On phases in weakly interacting finite Bose systems

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We study precursors of thermal phase transitions in finite systems of interacting Bose gases. For weakly repulsive interactions there is a phase transition to the one-vortex state. The distribution of zeros of the partition function indicates that this transition is first order, and the precursors of the phase transition are already displayed in systems of a few dozen bosons. Systems of this size do not exhibit new phases as more vortices are added to the system.

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I. INTRODUCTION

The study of vortices in dilute atomic Bose–Einstein condensates has received a lot of attention in recent years. The condensate wave function of a vortex state exhibits a quantized circulation of its velocity field. This state may experimentally be formed, e.g., by “phase imprinting” techniques or by directly transferring angular momentum to the condensating system. Current experiments are performed in the Thomas–Fermi regime of short coherence length. For a review of recent results see, e.g., [1]. The regime of long coherence length is of interest as well. Indeed, harmonically trapped Bose systems with perturbatively weak repulsive interactions display a rich structure [2]. At low ratios of angular momentum $L$ to particle number $N$, i.e. $L/N \ll 1$, the ground states are dominated by quadrupole and octupole excitations [3]. The ground state structure changes smoothly until the one-vortex state $L/N = 1$ is approached. In particular, the ground state wave function is known analytically and the ground state energy depends linearly on $L$ for $L/N < 1$ [4]. The one-vortex state is a Bose–Einstein condensed state where a macroscopic number of particles carries one quantum of angular momentum each [5]. The structure of ground states changes considerably as further angular momentum is put into the system. Results from mean-field calculations exhibit changing symmetries of the developing vortex array which correspond to changes in the occupation numbers of single-particle states [6]. This goes along with an increasing complexity of higher vortex states. The two-vortex state $L/N = 2$, for instance, already exhibits a complicated structure and is dominated by excitations that carry 0, 2, and 4 units of angular momentum [7]. Naturally, the question arises whether the observed changes in the condensate wave function structure and the formation of quantized vortices are associated with thermal phase transitions.

For the transition to the one-vortex state, the answer is affirmative. Wilkin et al. [8] showed that the one-particle reduced density matrix of the one-vortex state has one eigenvalue of order $N$ and thus meets a criterion for Bose–Einstein condensation in finite systems; see e.g. [9]. The order of this phase transition, however, is not known until now. It is the main purpose of the present paper to classify this phase transition from its precursors in finite systems.

We recall that small systems do not exhibit phase transitions. Nevertheless, finite systems may display precursors of phase transitions. Recently, Borrmann et al. proposed that the distributions of zeros of the canonical partition function “reveal the thermodynamic secrets of small systems in a distinct manner” [10]. We will apply this method to the case of weakly interacting Bose systems under rotation.

II. SYSTEM AND METHOD

We consider a system of $N$ bosons confined in a three-dimensional harmonic trap at total angular momentum $L$ and restrict ourselves to the sector of maximal magnetic quantum number, i.e. the particles are in the ground state with respect to excitations along the axis of rotation. The non-interacting system is highly degenerate. In what follows, we assume that the repulsive interaction between the bosons is perturbatively weak and simply lifts this degeneracy. This yields sets of now quasi-degenerate states that are separated by multiples of the oscillator spacing $\hbar \omega$. Under these conditions, the level spacing between quasi-degenerate states is much smaller than the oscillator spacing. We are interested in the thermal properties of the system while keeping the angular momentum $L$ fixed. For temperatures that are smaller than the oscillator spacing, we may restrict ourselves to the lowest-lying set of quasi-degenerate states with approximate energies $E \approx L \hbar \omega$. We set the ground state energy of the non-rotating system to zero.) Current experiments do not work within this low-temperature regime. We recall that the onset of Bose–Einstein condensation is already observed for temperatures $kT \sim N^{1/3} \hbar \omega$ [11]. Below we find that quantitative results concerning thermal phase transitions are already determined by a few hundred low-lying levels. It thus seems that one can lift the requirement of perturbatively small temperatures without facing the inclusion of highly excited states for the problem under consideration. In the low-temperature regime, the Hamiltonian of the $N$-boson system with contact interaction reads [12].
\[ \hat{H} = v_0 \sum_{i,j,k,l} \frac{(k+l)!}{2^{k+l}(i!)^{j!}(k!)^{l!}} \tilde{a}_{k+l}^{\dagger} \tilde{a}_{j}^{\dagger} \tilde{a}_{k} \tilde{a}_{l}. \]  

(1)

Here, \( v_0 \) denotes the strength of the contact interaction. The operators \( \tilde{a}_{j}^{\dagger} \) and \( \tilde{a}_{j} \) create and annihilate one boson in the single-particle state with angular momentum \( j \) with \( j = 0, 1, 2 \ldots \), respectively. The operators

\[ \tilde{N} = \sum_{j} \tilde{n}_j \]  

(2)

and

\[ \tilde{L} = \sum_{j} j\tilde{n}_j \]  

(3)

count the number of particles and the quanta of angular momentum and have quantum numbers \( N \) and \( L \), respectively. We have used the number operators \( \tilde{n}_j = \tilde{a}_{j}^{\dagger} \tilde{a}_j \).

Basis states are denoted as \( |n_0, n_1, n_2, \ldots \rangle \), where \( n_j \) denotes the number of particles with angular momentum \( j \).

Hilbert space is partition space, and the number of basis elements grows exponentially with increasing \( N \).\( N \) can be considered as the number of partitions of \( \hat{L} \) into at most \( N \) parts. The dimension of Hilbert space grows exponentially with increasing \( L \) while being only mildly dependent on \( N \) for \( L > N \).

Let us now turn to a description of the method proposed in Refs. \[ 10, 11 \]. It is based on an analysis of Hilbert space that Grossmann and Rosenhauer made for macroscopic systems about three decades ago \[ 13 \]. The canonical partition function \( Z(B) \) is evaluated at complex arguments \( B = \beta + i\tau \). Since \( Z(\beta) \) is real, it suffices to consider the partition function \( Z(B) \) for arguments in the upper complex plane. Two different phases of macroscopic systems are separated by a line of zeros which intersects the real axis at the critical temperature. Further information about the order of the phase transition is encoded in the slope of the line at the intersection point and the density of zeros close to the intersection point. This is physically plausible. We recall that thermodynamic quantities are given by logarithmic derivatives of the partition function and thus diverge at its zeros.

In finite systems, the line of zeros reduces to more or less closely spaced zeros that line up on a curve. Following Ref. \[ 10 \], one then studies the behavior of the zeros with smallest imaginary part and of the underlying curve while increasing the number of particles. This allows one to predict the critical temperature and order of the phase transition in the infinite system. Furthermore, the shape of the curve or the presence of several such curves allows one to identify different “phases” already in finite systems. These techniques have been used to study precursors of phase transitions in Bose–Einstein condensates of ideal gases and atomic cluster \[ 10, 11, 13 \]. Further applications include the classification of a pairing phase transition in finite Fermi systems \[ 13 \].

We compute the canonical partition function from the eigenvalues of the Hamiltonian \[ 1 \]. This requires the complete diagonalization of \( \hat{H} \) and is practicable only for moderately large values of \( L \). Zeros of the partition function are determined conveniently by locating the poles of the specific heat, which is given by

\[ C_v(B) = \frac{\partial^2 \ln Z(B)}{\partial^2 B}. \]  

(4)

For larger system sizes (i.e. larger values of angular momentum \( L \)), we restrict the computation to the lowest hundreds of levels and construct an approximate partition function only. Nevertheless, we find sufficiently well-converged zeros of the partition function close to the real axis of complex temperature \( B = \beta \pm i\tau \). This allows us to present quantitative data concerning the order of the phase transition in the macroscopic system.

### III. RESULTS

We investigate the transition to the one-vortex state first. To this purpose, we fix the number of particles to \( N = 30 \) and fully diagonalize the Hamiltonian for several values of angular momentum in the range \( 0.8 < L/N < 1.07 \) around the one-vortex state \( L/N = 1 \). The partition function is computed from the obtained energy levels. Figure \[ 1 \] shows the specific heat as a function of complex \( B = \beta + i\tau \). We restricted the plot to include only those zeros with smallest positive imaginary part. Figure \[ 2 \] demonstrates that the zeros approach the real axis with increasing \( L \). The closest encounter is found for the one-vortex state \( L = N = 30 \). This is a precursor of the condensation into the one-vortex state in the infinite system and supports earlier results \[ 8, 7, 6 \]. We are particularly interested in the order of this phase transition. To this purpose, we consider the one-vortex state \( L = N \) and compute eigenvalues of the Hamiltonian \[ 1 \] for increasing values of particle number \( N \). A complete diagonalization is prohibitively expensive for \( N \) exceeding values of about 35. Instead, we restrict ourselves to the computation of the lowest-lying eigenvalues. These are used for an approximate construction of the partition function. We found numerically that its zeros with smallest positive imaginary parts are already sufficiently well converged when only a few hundred eigenvalues are included in the computation. We considered systems up to \( L = N = 55 \), corresponding to a dimension of Hilbert space of the order \( 4.5 \times 10^5 \). The relevant eigenvalues are computed numerically using the ARPACK and PARPACK routines \[ 12 \].

Figure \[ 2 \] shows the distribution of poles in the complex plane of the specific heat at the one-vortex state for different system sizes. These plots are generated from the lowest-lying 300 eigenvalues. (Increasing the number of eigenvalues from 300 to 380 yields less than 1% change in the numerical results. Thus, the data is sufficiently well converged for our purposes.) It is clearly seen that the zeros line up and approach the real axis with increasing system size. The order of the phase transition
is determined as follows \([1]\). The distribution of zeros close to the real axis is approximately described by three parameters. Two of these parameters reflect the order of the phase transition, while the third indicates the size of the system. Let us assume that the zeros lie on a line. We label the zeros according to their closeness to the real axis. Thus \(\tau_1\) reflects the discreteness of the system. The density of zeros for a given \(\tau_k\) is given by

\[
\phi(\tau_k) = \frac{1}{2} \left( \frac{1}{|E_k - E_{k-1}|} + \frac{1}{|E_{k+1} - E_k|} \right), \quad (5)
\]

with \(k = 2, 3, 4, \ldots\). A simple power law describes the density of zeros for small \(\tau\), namely \(\phi(\tau) \sim \tau^\alpha\). If we use only the first three zeros, then \(\alpha\) is given by

\[
\alpha = \frac{\ln \phi(\tau_3) - \ln \phi(\tau_2)}{\ln \tau_3 - \ln \tau_2}. \quad (6)
\]

The final parameter that describes the distribution of zeros is given by \(\gamma = \tan \nu \sim (\beta_2 - \beta_3)/(\tau_2 - \tau_1)\).

In the thermodynamic limit, \(\tau_1 \to 0\), in which case the parameters \(\alpha\) and \(\gamma\) coincide with the infinite system limits discussed by Grossmann and Rosenhauer \([2]\). For infinite systems, \(\alpha = 0\) and \(\gamma = 0\) indicates a first-order phase transition, while \(0 < \alpha < 1\) and \(\gamma = 0\) or \(\gamma \neq 0\) indicates a second-order transition. For systems approaching infinite particle number, \(\alpha\) cannot be smaller than zero since this causes a divergence of the internal energy. In small systems, with finite \(\tau_1\), \(\alpha < 0\) is possible and is also indicative of a first-order transition. We show our results for \(\alpha, \gamma, \tau_1\) in Table \([3]\) for the \(N = 40, 50, 52, 55\) systems. \(\tau_1\) decreases with increasing system size as a power law. The fit is given by \(\tau_1 = 1.15N^{-1.53}\). From the table we note that \(\gamma\) is nearly zero, and \(\alpha\) is a small negative number for each system we studied here. The critical temperature \(kT_c\) is approximately given by \(1/\beta_1\). Our data suggests that \(kT_c \sim \tau_0N^{1.1\ldots 1.4}\). The \(N\)-dependence differs considerably from what is found for the ideal Bose gas in three-dimensional traps \([4]\).

We thus find that the phase transition to the one-vortex state is first order. This is the main result of this work and combines well with previous results found for the energy and wave function structure. We recall that the ground state energy of the \(N\)-boson system exhibits a kink at \(L = N\), and that the wave function structure changes strongly when increasing \(L\) beyond \(N\) \([5,6]\).

Are there further indications of phase transitions as one approaches the two-vortex state? Mean-field results by Kavoulakis et al. \([7,8]\) show that the structure of ground states changes considerably at certain ratios of \(L/N\). At \(L/N \approx 1.75\) the mean-field density develops a two-fold symmetry, and the expectation \(n_j\) for occupation of single-particle orbitals with odd \(j\) vanishes at \(L/N \approx 1.75\). A second change in ground state structure occurs at \(L/N \approx 2.03\) where the two-fold symmetry of the mean-field density changes into a three-fold symmetry. This is accompanied by a macroscopic occupation of single-particle orbitals with angular momentum \(j = 0, 3, 6, 9\). We numerically computed the ground states of Hamiltonian \([1]\) for systems with moderate particle numbers and confirm these results. We also computed the partition function from the fully diagonalized Hamiltonian for \(L = 30\) and \(N\) ranging from 10 to 20. However, the distribution of zeros of the partition function does not indicate a thermal phase transition. In particular, we do not find zeros that start to line up and approach the real axis at the corresponding values of \(L/N\). This is most likely due to the small system size.

Let us finally turn to Bose–Einstein condensates with attractive interaction. In this case, the ground state is the (Bose–Einstein condensed) state of the non-rotating system which executes pure center-of-mass motion, i.e. all angular momentum is carried by the motion of the center of mass \([3,4]\). A direct calculation of the one-particle reduced density matrix indicates the presence of a condensate that is fragmented over several states \([5,6]\). Only when the center-of-mass motion is separated does one find the condensation into one state \([6]\). The distribution of zeros of the partition function does not indicate a phase transition. This remains the case also when considering systems of size \(L, N \approx 50\).

In summary, we have investigated phases in weakly interacting Bose–Einstein condensates. The phase transition to the one-vortex state is first order, and its precursors are clearly seen in the distribution of zeros for systems comprising only 30 to 55 particles. The question about further phase transitions to states with several vortices remains open.

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| $N$ | $\tau_1$  | $\gamma$  | $\alpha$  |
|-----|-----------|-----------|-----------|
| 40  | 0.0775    | -0.03     | -0.1109   |
| 50  | 0.055     | 0.0       | -0.145    |
| 52  | 0.053     | 0.003     | -0.147    |
| 55  | 0.050     | 0.003     | -0.148    |

TABLE I. Calculated parameters $\tau_1$, $\gamma$, and $\alpha$ for the various boson systems at $L/N = 1$. 
FIG. 1. Contour plots of the specific heat in the complex temperature plane for the $N = 30$ system at a) $L = 20$, b) $L = 25$, and c) $L = 30$ units of angular momentum. The spots indicate the locations of the zeros of the canonical partition function.
FIG. 2. Contour plots of the specific heat in the complex temperature plane for the $L/N = 1$ systems with increasing numbers of particles: a) $N = 40$, b) $N = 50$, and c) $N = 55$. The spots indicate the locations of the zeros of the canonical partition function.