

Condensation of bosons with several degrees of freedom
Condensación de bosones con varios grados de libertad



Trabajo presentado por
Rafael Delgado López¹
para optar al título de
Máster en Física Fundamental
bajo la dirección del
Dr. Pedro Bargueño de Retes²
y del
Prof. Fernando Sols Lucia³

Universidad Complutense de Madrid

Junio de 2013

Calificación obtenida: 10 (MH)

1 rdelgadol@ucm.es, Dep. Física Teórica I, Universidad Complutense de Madrid

2 p.bargueno@fis.ucm.es, Dep. Física de Materiales, Universidad Complutense de Madrid

3 f.sols@fis.ucm.es, Dep. Física de Materiales, Universidad Complutense de Madrid

Abstract

The condensation of the spinless ideal charged Bose gas in the presence of a magnetic field is revisited as a first step to tackle the more complex case of a molecular condensate, where several degrees of freedom have to be taken into account.

In the charged bose gas, the conventional approach is extended to include the macroscopic occupation of excited kinetic states lying in the lowest Landau level, which plays an essential role in the case of large magnetic fields. In that limit, signatures of two diffuse phase transitions (crossovers) appear in the specific heat. In particular, at temperatures lower than the cyclotron frequency, the system behaves as an effectively one-dimensional free boson system, with the specific heat equal to $(1/2) Nk_B$ and a gradual condensation at lower temperatures.

In the molecular case, which is currently in progress, we have studied the condensation of rotational levels in a two-dimensional trap within the Bogoliubov approximation, showing that multi-step condensation also occurs.

statistical mechanics, macrocanonical ensemble, Bose Einstein condensation, density of states, degenerate matter, Bogoliubov interactions

Resumen

En este trabajo se analiza la condensación de un gas de Bose ideal de partículas cargadas y sin espín en presencia de un campo magnético como un primer paso para tratar el caso más complejo de un gas de Bose molecular, en el que se han de considerar varios grados de libertad.

Respecto al gas de Bose cargado, el tratamiento tradicional se extiende para incluir un término de niveles cinéticos excitados en el estado fundamental de niveles de Landau. Dicho término juega un papel especial en el límite de grandes campos magnéticos, en el que aparecen señales de dos transiciones de fase difusas (crossovers) en el calor específico. En particular, a temperaturas menores que la frecuencia ciclotrón, el sistema se comporta como un sistema unidimensional de bosones libres, con calor específico $(1/2) Nk_B$, y presenta una condensación gradual a temperaturas más bajas.

En el caso molecular, todavía en estudio, hemos estudiado la condensación de niveles rotacionales en una trampa bidimensional dentro de la aproximación de Bogoliubov, mostrando que también se da la condensación múltiple.

mecánica estadística, distribución macrocanónica, condensación de Bose Einstein, densidad de estados, materia degenerada, interacciones de Bogoliubov

Index

I. Introduction.....	1
II. Numerical approaches.....	3
III. Structure of the level population.....	5
IV. Numerical results for N_0 and N_k	6
V. Specific heat.....	7
VI. Conclusions.....	8

Condensation of bosons with several degrees of freedom

R. L. Delgado*

Departamento de Física Teórica I, Universidad Complutense de Madrid, E-28040, Madrid, Spain

The condensation of the spinless ideal charged Bose gas in the presence of a magnetic field is revisited as a first step to tackle the more complex case of a molecular condensate, in which several degrees of freedom have to be taken into account. In the charged Bose gas, the conventional approach is extended to include the macroscopic occupation of excited kinetic states lying in the lowest Landau level, which plays an essential role in the case of large magnetic fields. In that limit, signatures of two diffuse phase transitions (crossovers) appear in the specific heat. In particular, at temperatures lower than the cyclotron frequency, the system behaves as an effectively one-dimensional free boson system, with the specific heat equal to $\frac{1}{2}Nk_B$ and a gradual condensation at lower temperatures. In the molecular case, which is currently in progress, we have studied the condensation of rotational levels in a two-dimensional trap within the Bogoliubov approximation, showing that multi-step condensation also occurs.

I. INTRODUCTION

The equilibrium behavior of a charged Bose gas (CBG) in the presence of a magnetic field is a fundamental problem in quantum statistical mechanics. It was first addressed by Schafroth [1] at a time where the BCS theory of superconductivity had not yet been discovered. Although it was soon recognized that a model of non-interacting bosons had little predictive power for superconductivity, the CBG problem has continued to attract considerable attention because of its appealing simplicity and as a model to simulate astrophysical scenarios where charged particles are subject to extremely large magnetic fields, or neutral particles move in a fast rotating background. It is also interesting as a preliminary step in the study of the condensation of interacting bosons in a magnetic field or under rotation.

For the non-interacting case, Schafroth noticed that, in the presence of a magnetic field, Bose-Einstein condensation (BEC) no longer occurs in a strict sense, since at low enough temperatures, the system behaves as one-dimensional (1D) and a non-interacting 1D boson system is known to exhibit not a sharp but a gradual (diffuse) BEC transition. Later, May [2, 3] investigated the condensation in the non-relativistic case and showed that a sharp transition occurs for dimension ≥ 5 . Daicic and coworkers [4, 5] extended May's findings to the relativistic high-temperature case. Using a different definition of BEC, Toms [6–8] proved that BEC in the presence of a uniform magnetic field does not occur in any number of spatial dimensions and Elmfors and coworkers [9] considered that, in the three-dimensional (3D) case, although a true condensate is not formed, the Landau ground state can accommodate a large boson number. In this spirit, Rojas [10, 11] found that BEC may occur in the presence of a homogeneous magnetic field, but there is no critical temperature at which condensation starts, the phase transition being diffuse. Diffuse phase transitions

are those not having a definite critical temperature, but an interval of temperatures along which the transition occurs gradually. The concept was already introduced in the study of phase transitions which occur in certain ferroelectric materials [12]. In this work we treat the terms *diffuse transition* and *crossover* as synonyms. The notion of BEC of a CBG in the presence of a magnetic field in 3D continued to be studied by Toms and coworkers [13, 14], who showed that, although there is no BEC in the sense of a sharp phase transition, the specific heat exhibits a clear maximum that can be used to define a critical temperature. Using that definition, the authors inferred that the critical temperature increases with the magnetic field [14], reaching the usual value for the 3D free Bose gas when no magnetic field is present. The extension of these studies to the case of vector bosons in strong magnetic fields and at high temperatures was performed by Khalilov and coworkers [15–17]. Specifically, the condensation and effective magnetization of a charged vector boson gas were studied, showing that there is no true BEC as well, although a significant amount of bosons can accumulate in the ground state at low temperatures. More recently, the magnetic properties of charged spin-1 Bose gases in an external magnetic field have been revisited, with focus on the competition between diamagnetism and paramagnetism [18].

In the particular case of a large magnetic field, the main feature of a CBG is the coexistence of highly degenerate Landau levels and a fine structure of levels with nonzero momentum parallel to the magnetic field. We propose that a CBG under a large magnetic field can also be used as a crude model to understand basic features of systems where a fine sublevel structure coexists with sectors characterized by highly discrete quantum numbers. Specifically, we have in mind the condensation of bosonic molecules, whose level structure is hierarchical, with their rotational states structured into vibrational sectors which in turn can be grouped into largely spaced electronic levels.

Thus we are motivated by the study of molecular BECs, where a complex molecular level structure may give rise to multi-step BEC. Molecular condensates are

* rdelgadol@ucm.es

expected to display a wealth of fundamental phenomena. For instance, it has been proposed that molecular condensates may permit the experimental study of low-energy parity violation [19]. Specifically, the fact that recently both homonuclear [20], heteronuclear [21, 22] ultracold molecules and heteronuclear molecular ions [23, 24] have been produced in the rovibrational ground state, suggests that molecular BEC may not lie too far in the future. The conclusion is that the study of multi-step condensation of the CBG is interesting not only from an academic point of view, but it may provide a qualitative understanding of the condensation of molecules with a hierarchical level structure.

We consider a wide range of magnetic fields because we are interested in understanding the general trends. This means that in our analysis we include magnetic fields so large that would be unrealistic in some contexts [25–27]. Comparing our results with the previous related literature on the CBG (see, for example, Refs. 13 and 14), we notice the existence of a term that has so far been neglected. This is the occupation of states in the lowest Landau level but with arbitrary kinetic energy in the direction parallel to the magnetic field. This term is particularly important at large magnetic fields and in fact is responsible for the two-step condensation we refer to in the title and which we shall discuss in detail. We advance here that, as the temperature descends, a first step is defined by the onset of a preferential occupation of states in the lowest Landau level but without any of them absorbing a large fraction of the bosons. Then a plateau is reached where the system behaves as effectively one-dimensional. The second condensation step occurs at even lower temperatures, when the true one-particle ground state becomes host to a macroscopic fraction of the total boson number. By the time this occurs, the system behaves as one-dimensional, which translates into a diffuse Bose-Einstein condensation, as opposed to the conventional, sharp phase transition which is characteristic of three dimensions. Interestingly, these two distinct, both gradual condensation steps have been noted by Ketterle and coworkers [28, 29] in a different but somewhat analogous context, namely, that of condensation in a strongly anisotropic harmonic trap. As compared to a CBG in a large magnetic field, the role of the Landau levels is played there by the transverse subbands characterizing the motion in the most confined direction. In Refs. 28 and 29 the above mentioned term of the occupation of the states with the lowest value of the most discrete quantum number, was correctly included, which resulted in the prediction of a two-step condensation.

Although the macrocanonical ensemble of a non-interacting system is conceptually very simple, the calculations which it involves are challenging, specifically when several quantum numbers are considered. In addition, as the Bogoliubov approximation, when valid, transforms interacting to non-interacting problems [30, 32], it would be eventually analyzed through the same formalism.

As it is well known (see, for example, Refs. 30 and 32),

the energy of each individual boson in a non-interacting gas is given by a function like

$$\epsilon_{\vec{k}} = \epsilon(k_1, k_2, \dots), \quad (1)$$

where the values (k_1, k_2, \dots) are the quantum numbers of the problem. The number of particles N is given by

$$N = \sum_{\vec{k} \in K} \frac{d_{\vec{k}}}{z^{-1} \exp(-\beta \epsilon_{\vec{k}}) - 1}. \quad (2)$$

In this expression, K represents the space of all possible combinations of non-degenerate quantum numbers (k_1, k_2, \dots) ; $d_{\vec{k}}$, the possible remaining degeneracy of \vec{k} state; z , the fugacity; and β , the inverse temperature ($k_B = 1$). Thus, the challenging task is: given the functions $d_{\vec{k}}$ and $\epsilon_{\vec{k}}$, to recover the value of the fugacity z from Eq. (2) for a given value of β and N . The functions $d_{\vec{k}}$ and $\epsilon_{\vec{k}}$ together with the space K are, actually, the solution of the eigenvalues problem for an individual boson.

Once the value of z for a given β and N has been obtained, the population of a certain subset of levels $\tilde{K} \subset K$ is given by

$$N_{\tilde{K}} = \sum_{\vec{k} \in \tilde{K}} \frac{d_{\vec{k}}}{z^{-1} \exp(-\beta \epsilon_{\vec{k}}) - 1}, \quad (3)$$

the total internal energy U , by

$$U = \sum_{\vec{k} \in K} \frac{d_{\vec{k}} \epsilon_{\vec{k}}}{z^{-1} \exp(-\beta \epsilon_{\vec{k}}) - 1} \quad (4)$$

and the heat capacity at constant volume, by

$$C_v = \frac{\partial U}{\partial(\beta^{-1})}. \quad (5)$$

In practice, the space of quantum numbers K will be of the form \mathbb{N}^n , where n is the number of degrees of freedom. Therefore, the summations $\sum_{\vec{k} \in \tilde{K}}$ are finally numerical series in n variables. Thus, obtaining z requires the solution of an equation which includes in a non-trivial way such a series.

The usual (i.e., textbook) approach for dealing with Eq. (2) is replacing the summations over all quantum numbers by integrals. For Hamiltonians such harmonic or hard wall boundaries ones, there is a change of variables which allows to reduce the number of variables of integration. And the resulting unidimensional integral result to be a polylogarithm function, whose properties are well known [30, 32].

Lastly, a numerical treatment, a truncated series or the properties of the resulting polylogarithm function is used. Anyway, the crucial point is the reduction of the number of variables. Even if a computational library is used to evaluate the resulting polylogarithm function, such a library may use a (conveniently tuned) numerical series instead of a quadrature method.

The problem is that this classical approach fails if a large fraction of bosons is concentrated in a reduce subset of K or, eventually, in a unique value of \vec{k} . Of course, as we are dealing with Bose-Einstein condensation, it is expected that, for sufficiently low temperatures (high β), the population of bosons tends to concentrate in the level of minimum energy [30, 32]. This fact is usually taken into account by adding a term of the form

$$N_0 = \frac{d_0}{z^{-1} \exp(-\beta\epsilon_0) - 1} \quad (6)$$

to the resulting polylogarithm function, and the corresponding correction to the internal energy U .

For instance, the usual case of a 3D Bose gas in a box trap is described by

$$N = \sum_{k_x=1}^{\infty} \sum_{k_y=1}^{\infty} \sum_{k_z=1}^{\infty} \frac{1}{z^{-1} e^{\beta\epsilon(k_x^2+k_y^2+k_z^2)} - 1}, \quad (7)$$

where $\epsilon = \hbar^2/(2mL^2)$ is a constant. This expression is approximated by

$$N = \frac{1}{z^{-1} e^{\beta\epsilon(1^2+1^2+1^2)}} + \int_0^{\infty} dr \frac{4\pi r^2}{z^{-1} e^{\beta\epsilon r^2} - 1} \quad (8)$$

$$N = \sum_{k_x=1}^{\infty} \sum_{k_y=1}^{\infty} \sum_{k_z=1}^{\infty} \frac{1}{z^{-1} e^{\beta\epsilon(k_x^2+k_y^2+k_z^2)} - 1} \simeq \frac{1}{z^{-1} e^{3\beta\epsilon} - 1} + \int_0^{\infty} dx \int_0^{\infty} dy \int_0^{\infty} dz \frac{1}{z^{-1} e^{\beta\epsilon(x^2+y^2+z^2)} - 1}, \quad (13)$$

At low temperatures, the condensate term will be even greater than the integral which approximates all the other terms of the series. If it were neglected, the effect would be the absence of such a condensed phase, thus qualitatively modifying the physics of the problem.

Merging all the other terms of the original series into the integral assumes that each of such terms is negligible compared to the whole series. Even more, it also assumes that the series summing over a given k_i for certain $i = x, y, z$ and evaluating the series over the other variables is also negligible. Although critical for some purposes, this is seldom explicitly noticed, the articles of Ketterle and coworkers [28, 29] and our own [34] being an exception.

II. NUMERICAL APPROACHES

In this work, we have followed three numerical approaches. The first one is based on the development of a C++ computer program which accepts a *finite* list of energetic levels ϵ_i and their degeneracies d_i ($i = 1, 2, \dots, N$)

Taking $\beta\epsilon r^2 = x$, the integral term remains as

$$N - \frac{1}{z^{-1} e^{3\beta\epsilon} - 1} = \frac{2\pi}{(\beta\epsilon)^{3/2}} \int_{x=0}^{\infty} dx \frac{x^{1/2}}{z^{-1} e^x - 1} \quad (9)$$

Now, defining the polylogarithm function as

$$g_n(z) = \frac{1}{\Gamma(n)} \int_0^{\infty} dx \frac{x^{n-1}}{z^{-1} e^x - 1}, \quad (10)$$

Eq. (9) can be written as

$$N - \frac{1}{z^{-1} e^{3\beta\epsilon} - 1} = \frac{2\pi\Gamma(3/2)}{(\beta\epsilon)^{3/2}} g_{3/2}(z). \quad (11)$$

We notice that the complexity of evaluating the three-variable series of Eq. (7) has been reduced to that of evaluating a polylogarithm function $g_{3/2}(z)$, which actually can be written as

$$g_{3/2}(z) = \sum_{j=1}^{\infty} \frac{z^j}{j^{3/2}}. \quad (12)$$

Therefore, we arrive at a single-variable series. In the process, the only approximation made is that of substituting the numerical series by integrals but maintaining the term corresponding to the fundamental level $k_x = k_y = k_z = 1$, that is

and computes numerically the values of z (actually, the chemical potential μ , where $z = e^{\beta\mu}$), U and C_v by numerically solving Eq. (2). The Newton-Raphson algorithm is used and the derivative $\partial N/\partial z$ was explicitly hard-coded. Thus, the f function whose zeros are sought through the Newton-Raphson algorithm is

$$f(\mu) = \sum_{i=1}^N \frac{1}{e^{\beta(\epsilon_i - \mu)} - 1} \quad (14)$$

and its derivative,

$$\frac{df(\mu)}{d\mu} = \sum_{i=1}^N \frac{d_i \beta e^{\beta(\epsilon_i - \mu)}}{(e^{\beta(\epsilon_i - \mu)} - 1)^2} \quad (15)$$

Then, one of the tasks is that of computing a list of energetic levels which has to be large enough to include all the relevant levels, so that the effect of the finiteness of such a list can be neglected. This is computationally cheap when we are dealing with one degree of freedom, but becomes demanding when we have to sum contributions from several degrees of freedom, to sort the levels

by energies and to sum the degeneracies where the same energy levels are found as a result of the sum. And, at the same time, special care must be taken in order not to forget levels with less energy than a certain cutoff.

This has been successfully solved by using the program PARI/GP [33]. Actually, it is a Computer Algebra System (CAS) developed by Henri Cohen and coworkers for fast calculations in the field of number theory, which can deal with finite but extremely large series. When multiplying and powering the series, PARI/GP computes the order of the resulting series correctly, without computing or keeping unnecessary terms.

Thus, for each degree of freedom, a list of energy levels is computed. The energies are coded in the power of the monomials and the associated degeneracies in the multiplicative terms. That is, if they have a list of N levels with energies ϵ_i and degeneracies d_i , the associated truncated series will be

$$S[N, \epsilon_i, d_i] = \left(\sum_{i=1}^N d_i x^{\epsilon_i} \right) + O(x^{\epsilon_{N+1}}) \quad (16)$$

PARI/GP does not accept series with rational coefficients, but this can be bypassed by multiplying the column of energies by a common multiple of the denominators, and adding constants if needed (i.e., for dealing with a constant $+1/2$). This transformation must be reversed before using the list, although the addition of a finite constant c only adds a constant cN to the total internal energy U and a rescaling factor to the fugacity z , which is not directly measurable. Of course, this approach cannot deal with irrational energetic levels. But all the energetic levels considered in this work are integer or multiples of $1/2$. They come from potential wells ($\epsilon_k \propto k^2 + C$), harmonic traps ($\epsilon_k \propto k + C$), and vibro-rotational levels ($\epsilon_{\nu, J} = A\nu + BJ(J+1) + C$). In the vibro-rotational case, $\nu = 0, 1, \dots$ and $J = 0, 1, \dots$ are, respectively, the quantum number associated with the vibrational and rotational levels. And A, B and C are constants which depend on the properties of the molecule.

Thus, it can be proved that the task of merging several lists of energetic levels is reduced to that of multiplying the series associated to such lists. This is actually a non-trivial computation, but PARI/GP can deal efficiently with it, both in terms of processor and memory usage. The only handicap is that PARI/GP does not provide a method to parallelize this computation, and that the available RAM memory on a single computer is a practical limit. This could be problematic if several energy hierarchies separated by some orders of magnitude were taken into account.

To test this approach, we have compared in figs. 1 and 2 the approximate cumulative density of states of a 3D gas confined in a potential well (eigenstates $\epsilon_{\vec{k}} = k_x^2 + k_y^2 + k_z^2$, normalization $\epsilon = 1$), i.e.,

$$\int_0^\epsilon \rho(\epsilon') d\epsilon' = \int_0^\epsilon \frac{\pi}{4} \epsilon'^{1/2} d\epsilon' = \frac{\pi}{6} \epsilon^{3/2}, \quad (17)$$

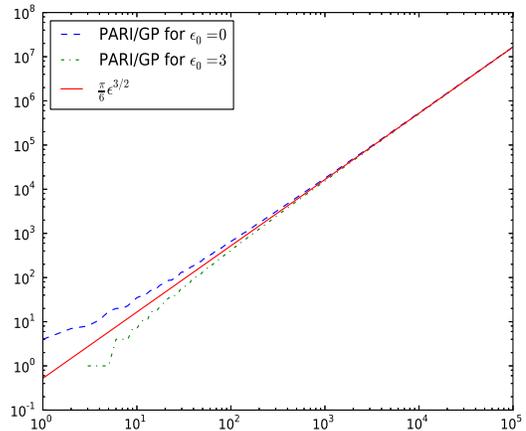


Figure 1. Exact solutions for the cumulative density of states versus energy computed with PARI/GP [33] for the cases of $\epsilon_0 = 0$ and $\epsilon_0 = 3$, compared with the approximation of the continuous limit $\int_0^\epsilon \rho(\epsilon') d\epsilon' = \frac{\pi}{6} \epsilon^{3/2}$.

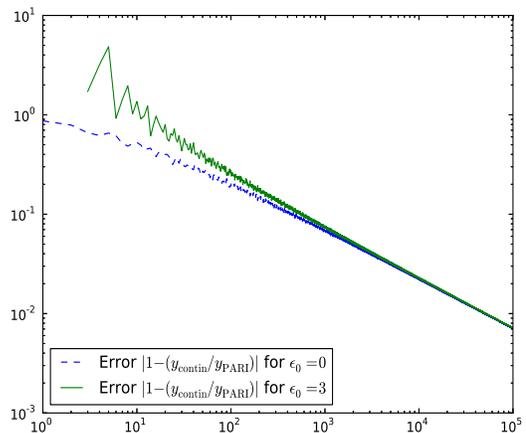


Figure 2. Relative error of the approximation of the continuous limit given two models ($\epsilon_0 = 0$ and $\epsilon_0 = 3$). The exact solutions have been computed with PARI/GP [33].

with the exact (and discrete) solution for both cases $k_i = 0, 1, 2, \dots$ ($\epsilon_0 = 0$) and $k_i = 1, 2, 3, \dots$ ($\epsilon_0 = 3$). Actually, the true solution would be that corresponding to $\epsilon_{\vec{k}} = k_x^2 + k_y^2 + k_z^2$ with $k_i = 1, 2, 3, \dots$

It is remarkable that these results apply to the case of both bosons and fermions, if the respective statistics are used. However, when dealing with a large number of particles (thermodynamic limit), the effect is negligible. Specially in the case of fermions, where the so called Fermi level (ϵ_F) tends to be far away from the ground state of a single fermion. This effect is likely to be dominant in the regime of very few particles and even with an isolated particle in a well trap.

Thus, a mixed formalism could be developed where several degrees of freedom could be fitted by a continuous function while the others should be kept discrete. Actually, those quasi-continuous levels would be approximated by a discrete structure of levels separated by a small distance compared with the other quantum numbers but much larger than the exact separation. This procedure allow us to perform the computations with limited resources. Special care should be taken on the validity of such approximations in the various regions of the spectrum. Such an analysis has not been performed because it is beyond the scope of our present work.

The second approach, followed by us in Ref. [34], was based on the use of the usual analysis which involves the approximation of substituting series by integrals and using the properties of polylogarithm functions to reduce the integration variables to just one. However, for solving Eq. (2), a numerical method for extracting the zero of a function has been used. Furthermore, like in Refs. [28, 29], several terms have been treated separately from the integral over all variables. These terms correspond to the ground level of a certain variable while summing over the rest. This approach was explained in section I, when describing the usual approaches to the macrocanonical problem. Furthermore, as this approach was chosen to deal with the case of a charged Bose gas in a large magnetic field [34], it will be explained in more detail in section III.

And the third approach is the numerical evaluation of the original multi-variable series, by using the program PARI/GP [33], which also has very fast methods for directly evaluating numerical series of different kinds. No ad hoc cutoff is needed except for the working precision. It can handle two-variable series easily and it can compute up to three-variable series in a reasonable time, although some optimization has to be manually performed. Specifically, the optimal method to sum the series depends on the space of parameters (i.e., β and the different parameters which define the hierarchy of energy levels).

This method, although overlaps with the first one (that of the truncated series), has been used to deal with the case of a molecular condensate with rotational levels within the Bogoliubov approximation. It is remarkable that in that case there is no clear possibility of reducing degrees of freedom via a change of variable in the integral approximation, thus making it impossible to follow the usual approach of using either polylogarithm functions or integrals. Of course, changing the series by multivariate integrals still remains possible (within the limits of such approximations). But this does not allow to reduce the number of variables.

However, if we were to deal with the more general case of an experimental rovibrational spectrum, or a more detailed model, it would be necessary to use the first approach of summing over a finite (but large) set of energy levels. Even more, including a limited set of levels is unavoidable, since the theory itself is limited in energies. For instance, in the molecular case, chemical reactions

are expected over a certain energy level [35].

Nevertheless, the most general case would be that of a Bose Einstein condensate with strong interactions, which would invalidate the hypothesis of non-interacting particles without giving a feasible way of recovering it via a change of variables. In either case, there is a brute-force method, namely lattice Monte Carlo, which would allow to extract the internal energy and almost any thermodynamical variable (spending enough computer time). The price to be paid would be the loss of simplicity of our semi-analytical approaches and the clear identification of the physical interactions which are responsible for the thermodynamical behavior of the Bose gas. Such method have indeed been widely used to study phase transitions, and constitutes a wide field of current research. See, for example, Refs. [36–39].

Finally, we note that the described methods give us $U(\beta)$, but the specific heat at constant volume, $C_V = -\beta^2 (\partial U / \partial \beta)_V$, must be obtained numerically from such expression. That is, through a numerical derivation. When using `Maple`, its numerical libraries are used. But when using either `PARI/GP` [33] or the finite series approach, we have to compute with a numerical derivation method implemented by ourselves. The simplest one has been selected. That is, simply taking $df/dx \approx (f(x+h) - f(x))/h + O(h)$.

III. STRUCTURE OF THE LEVEL POPULATION

Let us consider a charged gas of bosonic particles confined in a 3D box of volume AL , where A is the area in the x - y plane and L is the length in the z direction. Away from the edges of the box, the energy of a charged particle in a uniform magnetic field B pointing in the z direction is quantized as [30]

$$E_n(n_z) = \hbar\omega \left(n + \frac{1}{2} \right) + \varepsilon n_z^2, \quad (18)$$

where $\omega = qB/mc$ is the cyclotron frequency, $\varepsilon \equiv \hbar^2 \pi^2 / 2mL^2$ characterizes the level spacing in the z direction, and both n and n_z run over natural numbers (we assume hard wall boundary conditions at $z = 0$ and $z = L$). The index n is said to characterize the Landau level.

The area A is assumed to be large enough for the role of edge states in the x - y plane to be negligible. Specifically, $l^2 \ll A$, where $l^2 = \hbar c / qB$ is the magnetic length squared.

We start by writing the total number of particles N as ($\hbar = 1$)

$$N = d \sum_{n_z=0}^{\infty} \sum_{n=0}^{\infty} \frac{z}{\exp(\beta\varepsilon n_z^2 + \beta\omega n) - z}, \quad (19)$$

where $\beta \equiv (k_B T)^{-1}$, $d = A/l^2$ is the Landau degeneracy, and $z \equiv \exp(\beta\mu)$ is the fugacity, with μ the chemical po-

tential [which absorbs the $1/2$ term in (18)]. We partition the total particle number into four different groups:

$$N = N_0 + N_k + N_m + N_{mk}. \quad (20)$$

N_0 is the number of particles in the one-particle ground state ($n = n_z = 0$),

$$N_0 = d \frac{z}{1-z}; \quad (21)$$

N_k is the number of particles in the ground state of the magnetic level but in excited kinetic levels ($n = 0$ and $n_z \neq 0$),

$$N_k = d \sum_{n_z=1}^{\infty} \frac{z}{\exp(\beta \varepsilon n_z^2) - z}; \quad (22)$$

N_m is the number of particles in the kinetic ground state but in excited magnetic states,

$$N_m = d \sum_{n=1}^{\infty} \frac{z}{\exp(\beta \omega n) - z}; \quad (23)$$

and N_{mk} is the number of particles in excited states of both magnetic and kinetic degrees of freedom,

$$N_{mk} = d \sum_{n=1}^{\infty} \sum_{n_z=1}^{\infty} \frac{z}{\exp(\beta \varepsilon n_z^2 + \beta \omega n) - z}. \quad (24)$$

The term N_k can be approximated by

$$N_k \simeq d \eta_k g_{1/2}(z). \quad (25)$$

where $\eta_k = (\pi/4)^{1/2} (\beta \varepsilon)^{-1/2}$ and $g_\alpha(z) \equiv \sum_{j=1}^{\infty} z^j / j^\alpha$ stands for the polylogarithm function of order n [31]. Here, the identity $\lim_{\lambda \rightarrow 0} \sum_{j=1}^{\infty} \lambda f(\lambda j) = \int_0^{\infty} f(x)$ has been used assuming that $\lambda = \sqrt{\beta \varepsilon}$ is sufficiently small. Similarly, N_m and N_{mk} can be approximated as:

$$N_m \simeq d \eta_m g_1(z) \quad (26)$$

and

$$N_{mk} \simeq d \eta_m \eta_k g_{3/2}(z), \quad (27)$$

where $\eta_m \equiv (\beta \omega)^{-1}$. We can group these approximations to write the total particle number as

$$\frac{N}{d} = g_0(z) + \eta_k g_{1/2}(z) + \eta_m g_1(z) + \eta_k \eta_m g_{3/2}(z). \quad (28)$$

As noted by the authors of Ref. 29 in a similar context (with harmonic instead of hard-wall confinement), the expression Eq. (28) is an excellent and controlled approximation for the whole temperature regime. We note that, in this equation, the second, third, and fourth terms become dominant in the respective cases $\eta_k \gg 1$, $\eta_m \gg 1$ and both $\eta_k, \eta_m \gg 1$.

The factor d appearing in all the occupation numbers, Eqs. (21)-(28), reveals the existence of Landau degeneracy, which in particular reflects a multiplicity of one-particle ground states where bosons are in both the kinetic and magnetic ground state ($n = n_z = 0$).

The second term, N_k , represents the occupation of particles lying in the ground Landau manifold but in excited kinetic states (with motion in the z direction). We point out that this term has often been neglected in studies of the CBG. We show below that N_k plays a most important role in the thermodynamic properties of the CBG under large magnetic fields. The third term, N_m , which accounts for those bosons which are in the kinetic ground state but in excited magnetic states, will not be studied here because it acquires importance only for very small magnetic fields, that is, when the energy of the first magnetic excited state is much lower than the energy of the first kinetic state ($\omega \ll \varepsilon$). This would describe a two-dimensional boson gas which will not be considered here. The last term, N_{mk} , corresponds to the conventional term in which the bosons are in both magnetic and kinetic excited states. It is the dominant term at high enough temperature, where the 3D limit is recovered ($\eta_m, \eta_k \gg 1$).

Finally, we note that the order of the polylogarithm functions appearing in Eq. (28), $g_{d/2}(z)$, corresponds to the population of excited states of free particles in d dimensions.

IV. NUMERICAL RESULTS FOR N_0 AND N_k

For zero magnetic field and vanishing ε the CBG resembles a 3D free Bose gas, showing BEC at the usual critical temperature. In this case, a discontinuous phase transition occurs [32]. However, for large values of the magnetic field ($\omega \gg \varepsilon$), the transition becomes diffuse [10, 11] and only crossover temperatures can be defined. Specifically, due to the presence of the N_k term, two different crossover temperatures will be identified.

It is quite remarkable that, for these high magnetic fields, N_k gives a significant contribution to N , as revealed in Fig. 3, where we show the relative weight of $N_0(T)$ described by both the conventional and extended approaches ($N_k = 0$ and $N_k \neq 0$, respectively) for several values of the magnetic field. From this figure it can be noted not only that the phase transition becomes diffuse, but also that the macroscopic occupation of bosons with kinetic excited states lying in the ground Landau manifold is very important at large magnetic fields.

We note that, within this limit of large magnetic fields and for $z \ll 1$ (i.e. $\beta|\mu| = -\beta\mu \gg 1$, high temperature limit for the effective 1D system), the temperature dependence of N_0/N tends to

$$\frac{N_0}{N} = \frac{1}{1 + \eta_k}, \quad (29)$$

as shown in Fig. 3. In fact, this limit function cannot be

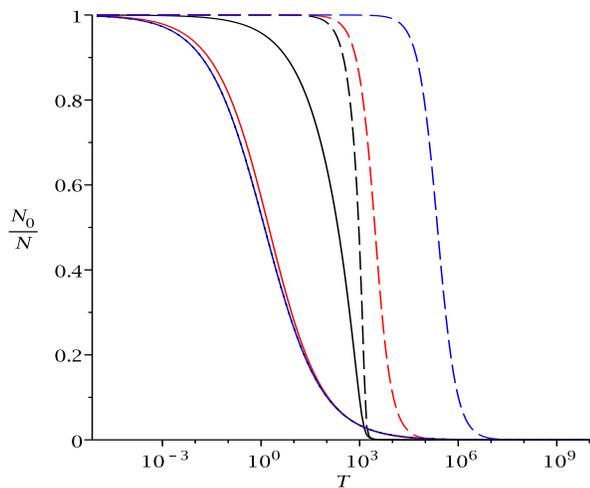


Figure 3. Computed relative weight of N_0 for $N = 10^5$ and $\omega = 10^2$ (black lines), $\omega = 10^5$ (red -light gray- lines) and $\omega = 10^8$ (blue -gray- lines), in units of ε . Temperature is given in units of ε/k_B . The conventional approach (which ignores N_k) is plotted with dashed lines. The effect of including the N_k in the relative weight of N_0 is plotted with solid lines. The limiting function $(1 + \eta_k)^{-1}$ is represented with black dotted lines (it overlaps with the solid blue (gray) line) [see Eq. (29)].

distinguished from the case $\omega = 10^8$ depicted in Fig. 3.

The origin of the discrepancy shown between the conventional and the extended approach (which increases with the magnetic field) can be traced to the relative weights of the different terms entering Eq. (28), which explicitly includes the contribution of N_k . Take for example $\omega = 10^5$ and $N = 10^5$. In this case, as shown in Fig. 4, N_k represents a significant (and occasionally dominant) amount of the total particle number. Moreover, two different crossover temperatures appear when either N_k or N_0 begin to grow substantially. In particular, the phase transition that occurs at a lower temperature remains somewhat more diffuse than the high-temperature one, because of its effective 1D nature.

V. SPECIFIC HEAT

The essential features of BEC as a phase transition are clearly exhibited in the behavior of the specific heat. In particular, we consider the specific heat at constant volume, defined by $C_V = -\beta^2 (\partial U / \partial \beta)_V$. In the extended approach, the internal energy can be expressed as

$$U(\beta, z) = \frac{d}{2} \eta_k \beta^{-1} g_{3/2}(z) + \frac{3d}{2} \eta_k \eta_\omega \beta^{-1} g_{5/2}(z). \quad (30)$$

When no magnetic field is present, C_V tends to the 3D free Bose gas, displaying a sharp maximum and a discontinuous first derivative. The effect of a nonzero magnetic field is that of smoothing out that maximum [14]. This can be clearly appreciated in Fig. 5. Although the

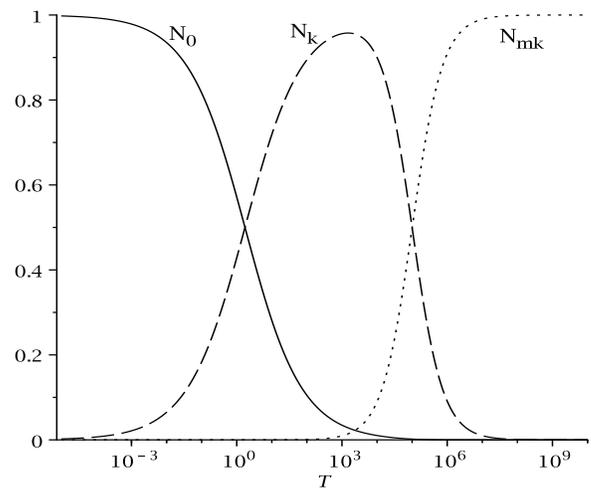


Figure 4. Computed relative weights of N_0 (solid line), N_k (dashed line) and N_{mk} (dotted line) for $\omega = 10^5$ and $N = 10^5$. See text for details.

phase transition remains diffuse in the presence of a magnetic field, as previously discussed, one can still associate a critical temperature to the maximum of the specific heat, as in the free gas case [14]. In Fig. 5 it can also be seen that, for $\omega = 10^2$, no significant deviations from the conventional approach are found except for one: the inclusion of the N_k terms tends to round off the relatively sharp maximum shown in the specific heat calculated from the conventional approach. On the contrary, for $\omega = 10^8$, significant differences between the conventional (dashed line) and extended (solid line) persist in a wide range of temperatures. Specifically, for large magnetic fields ($\omega \gg \varepsilon$) and high temperatures ($\beta\omega \ll 1$, or $\eta_m \gg 1$), C_V/N approaches the classical value of $3/2$. Within this regime, the classical limit can be obtained by taking $N \simeq d\eta_k \eta_\omega z$ and $U \simeq \frac{3}{2} d\eta_k \eta_\omega \beta^{-1} z$, which results in $U = 3N/2\beta$. This is the classical limit for a system in three dimensions.

It is interesting to note that signatures of a double phase transition appear in the specific heat. In particular, Fig. 5 shows a plateau-like structure in the specific heat when the effective number of particles, N/d , is of the order of 10^{-3} (solid blue -gray- line). This plateau spans the temperature range $\varepsilon \ll k_B T \ll \omega$. As T decreases, the first phase transition, observed at a high temperature, reveals the transition from states which have both kinetic and magnetic excitations to those which are in excited kinetic states but in the ground Landau manifold. The second phase transition shows how the absolute ground state (kinetic and magnetic) is reached. In fact, the existence of two crossovers can be understood from Fig. 4. This is in accordance with the large slope of the $C_V(T)$ curve observed for the high-temperature crossover, compared to the low-temperature one. On the contrary, the specific heat calculated within the conventional approach (that which ignores N_k) does not show

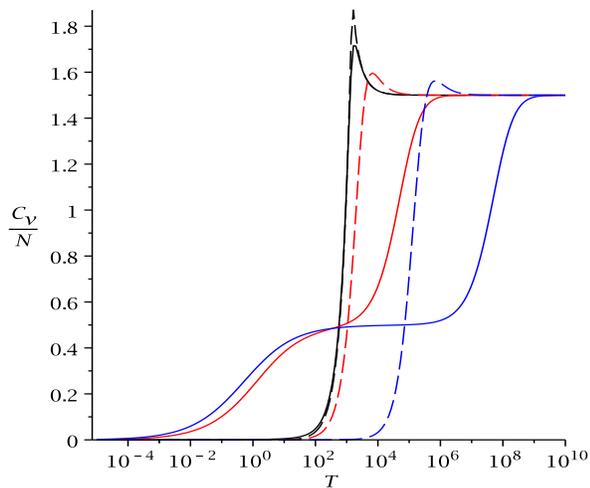


Figure 5. Specific heat at constant volume as a function of temperature. The extended and conventional approaches are plotted with solid and dashed lines, respectively. We have taken $N = 10^5$ and $\omega = 10^2$ (black lines), $\omega = 10^5$ (red - light gray- lines) and $\omega = 10^8$ (blue -gray- lines). See text for details.

signatures of double phase transitions, as expected.

We remark that, in the plateau $\varepsilon \ll k_B T \ll \omega$, a constant value for the specific heat is obtained between the two crossover temperatures. Within this temperature range, $N \simeq d\eta_k z$ and $U \simeq \frac{1}{2}d\eta_k \beta^{-1}z$. Finally, we get $U \simeq N/2\beta$. Thus, the plateau of the specific heat lies in the value $C_V = Nk_B/2$, as shown in Fig. 5, which corresponds to that of a Bose gas in one dimension. We note that, although the value of the specific heat in the intermediate temperature plateau is independent of the degeneracy d , the details of the low and high temperature behavior depend on the particular value of d . In fact, we recall that the very existence of the plateau relies essentially on the degeneracy being much greater than unity.

VI. CONCLUSIONS

In this work we have revisited the free charged Bose gas focusing on the case of a large magnetic field, in principle as a toy model to tackle in the future the more complex molecular case. Although a sharp Bose–Einstein condensation does not occur, two diffuse phase transitions (or crossovers) are found. As the temperature is decreased, the first crossover reflects the enhanced occupation of states in the lowest Landau level. Then a range of intermediate temperature is found where the system behaves as an effectively one-dimensional system in its high-temperature regime. At even lower temperatures, the system undergoes a 1D Bose condensation, which is known to be a diffuse phase transition. To account for this two-step condensation, it has proved essential to in-

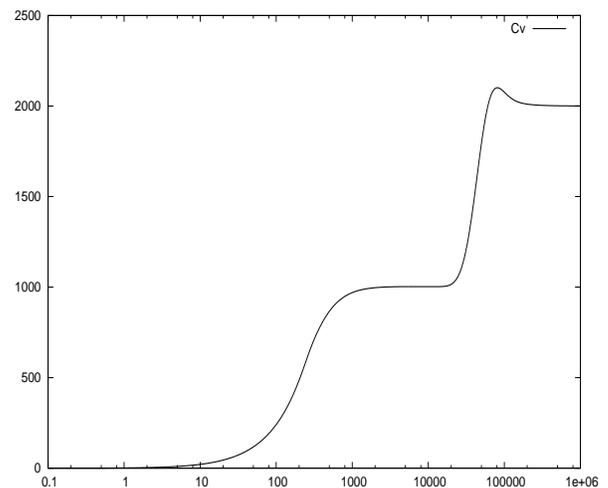


Figure 6. Specific heat of a molecular Bose gas in a 2D trap as a function of T . We have taken $\varepsilon = 1$, $B = 10^5$, $C = 10^0$.

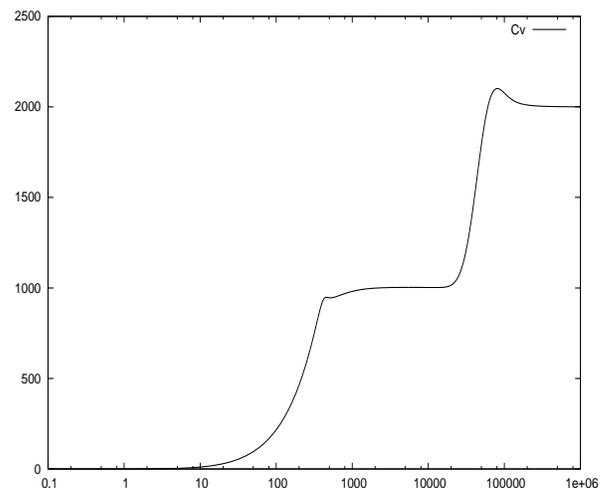


Figure 7. As in fig. 6, for $C = 10^2$.

clude the occupation of states in the lowest Landau level but with arbitrary kinetic energy in the direction parallel to the magnetic field.

Furthermore, three different numerical approaches to the macrocanonical ensemble problem have been studied. In one of them, to solve the case of a free charged Bose gas [34], the usual approximation of polylogarithm functions (which amounts to a change of variable in a multidimensional integration) has been eventually used. The approximation really simplifies the numerically challenging task of summing a series over several variables.

But such approximation will not be so useful when dealing with the rotational levels or the Bogoliubov cases, because the change of variables relies on a specific structure for the energetic levels. So, to deal with the more general case of a diatomic Bose gas with rotational levels and a kinetic term corrected by the Bogoliubov ap-

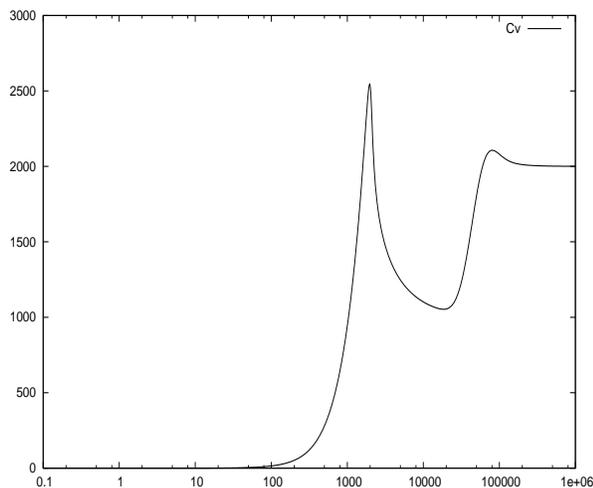


Figure 8. As in fig. 6, for $C = 10^4$.

proximation, we find more useful the approach of direct summation of the series through PARI/GP [33] or even the truncated series. To show the complexity of those models, we include here a simulation of a case with

$$\epsilon_{\vec{k}} = \sqrt{\epsilon_{\text{kin}}^2 + C\epsilon_{\text{kin}} + B \cdot J(J+1)}, \quad \epsilon_{\text{kin}} = \epsilon(k_x^2 + k_y^2), \quad (31)$$

where $C = 2nV_0$, with n and V_0 standing for the density and interaction energy, respectively; and the degeneration term is given by $g_{\vec{k}} = 2J + 1$. That is, a 2D Bose condensation of molecules with a rotational structure level and a Bogoliubov correction which affects the kinetic structure. The specific heat is shown in figs. 6 ($C = 10^0$), 7 ($C = 10^2$) and 8 ($C = 10^4$). In all the cases, $\epsilon = 1$ and $B = 10^5$. This work is currently in progress.

Even more, if an experimental or more realistic model of molecular levels were used, the approach of mixing the molecular levels with the kinetic ones through the formalism of multiplying truncated series (eq. 16) would be necessary. And, finally, if a model of strong interactions were used (where the Bogoliubov approximation would break down), then using a lattice Monte Carlo method (Refs. [36, 37]) could be a good choice, although it does not allow to perform directly a simple study of the actual energetic level structure.

To sum up, in the considered cases, if we have a complex level structure composed by several substructures associated with each quantum number, and those substructures have different level separations, several condensations emerge for each substructure. The corresponding critical temperature emerges when the excited states of the associated substructure are macroscopically populated. When several substructures have equal or comparable level separations, as in the case of the textbook example of a 3D Bose gas in a box, they give rise to a simple condensation, which tends to be sharper, as if several condensations were occurring at the same temperature (see fig. 5 for instance).

In fact, the specific heat of simple molecules at moderate temperatures is nearly constant along a wide range of temperatures, as required by the equipartition theorem, but presents steps when the temperature is high enough to excite additional degrees of freedom. However, it is not so easy to find a case in which several of those steps are degenerate. That is, in which they occur at temperatures which are close enough to observe an overlapping.

To conclude, we note that another interesting task would be the analysis of a Dirac gas with several energetic hierarchies, so that, even if there is no condensation associated to the lowest energetic excitation, a macroscopic fraction of particles can condensate in the ground state of a highly spaced quantum number.

-
- [1] M. R. Schafroth, Phys. Rev. **100**, 476 (1955).
 - [2] R. M. May, Phys. Rev. **115**, 254 (1959).
 - [3] R. M. May, J. Math. Phys. **6**, 1462 (1965).
 - [4] J. Daicic, N. E. Frankel and V. Kowalenko, Phys. Rev. Lett. **71**, 1779 (1993).
 - [5] J. Daicic, N. E. Frankel, R. M. Gailis and V. Kowalenko, Phys. Rep. **237**, 63 (1994).
 - [6] D.J. Toms, Phys. Rev. Lett. **69** 1152 (1992).
 - [7] D. J. Toms, Phys. Rev. D **47** 2483 (1993).
 - [8] D. J. Toms, Phys. Lett. B **343** 259 (1995).
 - [9] P. Elmfors, P. Liljenberg, D. Persson and B. -S. Skagerstam, Phys. Lett. B **348** 462 (1995).
 - [10] H. -P- Rojas, Phys. Lett. B **379**, 148 (1996).
 - [11] H. -P- Rojas, Phys. Lett. A **234**, 13 (1997).
 - [12] G. A. Smolenski and V. A. Isupov, Sov. Journal of Techn. Phys. **24**, 1375 (1954).
 - [13] G. B. Standen and D. J. Toms, Phys. Lett. A **239**, 401 (1998).
 - [14] G. B. Standen and D. J. Toms, Phys. Rev. E **60**, 5275 (1999).
 - [15] V. R. Khalilov, C. -L. Ho and C. Yang, Mod. Phys. Lett. A **12**, 1973 (1997).
 - [16] V. R. Khalilov, Theor. Math. Phys., **114**, 345 (1998).
 - [17] V. R. Khalilov and C. -L. Ho, Phys. Rev. D, **60**, 033003 (1999).
 - [18] X. Jian, J. Qin and Q. Gu, J. Phys.: Condens. Matter **23**, 026003 (2011).
 - [19] P. Bargeño and F. Sols, Phys. Rev. A, **85**, 021605(R) (2012).
 - [20] J. G. Danzl, M. J. Mark, E. Haller, M. Gustavsson, R. Hart, J. Aldegunde, J. M. Hutson, and H.-C. Nägerl, Nat. Phys. **6**, 265 (2010).
 - [21] K. Aikawa, D. Akamatsu, M. Hayashi, K. Oasa, J. Kobayashi, P. Naidon, T. Kishimoto, M. Ueda, and S. Inouye, Phys. Rev. Lett. **105**, 203001 (2010).
 - [22] K.-K. Ni, S. Ospelkaus, D. Wang, G. Quémener, B. Neyenhuis, M. H. G. de Miranda, J. L. Bohn, J. Ye, and

- D. S. Jin, *Nature (London)* **464**, 1324 (2010).
- [23] P. F. Staantum, K. Hojbjerg, P. S. Skyt, A. K. Hansen and M. Drewsen, *Nat. Phys.* **6**, 271 (2010).
- [24] T. Schneider, B. Roth, H. Duncker, I. Ernsting and S. Schiller, *Nat. Phys.* **6**, 275 (2010).
- [25] We note however that huge magnetic fields can be generated in stellar objects like supernovae and neutron stars. Specifically, magnetic fields of the order 10^{20} G and larger have been suggested to exist in the cores of neutron stars [26], where kaon condensation was proposed [27].
- [26] S. Chakrabarty, D. Bandyopadhyay, and S. Pal, *Phys. Rev. Lett.* **78**, 2898 (1997).
- [27] D.B. Kaplan and A. E. Nelson, *Phys. Lett. B*, **175**, 57 (1986).
- [28] W. Ketterle and N. J. van Druten, *Phys. Rev. A*, **54**, 656 (1996).
- [29] N. J. van Druten and W. Ketterle, *Phys. Rev. Lett.*, **79**, 549 (1997).
- [30] L. Landau and L. Lifschitz, *Quantum Mechanics*, Pergamon, Oxford (1987).
- [31] K. Huang, *Statistical Mechanics (2nd edition)*, John Wiley and Sons (1987).
- [32] L. Pitaevskii and S. Stringari, *Bose–Einstein Condensation*, Oxford University Press, Oxford (2003).
- [33] PARI/GP, version 2.5.1, Bordeaux, 2012, <http://pari.math.u-bordeaux.fr/>.
- [34] Delgado, R. L., Bargueño, P., & Sols, F. 2012, *Phys. Rev. E*, **86**, 031102
- [35] Paul S. Julienne, Thomas M. Hanna and Zbigniew Idziaszek, *Phys. Chem. Chem. Phys.*, 2011, **13**, 19114–19124
- [36] G. Parisi, *Statistical Field Theory*, Perseus Books Group, 1998.
- [37] D. J. Amit and V. Martín Mayor, *Field Theory, the Renormalization Group and Critical Phenomena*, World-Scientific Singapore, third edition, 2005.
- [38] Fernandez, L. A., Martín-Mayor, V., & Yllanes, D. 2011, arXiv:1106.1555
- [39] Janus Collaboration, Baños, R. A., Cruz, A., et al. 2012, arXiv:1202.5593