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Phase transition of a Bose gas in a harmonic potential

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Abstract. – We consider a Bose gas confined by a harmonic potential. We define an appropriate thermodynamic limit and analyze the properties of the phases and phase transition in this limit. Critical properties in the presence of the potential are found to be different from, though simply related to, those in the usual translationally invariant case. We argue that the properties of magnetically trapped rubidium and sodium gases (in which Bose-Einstein condensation has recently been observed) are well approximated by our thermodynamic limit except in a narrow window of temperature around the critical temperature. We also consider the effect of the confining potential on the non-equilibrium dynamics following a rapid quench to the ordered side and give a scaling description of the late-time universal dynamics.

Much excitement has been generated in the last few months by the observation of Bose-Einstein condensation (BEC) in magnetically trapped alkali atoms [1]. Since the original observation of BEC in rubidium atoms, two other groups have reported evidence for the same in lithium [2] and sodium [3] atoms. A key feature of these experiments is the presence of a confining harmonic potential that the atoms feel. In this paper, we study the effects of such a confining potential on the statistical mechanics of ideal and interacting Bose systems (we confine our attention to repulsive interactions —so our results are not directly applicable to the lithium experiment). In particular, we study the effects of this confining potential on the equilibrium critical properties of the finite-temperature phase transition at which the Bose condensate first appears. We show how to define a sensible thermodynamic limit in which the critical singularities are present; the experiments are, of course, in finite systems —this is accounted for by finite-size scaling crossover functions which smooth out the singularities, in a manner quite analogous to that for familiar phase transitions in translationally invariant systems placed in a finite box. We will find that the exponents of the critical singularities are related, but *not* identical, to those of translationally invariant systems. The finite-size scaling crossover functions are expected to be new and not simply related to known crossover functions. We also consider the non-equilibrium dynamics associated with the establishment of long-range order following a rapid quench to the superfluid phase. We argue that recent

results [4] obtained for the case of a translationally invariant system placed in a finite box may be used to understand the effects of the confining potential on this dynamics.

On general grounds, there is no true phase transition to a Bose condensed phase in the presence of a confining potential for a finite number of particles. Such a transition is expected to appear only in a suitable “thermodynamic” limit; we will argue here that the experimentally appropriate limit is one in which the frequency, ω , of the confining potential goes to zero, and the number of particles, N , to infinity, while keeping $N\omega^3$, the interaction strength, and the temperature (T) fixed. We will show that the critical properties in this limit can be understood by an application of the “local density approximation” of Oliva [5]. In this approximation, the system is viewed as a collection of homogenous semi-macroscopic blocks, each with its own local chemical potential. Each of these blocks can be treated independently of the others, and have properties characteristic of large uniform systems. The properties of the system with the confining potential can then be related to the corresponding properties of the usual translationally invariant systems. Many aspects of our general discussion below can be checked explicitly in a Hartree-Fock calculation [6]. We thus obtain a complete understanding of the properties of the system in the thermodynamic limit. (In earlier treatments [5], [7], this approach was used for an approximate treatment of the non-critical properties of the inhomogenous Bose gases, but the importance of the thermodynamic limit in justifying it was not noted.) For the phase transition, we estimate by the usual Ginzburg criterion ⁽¹⁾[8] that the system crosses over to the critical non-ideal regime only at small deviations from criticality ($|T - T_c|/T_c \simeq 10^{-3}$ for the existing experimental systems); some properties of the system in this regime are quite significantly modified by the presence of the potential. Further, we show that the experimental systems are quite accurately described by our thermodynamic limit except in a narrow window of temperatures near the critical temperature, where finite-size crossovers need to be considered. However, this window is somewhat bigger than the temperature range for non-ideal behaviour; thus the crossover to non-ideal critical behaviour will be complicated by the presence of finite-size effects.

We will describe our results using the Hamiltonian (in second-quantized notation)

$$\mathcal{H} = \int d^3x \left[\frac{\hbar^2}{2m} |\nabla\psi|^2 + \left(\frac{1}{2}m\omega^2(x^2 + y^2 + \lambda^2z^2) - \mu \right) |\psi|^2 + \frac{u}{2} |\psi|^4 \right], \quad (1)$$

where m is the mass of the bosons, the interaction strength u is related to the scattering length a by $u = 4\pi\hbar^2a/m$, and λ is the anisotropy in the harmonic potential. When ω is finite, the system is confined to a finite region and will not have a true phase transition to a phase with long-range order. We expect “thermodynamic” behaviour to emerge only in the limit in which ω is sent to zero and the number of particles to infinity. In the usual case of a system confined in a box, this is achieved by keeping the density constant while sending the box size to infinity. For the oscillator case, this suggests that we scale the number of particles N with the volume over which the system is confined. This can be estimated at high temperatures (where interactions and quantum effects may be neglected) to be $\simeq (k_B T/m\omega^2)^{3/2}$. Thus, we guess that the thermodynamic limit is defined by sending ω to zero while keeping $N\omega^3$ fixed. As shown below, this does turn out to be a perfectly sensible limit in which there is a true phase transition at a finite non-zero temperature and the free energy per particle is finite ⁽²⁾.

First consider the system in its high-temperature phase. As ω goes to zero, the potential varies over a macroscopic length scale $\sim 1/\omega$. Divide the system up into blocks, such that

⁽¹⁾ The Ginzburg criterion measures when mean-field results for a phase transition breakdown by estimating the magnitude of fluctuation corrections; see ref. [8] for more details.

⁽²⁾ This thermodynamic limit has been discussed earlier for the case of an ideal Bose gas by Masut *et al.* [9].

the potential does not vary significantly across any block. Each of these blocks is macroscopic in size and uniform. The correlation length in any block is some microscopic number (much smaller than the size of the block) determined by the local chemical potential. The different blocks can therefore be treated independently of each other. Furthermore, the properties of any block are well approximated by the thermodynamic behaviour of the corresponding uniform system. *Extensive* quantities such as the free energy are then a sum over the free energies of the individual blocks. For the total free energy F we thus have

$$F = \sum_{\text{blocks}} F_{\text{block}} = \int d^3r \mathcal{F}(\mathbf{r}), \quad (2)$$

where $\mathcal{F}(\mathbf{r})$ is the free-energy density of a block of size d^3r centered at the point labelled by \mathbf{r} . Note that we have replaced the sum over blocks by an integral, as the free-energy density varies slowly from one block to another. The only \mathbf{r} - and ω -dependence of $\mathcal{F}(\mathbf{r})$ is through the local chemical potential $\mu(\mathbf{r}) = \mu - \frac{1}{2}m\omega^2(x^2 + y^2 + \lambda^2z^2)$ and, therefore, $\mathcal{F}(\mathbf{r}) = f(\omega x, \omega y, \omega \lambda z)$. Thus

$$F = \frac{1}{\lambda\omega^3} \int d^3\tilde{r} f(\tilde{r}), \quad (3)$$

where $\tilde{x} = \omega x$, $\tilde{y} = \omega y$ and $\tilde{z} = \lambda\omega z$. Note that the function $f(\tilde{r})$ has no ω -dependence. We immediately see that the free energy per particle F/N is finite in the limit $N \rightarrow \infty$, $\omega \rightarrow 0$, $N\omega^3$ fixed. Thus the properties of the high-temperature phase are related trivially to the corresponding properties of the uniform system.

This approach will fail if the correlation length in some of the blocks becomes bigger than the block size. For a small but non-zero ω , this would happen close enough to a critical point. *The true thermodynamic behaviour is accessed by first sending ω to zero and then approaching the critical point.* When the limits are taken in this order, the block sizes can always be taken larger than the correlation lengths and so eqs. (2) and (3) remain valid all the way up to a critical point. It is now easy to see that there is indeed a phase transition at a finite non-zero value of the temperature. As we have already seen, at high enough temperature there is a well-defined disordered phase; now consider the system at low enough temperature — there will always be some blocks with density bigger than the threshold value required for condensation at that temperature. These blocks will then become superfluid. Thus below a certain non-zero finite critical temperature the disordered phase is unstable to superfluid ordering.

The properties of the system in the critical regime can be obtained straightforwardly from equations like (2) and (3). The singular part of the free-energy density at point \mathbf{r} satisfies the hyperscaling relation ⁽³⁾ $\mathcal{F}(\mathbf{r}) = C/(\xi(\mathbf{r}))^3$, where $\xi(\mathbf{r})$ is the correlation length in the block centered at \mathbf{r} and C is a constant. For $\mu(\mathbf{r})$ sufficiently close to μ_c , the critical point of the uniform system, the correlation length diverges as $\xi(\mathbf{r}) \sim (\mu_c - \mu(\mathbf{r}))^{-\nu}$, where $\nu \simeq 0.67$ is the correlation length exponent of the three-dimensional XY universality class [8]. The total free energy is given by

$$F = \int d^3r \frac{C}{(\xi(\mathbf{r}))^3} + \dots \sim (\mu_c - \mu)^{3(\nu+\frac{1}{2})} + \dots \quad (4)$$

The integral is up to a value of r which is of the order of, but smaller than $\sqrt{k_B T/m\omega^2}$, and the ellipses denote terms regular in $\mu - \mu_c$. Note the extra factor of $\frac{3}{2}$ in the exponent. This is a consequence of the quadratic potential in the system and leads to a violation of naive hyperscaling. Now, at fixed density, $T - T_c$ is analytic in $\mu_c - \mu$ ⁽⁴⁾ and hence the singular

⁽³⁾ This is the statement that the free energy is of order $k_B T$ per correlation volume [8].

⁽⁴⁾ This is generally the case when the specific-heat exponent is negative, as happens here. See [10].

of F as a function of T is similar ($F \sim (T - T_c)^{3(\nu + \frac{1}{2})}$), and the specific exponent, obtained by taking two derivatives of F with T , is $2 - 3(\nu + \frac{1}{2}) \simeq -1.52$. This very weak singularity is likely to be masked by analytic background terms even if one could access the critical region.

The order parameter correlation function for two points separated by \vec{x} , in a block labelled by \mathbf{r} , for $x \gg \xi(\mathbf{r})$, is $G(\mathbf{r}; \mathbf{x}) \sim \exp[-x/\xi(\mathbf{r})]/x^{1+\eta}$, where η , the anomalous dimension, is approximately 0.03 in this case [8]. The order parameter susceptibility is given by the integral of the correlation function over both its arguments. The singular part of the order parameter susceptibility, χ (which is of physical importance in magnetic systems) varies as $(T - T_c)^{\frac{3}{2} - \nu(2-\eta)}$. This exponent is *positive* (approximately 0.18), implying that the susceptibility is *finite* at the transition (even though there is a divergent correlation length associated with the transition) in contrast to the uniform case.

We now consider the ordered phase. This phase is characterised by a non-zero expectation value for the Bose field Ψ . The magnitude of this order parameter will be spatially inhomogeneous (due to the confining potential), while its phase will be constant. First, we argue that there is indeed a well-defined ordered phase in the thermodynamic limit defined above. Again, we imagine that the entire system is divided into semi-macroscopic blocks as before. We expect that both the density and the magnitude of the order parameter have short-range correlations and hence their values in each block are determined by the local chemical potential ⁽⁵⁾. This immediately implies that the total number of particles scales as $1/\omega^3$. Similarly, we also expect the free-energy density to be determined just by the local chemical potential, and hence the total free energy also scales as $1/\omega^3$. Thus the free energy per particle is again finite in the thermodynamic limit.

Since the local chemical potential is a maximum at the center of the trap, the magnitude of the order parameter will be the largest at the center and will decrease as one moves away from the center. It eventually becomes zero when the local chemical potential becomes smaller than μ_c . The position of this edge, denoted by \mathbf{r}_c , is given by $\mu(\mathbf{r}_c) = \mu_c$. Near the edge, $|\langle \Psi \rangle| \sim (\mu(\mathbf{r}) - \mu_c)^\beta \sim (r_c - r)^\beta$, where $\beta \simeq 0.34$ is the usual order parameter exponent for the uniform system [8]. This is an important point as it may be possible to study *critical* properties of the system by studying it close to the edge of the condensate in the *ordered* phase.

The fraction of particles in the $k = 0$ mode, $n(k = 0)$ (which is of direct experimental significance) is proportional to $(\omega^3 \int d^3r |\langle \Psi(\mathbf{r}) \rangle|)^2$ in the thermodynamic limit. As one approaches the critical point from the ordered phase, the spatial extent of the condensed region shrinks to zero as $(\mu - \mu_c)^{\frac{1}{2}} \sim (T_c - T)^{\frac{1}{2}}$. The maximum value of the order parameter (*i.e.* at $r = 0$) vanishes as $(\mu - \mu_c)^\beta \sim (T_c - T)^\beta$. This implies that $n(k = 0) \sim (T_c - T)^{2(\beta + \frac{3}{2})} \sim (T_c - T)^{3.68}$. An explicit calculation of the order parameter profile at $T = 0$ within a Hartree-Fock approximation was performed in ref. [11]. Note that the ‘‘Thomas-Fermi’’ approximation used there becomes exact away from the origin in the thermodynamic limit we have discussed. An extension of such a calculation to the critical regime [6] provides an illustration of the general discussion above (see also ref. [12]).

As before, the free energy is determined completely once the free-energy density of the uniform system is known as a function of μ . Thus the low-temperature specific heat is proportional to T^3 , as in the uniform case, though the prefactor will be different.

The phase of the order parameter, of course, has long-range correlations. Associated with slow variations of this phase, we have the usual sound wave. The character of this mode is not different from the uniform case as long as the wavelength is small compared to a typical block

⁽⁵⁾For this to be true, we must require that the size of any block is much bigger than the local Josephson correlation length.

size. The sound wave velocity will be determined in the usual way by the local superfluid density and compressibility. This spatial variation will cause the wave to be “refracted” as it propagates.

The critical behaviour described above will become observable only in a window around T_c which is given by the Ginzburg criterion [8] (see footnote ⁽¹⁾). This predicts that the system crosses over to the critical regime when $\xi \sim \lambda_T^2/a$, where $\lambda_T = (\hbar^2/2mk_B T)^{1/2}$ is the thermal de Broglie wavelength and a is the scattering length. This corresponds to $|(T - T_c)/T_c| \sim (a/\lambda_T)^2 \sim 10^{-3}$ – 10^{-4} for the Rb [1] and Na [3] experiments. Outside of this window in the high-temperature phase, the behaviour of the system can be well approximated by the thermodynamic limit of the ideal Bose gas in a harmonic potential and the calculations of [13] are expected to apply.

A small but non-zero value of ω leads to deviations from the theory described above, which is valid in the thermodynamic limit. “Finite-size” corrections are most significant near the critical point where the non-zero ω rounds off any singular behaviour of physical quantities. A crude estimate of the width of this region where finite-size effects are important may be obtained as follows: Near the bottom of the well, the correlation length varies appreciably over a length $r \sim \sqrt{(\mu_c - \mu)/(m\omega^2)}$. Finite-size effects will be negligible so long as this length is much larger than $\xi(r=0)$. In the high-temperature phase, by using the ideal Bose gas expression for $\xi(r=0)$, this can be converted to the condition $(T - T_c)/T_c < \hbar\omega/(k_B T_c) \sim 10^{-2}$. A similar estimate is expected to hold below T_c as well. Note that this window is at least an order of magnitude bigger than the temperature range where the system crosses over to the critical regime. Thus “finite-size” effects will prohibit observation of the true critical behaviour in the current range of experimental parameters. Increasing the scattering length and/or decreasing the frequency of the trap will enhance the possibility of measuring critical properties.

So far we have restricted ourselves to the equilibrium properties of the system. However, an interesting question which may also be experimentally relevant [1] is: How does the condensate grow in time to its final equilibrium value after a rapid quench in temperature from above T_c to below? This non-equilibrium question has been addressed recently [4] for a translationally invariant Bose gas. It was shown that the standard phenomenology of phase-ordering kinetics [14] (which predicts, at late times, the existence of a single time-dependent length scale $\sim t^{1/2}$) can be used to obtain a scaling form for the equal-time correlation function of the boson field Ψ :

$$G(r, r', t, L) \equiv \langle \psi^*(r, t)\psi(r', t) \rangle = |\langle \psi \rangle|^2 F\left(\frac{|r - r'|}{L}, \frac{ct}{L^z}\right), \quad (5)$$

where L is the linear size of the system, c is a scale factor that depends on the final temperature (or equivalently, the final chemical potential), $\langle \psi \rangle$ is the equilibrium order parameter at that temperature and $|r - r'|$ is much larger than all microscopic scales in the problem. The value of z was numerically estimated to be close to 1 and it was argued that z should be exactly equal to 1 [4].

We now consider the effect of the confining potential on this dynamics. Imagine, as before, splitting the system up into many blocks (of size $l \sim 1/\omega$) such that the potential does not vary significantly within any block. As long as $t^{1/2} \leq l$, the equal-time correlation function within each block scales as

$$G(r, r', t, \omega) = |\langle \psi(R\omega) \rangle|^2 H(|r - r'|_\omega, c'(R\omega)t\omega^z), \quad (6)$$

where R is the coordinate of the center of the block, c' is a scale factor that depends on the local chemical potential and the value of z is *unchanged* from the translationally invariant case. Motivated by this, we can now make the following ansatz for the scaling form valid for

arbitrarily large values of t and $|r - r'|$ (in particular, r and r' may belong to different blocks):

$$G = P(r\omega, r'\omega, t\omega^z), \quad (7)$$

where z is *the same as before*. Note that as $t \rightarrow \infty$ P must reduce to $\langle \psi(r) \rangle \langle \psi^*(r') \rangle$ which is consistent as $\langle \psi(r) \rangle$ depends on r only through $\mu(\omega r)$.

The total number of particles in the $k = 0$ mode is proportional to $\omega^3 \int d^3r \int d^3r' P$ and thus satisfies the scaling form

$$n(k = 0, t) = \omega^{-3} f(t\omega^z). \quad (8)$$

The fraction of particles in the $k = 0$ mode is given as $n(k = 0, t)/N = (1/(N\omega^3))f(t\omega^z)$. The function f , of course, depends on the value of temperature we quench to and the value of the anisotropy λ . We thus conclude that the time dependence of $n(k = 0)/N$ for fixed T , $N\omega^3$ and λ but different values of ω *should exhibit scaling collapse at late times*. For small values of its argument $f(x) \sim x^{\frac{3}{z}}$. For small enough ω (*i.e.* for a large enough system) it may be possible to observe a corresponding window in time in which *the condensate fraction has power law growth* $n(k = 0, t)/N \sim t^{\frac{3}{z}}$.

In summary, we have presented a rather complete understanding of the effects of the confining potential on the equilibrium properties of a Bose gas. In particular, we have demonstrated that the critical properties of the system in a confining potential are different from but simply related to the uniform case. We have also provided a scaling description for the late-time universal dynamics following a rapid quench to the ordered phase.

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