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Bose–Einstein condensation in the three-sphere and in the infinite slab: Analytical results

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HIGHLIGHTS

- We study analytically finite size effects on the thermodynamics of an ideal Bose gas.
- The geometries considered are the three-sphere, the 1D box and the infinite slab.
- Expressions obtained are valid throughout the quantum regime and BEC transition.
- Specific heat and number of particles are given as explicit functions of temperature.
- The effect of the different finite geometries on the thermodynamics is highlighted.

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ABSTRACT

We study the finite size effects on Bose–Einstein condensation (BEC) of an ideal non-relativistic Bose gas in the three-sphere (spatial section of the Einstein universe) and in a partially finite box which is infinite in two of the spatial directions (infinite slab). Using the framework of grand-canonical statistics, we consider the number of particles, the condensate fraction and the specific heat. After obtaining asymptotic expansions for large system size, which are valid throughout the BEC regime, we describe analytically how the thermodynamic limit behaviour is approached. In particular, in the critical region of the BEC transition, we express the chemical potential and the specific heat as simple explicit functions of the temperature, highlighting the effects of finite size. These effects are seen to be different for the two different geometries. We also consider the Bose gas in a one-dimensional box, a system which does not possess BEC in the sense of a phase transition even in the infinite volume limit.

1. Introduction

The phenomenon of Bose–Einstein condensation (BEC) is described in statistical mechanics textbooks (e.g. Refs. [1,2]). Given an ideal gas of particles obeying Bose statistics inside a box with sides of length L_1, L_2, L_3, as the thermodynamic limit is taken in the usual way ($N \to \infty, V \to \infty$ while N/V and L_i/L_j are held fixed), the fraction of particles in any excited state i, N_i/N, goes to zero. This is expected since the single particle energy levels get closer and closer to each other, eventually forming a continuum in the thermodynamic limit. The ground state is the exception. Indeed, below a certain critical temperature, the fraction of particles in the ground state, N_{gr}/N, will be non-vanishing in the thermodynamic limit, which means that the probability distribution of particles as a function of their energy has a Dirac δ component at zero energy. Because of this, the chemical potential and, as a consequence thermodynamic functions in general, are non-analytical at the critical temperature, signalling the BEC phase transition.

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In finite systems, however, we are away from the thermodynamic limit and, strictly speaking, a phase transition does not happen, all thermodynamic functions being smooth functions of the temperature at the critical point. Nevertheless, a large finite system can be practically indistinguishable from an infinite one. For example, in the thermodynamic limit as described above, the specific heat for the three-dimensional gas has a sharp peak with a discontinuous first derivative at the onset of BEC. For a finite large system, there will still be a more or less sharp peak but all thermodynamic functions will be analytical. The larger the volume that the finite system has, the sharper the peak. The difference between a finite system and its infinite counterpart can be brought out analytically in the form of finite size correction terms. Furthermore, these finite size corrections are dependent on the particular way the gas is confined; namely, they depend on the geometry of the system.

It is our aim in this article to obtain analytically finite size corrections to the thermodynamics of an ideal non-relativistic Bose gas in the quantum degenerate regime in three distinct physical situations: the three-sphere (spatial section of the Einstein universe), the three-dimensional box which is infinite in two of the directions and finite in the other one (we will call this the infinite slab) and the one-dimensional box. The choice of these models enables us to perform a full analytical treatment showing very explicitly in simple expressions the finite size effects and the impact that different geometries can have in these effects. The three seemingly disparate situations under consideration have mathematical aspects in common, allowing for a unified treatment as will be seen. Actually, it is well known that the one-dimensional box does not possess BEC, but once we have all the mathematical apparatus set up, the study of this system requires no extra effort. The infinite slab is an example of generalized BEC, in which the particles condense into a low lying set of states rather than the ground state, as described early on in Ref. [3] (and which the work in Ref. [4] already hinted at) and later systematically studied by van den Berg and collaborators [5–7] (see Refs. [8,9] for recent articles on this topic). From the systems we study here, the only one having the usual form of BEC is the three-sphere.

Our point of departure in the analytical treatment of the thermodynamic sums will be the Mellin–Barnes transform, a tool used in the past in Refs. [10–13], to study respectively the ideal Bose gas in a harmonic oscillator potential, in the infinite flat space subject to a magnetic field and in the three-dimensional space in which one of the directions is compactified to form a circle. This transform can also be used to obtain high temperature expansions for the ideal Bose gas in quite general settings, as was shown for the Bose gas under arbitrary background potentials and in boxes of arbitrary shape [14,15] and, more recently, for the Bose gas in product manifolds [16]. Although these high temperature expansions can provide a way of calculating a BEC critical temperature in each setting, they cannot be used to study the BEC transition itself or the BEC regime. Our approach allows us to obtain large size expansions, in terms of temperature and chemical potential, which are valid and very effective throughout the quantum degenerate regime and in the vicinity of the critical region. This is done in Section 2. For the first two systems mentioned above, we will then obtain, in Section 3, an analytical description of the approach to the critical behaviour which signals the onset of BEC in the thermodynamic limit. Specifically, in the critical region we obtain the chemical potential, fraction of condensed particles and the specific heat as explicit functions of the temperature only. From the results thus obtained, it will be clear that the geometry of the system has a crucial role in the nature of the finite size corrections in each situation. For example, while in the three-sphere the specific heat peak happens at a slightly higher temperature than the temperature at which the chemical potential is zero, the opposite happens in the infinite slab scenario.

The case of the one-dimensional box has been treated before by Pathria [17] who obtained finite size corrections to the number of particles (as a function of temperature and chemical potential) using the Poisson summation formula. However, his procedure is valid only away from the quantum degenerate regime. Finite size corrections to non-relativistic BEC in the three-sphere have also been treated before by Altaie [18]. His procedure is similar to that of Pathria's article mentioned above. In particular, it is based on the use of the Poisson summation formula and likewise, it is valid only away from the quantum degenerate regime. A physical system analogous to our infinite slab case was considered before in the context of the thermal Casimir effect in Refs. [19,20], where the authors obtain high temperature (classical region) expansions for the thermodynamic potential and tackle the quantum degenerate regime by setting the chemical potential identically equal to its (thermodynamic limit) critical value. Some developments were also made in the finite size effects of a relativistic Bose gas in the three-sphere [21,22]. These works used a combination of analytical and numerical techniques and were very much inspired by an earlier study by Singh and Pathria [23]. Other work on BEC for the relativistic Bose gas on the three-sphere includes [24]. Some work on finite size effects for the uncharged relativistic Bose gas on the three-sphere have been considered [25].

2. Number of particles and specific heat

Consider an ideal Bose gas with particle eigenstates of energy E_n. The grand-canonical average number of particles is

$$N = \sum_i [\mathrm{e}^{\beta(E_i-\mu)} - 1]^{-1}, \tag{1}$$

where β is the inverse of the temperature T, μ is the chemical potential and the sum is over all particle eigenstates. We will use the natural units system with $\hbar = 1$, $c = 1$, and Boltzmann's constant $k = 1$ throughout. Expression (1) gives us $\mu(T)$ implicitly if we fix N. The internal energy is

$$U = \sum_i E_i [\mathrm{e}^{\beta(E_i-\mu)} - 1]^{-1}. \tag{2}$$