu}{2}(\omega_x^2 r_x^2 + \omega_y^2 r_y^2) \qquad (3)$$

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where $\mu = m/2$ is the reduced mass. With the Trotter breakup, the quotient in (2), which plays the role of a correction term, can be transformed to

$$\rho_{HC}(r, r') \frac{X(r)X(r')}{\rho_{1,\mu}(r, r')} \tag{4}$$

with $X(r) = \exp(-\tau\mu(\omega_x^2 r_x^2 + \omega_y^2 r_y^2)/4)$ and the relative coordinates $r = r_i - r_j$ and $r' = r'_i - r'_j$. $\rho_{HC}(r, r')$ is the density matrix for the Hamiltonian H_{HC} (Eq. (3)) describing the interaction between two interacting particles without confining potential and $\rho_{1,\mu}(r, r')$ is the density matrix for a single particle of reduced mass μ in the harmonic potential.[4]

Calculating $\rho_{HC}(r, r')$ for a hard-core potential using an eigenfunction expansion yields

$$\rho_{HC}(r, r'; \tau) = \sum_{l=-\infty}^{\infty} \frac{1}{2\pi} e^{il\varphi} \int_0^\infty dk R_{kl}(r) R_{kl}(r') e^{-\tau \frac{\hbar^2 k^2}{2\mu}} \tag{5}$$

with the radial wave functions

$$R_{kl}(r) = \sqrt{k}(\cos\delta_{kl}\, \mathrm{J}_l(kr) - \sin\delta_{kl}\, \mathrm{N}_l(kr)) \quad \text{and} \quad \tan\delta_{kl} = \frac{\mathrm{J}_l(ka_0)}{\mathrm{N}_l(ka_0)}$$

where J_l and N_l are the Bessel and Neumann functions and φ is the angle between r and r'.

Since the numerical evaluation of this function is quite time consuming, values distributed over a mesh with parameters $|r|, |r'|$ and φ are computed for each value of τ. A simple linear interpolation method proved to be sufficient to reach the required degree of accuracy for evaluation in the simulation. The full correction factor (Eq. (4)) with dependence on the confining potential can then be calculated very efficiently during the Monte-Carlo simulation.

To further speed up the calculation, a boxing algorithm[3] is used that divides the space of the system into boxes with a size of at least the "healing length" of the pair interaction. When we compute the effects of the interaction of a given particle, it is necessary to consider only a small number of interactions with particles in boxes neighbouring that of the particle in question. Furthermore, attempting only permutations with particles from the same box, increases the acceptance probability for these moves and results in a more effective sampling of permutation space.[3]

The value of τ has to be chosen carefully for each particle density to accommodate both the Trotter breakup and the approximation of pair interactions (Eq. (2)). For the density used, tests with values for τ ranging over orders of magnitude have been performed, showing that a further decrease below $\tau = 0.01$ yield the same results within statistical errors.

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2. DENSITY PROFILES AND CONDENSATE FRACTION

In 2D, with interactions, there is no phase transition to a Bose condensed state[5] even in a trap, nevertheless there should be a macroscopic fraction of particles in the ground state at finite temperature when the particle number is finite.

We tentatively assume that, in 2D, the condensation fraction can be determined, as in 3D,[3] by observing a macroscopic number of particles with long exchange cycles in the lowest state of their subsystem. For each temperature a characteristic length of permutation cycles l_0 can be chosen so that the density profiles for particles on cycles longer than l_0 are essentially the same. Particles on shorter cycles will have a broader density profile. Particles on cycles longer than l_0 are identified with the condensate (Fig. 1). What is plotted is the average distribution in one coordinate after integrating over the other coordinate. We have fit the lowest temperature curve in Fig. 1 with the infinite-N solution of the zero-temperature GP equation.[6] The interaction coefficient has been determined by the fit since, in 2D, there is no straightforward connection between a hard-core interaction and a contact pseudopotential. We observe no obvious bimodality, due to separate distributions of condensed and non-condensed particles in the overall density in Fig. 1; if a kink did exist in the density it would likely be washed out by the integration over one coordinate.

In two dimensions interactions seem to lead to a comparatively stronger depletion of the condensate (Fig. 2) than in three dimensions (Cf., Ref. 3). This is expected, since there is no condensate at finite temperature in the thermodynamic limit for the interacting system and therefore the critical temperature has to approach zero (for large numbers of particles) when interactions are turned on.[5]

3. SUPERFLUID FRACTION

Recently one of the authors[7] showed that the Hartree-Fock-Bogoliubov equations indicated that there is a phase transition in 2D, although it cannot be to the BEC state. Perhaps this transition is of the Kosterlitz-Thouless (KT) type[8] and involves superfluidity. The superfluid fraction can be related to the mean square surface area enclosed by Feynman paths. Sindzingre *et. al.* have shown that[9]

$$\rho_s/\rho = \frac{4m^2\langle A^2\rangle}{\beta h^2 I_c} \tag{6}$$

with A the area swept out by the paths and I_c the classical moment of inertia. The average is taken over configurations in the simulation.

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The resulting superfluid densities are very small (Fig. 2). A smaller ρ_s than in the translationally invariant system is expected because the formation of the superfluid begins in the middle of the potential well where the contribution to the moment of inertia is small. Paths with different orientations will contribute with different signs to the area making cancellation possible.

The simulation results for the 2D system without confining potential[10] are in agreement with the KT theory for the superfluid transition. If this description is also appropriate with confining potential, the vortex picture of the KT-transition suggests an additional mechanism leading to a decrease of ρ_s[8] : Superfluidity is destroyed by dissipation through vortices which are not paired. At low temperatures vortices form pairs which unbind at higher temperatures. In the non-uniform system the two vortices forming a pair will in general experience a slightly different potential leading to imperfect pairing and thereby a lowering of the superfluid fraction.
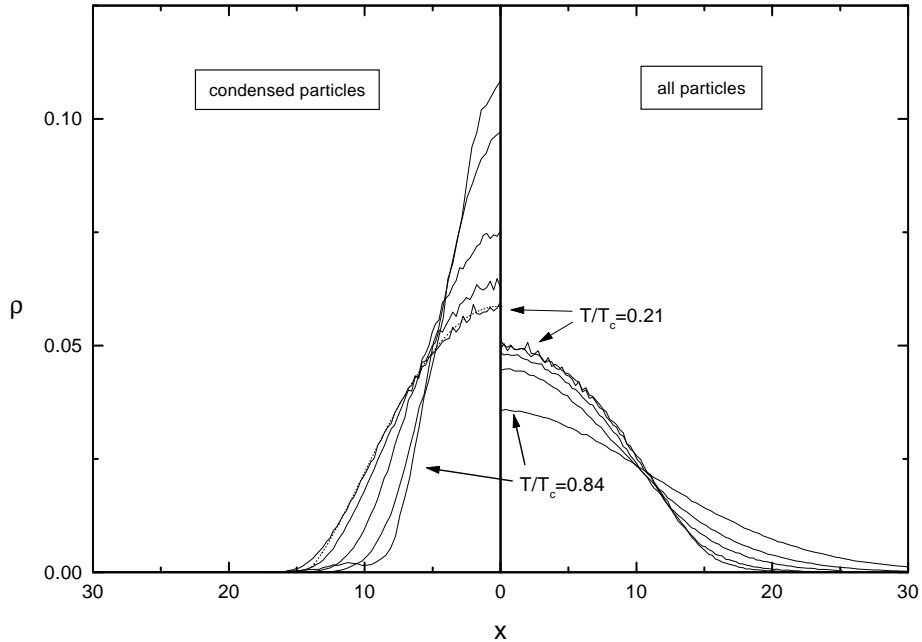

Fig. 1. Density profiles for 1000 particles at temperatures $T/T_c = 0.84, 0.56, 0.42, 0.28, 0.21$ for $\omega = 0.15$. The condensate parts are displayed on the left and the profiles for all particles on the right. All profiles are normalised to unity. Temperatures are given with reference to the critical temperature T_c of the ideal system in the thermodynamic limit. The smooth dotted curve through the 0.21 data is the infinite-N solution of the GP equation with interaction strength determined by the fit.
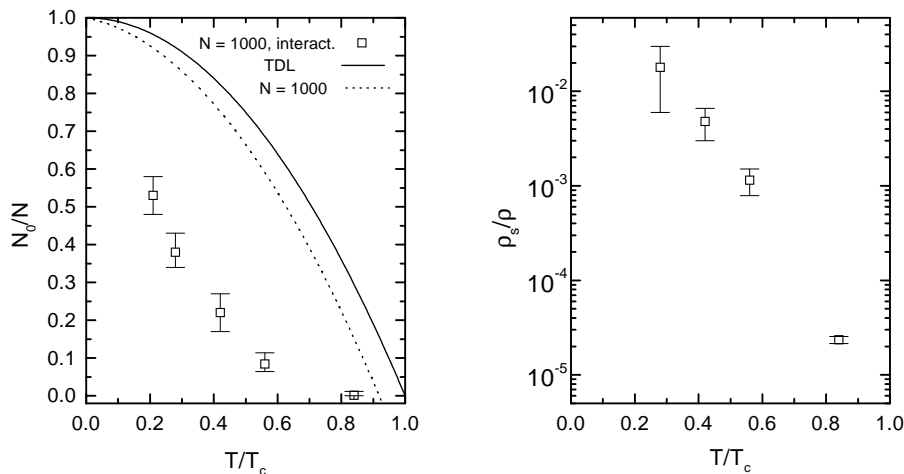
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Fig. 2. Left figure: Condensate fraction for the interacting system with N=1000 and $\omega = 0.15$ and comparison with theoretical prediction for the ideal gas in the thermodynamic limit (TDL) and with finite size corrections for 1000 particles. Right figure: Dependence of the superfluid fraction on temperature for 1000 particles.

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REFERENCES

1. D. Ceperley, *Rev. Mod. Phys.* **67**, 279 (1995);
    E. L. Pollock, and D. M. Ceperley, *Phys. Rev. B* **30**, 2555 (1984).
2. F. Dalfovo, S. Stringari, *Phys. Rev. A*, **53**, 2477 (1996).
3. W. Krauth, *Phys. Rev. Lett.* **77**, 3695 (1996).
4. R. P. Feynman A. R. and Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill Inc., New York 1965).
    R. P. Feynman, *Statistical Mechanics*, (Benjamin, New York, 1972) .
5. W. J. Mullin, *J. Low Temp. Phys*, **106**, 615 (1997).
6. G. Baym and C. Pethick, *Phys. Rev Lett.*, **76**, 6 (1996).
7. W. J. Mullin, *J. Low Temp. Phys*, **110**, 167 (1998).
8. S. I. Shevchenko, *Sov. Phys. JETP*, **73**, 1009 (1991).
    S. I. Shevchenko, *Sov. J. Low. Temp. Phys.*, **18**, 223 (1992).
9. P. Sindzingre, M. Klein, and D. M. Ceperley, *Phys. Rev. Lett.* **63**, 1601 (1989).
10. D. M. Ceperley and E. L. Pollock, *Phys. Rev. B* **39**, 2084 (1989).