Magnetic Properties of a Bose-Einstein Condensate

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Three hyperfine states of Bose-condensed sodium atoms, recently optically trapped, can be described as a spin-1 Bose gas. We study the behaviour of this system in a magnetic field, and construct the phase diagram, where the temperature of the Bose condensation $T_{BEC}$ increases with magnetic field. In particular the system is ferromagnetic below $T_{BEC}$ and the magnetization is proportional to the condensate fraction in a vanishing magnetic field. Second derivatives of the magnetization with regard to temperature or magnetic field are discontinuous along the phase boundary.

Recently experimentalists confined three $f = 1$ hyperfine states of sodium in an optical trap [1]. This was impossible to do in a magnetic trap, which confines only one hyperfine state [2]. One can ask what are the properties of an $f = 1$ Bose-Einstein condensate in a magnetic field. In a weak magnetic field $H$ the electron $s$ and nuclear $i$ magnetic moments precess around $f$ and $f$ precesses around $H$. A simple calculation [3] gives that the average of the projection of the electron spin on the direction of the magnetic field (z-direction) is:

$$\bar{s}_z = \frac{m_f}{2f(f+1)}[f(f+1) - i(i+1) + j(j+1)]. \quad (1)$$

Sodium has a nuclear spin $i = \frac{3}{2}$ and electron spin $s = \frac{1}{2}$; and the electron is in an $l = 0$ state, so that $j = s$. Substituting these values in Eq. (1), we obtain:

$$\bar{s}_z = -\frac{1}{4}m_f. \quad (2)$$

The magnetic moment of the nucleus is negligible in comparison to that of the electron. Therefore, the system is equivalent to a spin-1 boson, with magnetic moment 4 times less than that of the electron. The projection of the magnetic moment on z-direction is:

$$\bar{\mu}_z = -2\mu_B \bar{s}_z = \frac{\mu_B}{2}m_f, \quad (3)$$

where $\mu_B$ is the Bohr magneton. As the hyperfine interactions are of the order of GHz, magnetic field much less than $GHz/\mu_B \approx 100$Gs is small.

As the densities of the Bose condensates of atomic vapes are very small, one can treat them as an ideal gas. We shall return to the validity of this assumption below.

An immediate observation is that the system is ferromagnetic [1], when Bose-condensed, as the condensate is aligned with the external magnetic field however small it is. Another observation is that the external magnetic field increases the temperature of the Bose condensation. A spin-$s$ Bose gas has a critical temperature which is $(2s+1)^{2/3}$ times less than a spin-0 one at the same density, due to the $2s+1$ spin states available for excitations. At high magnetic fields the gas is completely spin polarized and therefore equivalent to a spin-0 Bose gas, and has the same critical temperature as the latter. The aim of this paper is to construct the phase diagram of the system, to find the condensate density and magnetization as a function of temperature and magnetic field and investigate singularities of the latter along the phase boundary.

The number of particles in excited states is given by a standard formula [4] modified to include 2 extra spin states:

$$n_{ex} = \frac{(m_e T)^{3/2}}{\sqrt{2\pi^2\hbar}} \left[ \frac{\int_0^\infty \sqrt{z} dz}{e^{\alpha z} - 1} + \frac{\int_0^\infty \sqrt{z} dz}{e^{\alpha z + \gamma} - 1} + \int_0^\infty \frac{\sqrt{z} dz}{e^{\alpha z + 2\gamma} - 1} \right]. \quad (4)$$

Here

$$y = \frac{(\mu_B/2)H}{T}, \quad a = -\mu/T, \quad (5)$$

$\mu$ is the chemical potential and $m_e$ is the mass of the bosonic atom. The integrals in Eq. (4) can be rewritten following [5] as

$$\int_0^\infty \frac{\sqrt{z} dz}{e^{\alpha z} - 1} = \sqrt{\frac{\pi}{2}} \sum_{n=1}^\infty \frac{e^{-nx}}{n^2} = \frac{\sqrt{\pi}}{2} F_{\alpha}(x), \quad (6)$$

with $F$ defined as:

$$F_\alpha(x) = \sum_{n=1}^\infty e^{-nx}/n^\alpha, \quad (7)$$

which reduces to the Riemann function for $x = 0$: $F_\alpha(0) = \zeta(\alpha)$. Let us introduce new variables:

$$T_0 = T_{BEC}(H = 0) = \frac{2\pi \hbar^2}{(3\zeta(\frac{3}{2}))^{2/3} m_e^{1/3}}, \quad (8)$$

$$t = T/T_0, \quad b = \frac{(\mu_B/2)H}{T_0},$$

where $n_0$ is the total particle density.
Substituting this in Eq. (9) we obtain:

\[ n_{\text{ex}}/n_0 = \frac{t_f^2}{3 \zeta(2)} \left( F_{\frac{3}{2}}(a) + F_{\frac{3}{2}}(a + y) + F_{\frac{3}{2}}(a + 2y) \right). \]  

(9)

Here, as in the familiar spin-0 boson case [3], [4], \( a = 0 \) when \( n_{\text{ex}}(a = 0, t, y)/n_0 \leq 1 \) and \( a \) is determined from \( n_{\text{ex}}(a, t, y)/n_0 = 1 \) otherwise.

The temperature, \( t_c \) of BEC is obtained by equating the number of particles in excited states \( n_{\text{ex}} \) to the total number of particles: \( n_{\text{ex}} = n_0 \) at zero chemical potential. Substituting this in Eq. (9) we obtain:

\[ 1 = \frac{t_c^2}{3 \zeta(2)} \left( \zeta\left(\frac{3}{2}\right) + F_{\frac{3}{2}}(y) + F_{\frac{3}{2}}(2y) \right). \]  

(10)

This gives the phase diagram in a parametric form. In order to obtain it explicitly, one computes numerically \( t_c(y) \) from Eq. (10) and then finds \( b_c(y) = y/t_c(y) \). To obtain the condensate density, \( n = n_{\text{BEC}}/n_0 \), contour lines, we replace 1 in the left hand side of Eq. (10) with \( 1 - n \). Then for given \( y \) we get \( t_n = t_c(1 - n)^{2/3} \) and \( b_n = y/t_n(y) = b_c(y)/(1 - n)^{2/3} \). Therefore the condensate density contour lines are obtained from the phase transition line by a rescaling. The results are shown in Fig. 2. For small or large \( b \) one can find the asymptotic behavior of Eq. (10):

\[ t_c \sim 3^{2/3} \frac{2}{3^{1/3} \zeta\left(\frac{3}{2}\right)} \exp(-b/3^{2/3}), \text{when } b \gg 1. \]  

(11)

When \( b \to \infty \) all atoms are in the \( m_f = 1 \) state which is equivalent to having a spin-0 Bose gas at the same density, resulting in an increase of \( t_c \) by a factor of \( 3^{2/3} \).

The condensate fraction \( n = n_{\text{BEC}}/n_0 = 1 - n_{\text{ex}}/n_0 \), computed using Eq. (9) as a function of magnetic field or temperature is shown in Fig. 2. Asymptotically, the condensate density is \( n(b = 0) = 1 - t^{1/2} \) and \( n(b) - n(b = 0) \sim t \sqrt{b} \) for \( t \leq 1 \) and \( b \ll 1 \). For \( t > 1 \), \( n \) is linear in \( b - b_c \).

To calculate the magnetization per particle, \( m \), we note that (in units of \( \frac{\mu_B}{n_0} \)):

\[ m = \frac{(n(m_f = 1) - n(m_f = -1))/n_0}. \]  

(12)

This expression is inconvenient because there are both condensate and excited atoms in the \( m_f = 1 \) state. Taking into account that \( n(m_f = 1) + n(m_f = 0) + n(m_f = -1) = n_0 \), one has \( m = 1 - n(m_f = 0) - 2n(m_f = -1) \), or:

\[ m = 1 - \frac{t_f^2}{3 \zeta(2)} \left( F_{\frac{3}{2}}(a + y) + 2F_{\frac{3}{2}}(a + 2y) \right). \]  

(13)
FIG. 3. (a) Magnetization, \( m \), as a function of temperature \( t \equiv T/T_0 \) for several values of the magnetic field \( b \equiv (\mu_B/2)H/T_0 = 0, 0.01, 0.1, 0.3, 1, 3 \), from left to right). Dashed line is \( m(b_c(t), t) \). (b) derivatives of the \( m(t) \) curves in (a) with regard to temperature. The cusp is at the critical temperature.

Asymptotically:

\[
m = 1 - t^2, \quad (14)
\]

when \( b = 0^+ \), that is the magnetization is proportional to the condensate density in a vanishing field, and

\[
m \sim \sqrt{b}, \quad (15)
\]

when \( t = 1 \), \textit{i.e.} at the phase transition.

When \( b \) is finite, the magnetization is no longer zero in the normal phase, however BEC appears in a cusp in the derivatives \( \left( \frac{\partial m}{\partial t} \right) \) and \( \left( \frac{\partial m}{\partial b} \right) \), see Figures 3 and 4, where these curves were computed numerically, using equations (A1) and (A4). In other words, second derivatives of the magnetization are discontinuous along the phase boundary (see Equations (A5) and (A6)).

We have studied the magnetization of the Bose-ferromagnet in a vanishing but non zero magnetic field. A question remains what happens for strictly zero field. In the case of Bose condensate of \( N \) spin-1 particles projection of the magnetization per particle, \( m \) (in units of particle’s magnetic moment) on the z-axis is equal to \( m_z \), which satisfies the obvious restriction

\[
N(1) + N(0) + N(-1) = N, \quad (17)
\]

have equal probability. \( m_z = 1 \) is achieved only when \( N(1) = N, N(0) = 0, N(-1) = 0 \), while \( m_z = 0 \) can be achieved by many combinations: \( N(1) = 0, N(0) = N, N(-1) = 0 \), or \( N(1) = 1, N(0) = N - 2, N(-1) = 1 \) and so on. One can show by a generalization of this argument that the probability distribution is

\[
P_z(m_z) = 1 - |m_z|. \quad (18)
\]

To find how the absolute value of \( m \) is distributed we notice that the magnetization is macroscopic and therefore can be treated classically. Now if we know the distribution of its projection on the z-axis \( P_z(m_z) \), we can find the distribution of the absolute value \( P(m) \). Taking into account that the projection of a vector of unit
length uniformly distributed on a sphere is uniformly distributed between \(-1\) and \(+1\), we can write:

\[
P_z(m_z) = \int_{-1}^{1} dmP(m) \frac{1}{2} \int_{-1}^{1} dx \delta(mx - m_z) = \int_{m_z}^{1} dmP(m)/(2m).
\]  

By differentiating this equation with respect to \(m_z\) we get:

\[
P(m) = -2mP'(m),
\]  
or, taking into account Eq. (18)

\[
P(m) = 2m.
\]

These distributions are shown in Fig. 5. Let us compare this with classical systems. For instance in the familiar case of an Ising ferromagnet below the phase transition temperature the probability distribution of the magnetization consists of two one-half delta functions at positive and negative values of the magnetization. Applying a magnetic field changes this distribution to a single delta function. For the case of the Heisenberg ferromagnet magnetization can point in any direction, however the probability distribution of the absolute value of the magnetization is a delta function, an infinitely small external magnetic field will select the direction of the magnetization. In the case of a Bose-ferromagnet, an infinitely small applied magnetic field will not only select the direction, but also change the form of the probability distribution function of the magnetization from that of Fig. (b) to delta-function.

The experiments are done in a trap, which can be modeled by a weak external potential. It was shown that interatomic interactions, however small, have a strong effect on the properties of the condensate, when it is in an external potential. The effect is that the Bose condensate is not in the single-particle ground state of the potential, which has small spatial extent, but its wave function is spread to balance the interatomic repulsions and confining potential. The density of the condensate is then determined from this balance. Once it is determined, it is a reasonable approximation to treat the gas as ideal at \(\mu\)K, as if it was in a square box, which is in the optical trap \(
\sim 10^{15}/\text{cm}^3
\). This makes \(t = 1\) in our figures to be of the order of \(\mu\)K and \(b = 1\) of the order of 0.1Gs (which is also much less than the weak field requirement of 100Gs mentioned in the beginning of the paper). At this density spin-spin interactions are a few orders of magnitude less than the spin energy in a magnetic field, and can therefore be neglected. A disadvantage of this low density is that the magnetization is very small and difficult to observe directly. However one can measure the populations of the hyperfine states and calculate the magnetisation from Eq. (2).

Exchange interactions have been found to be important in a related problem of a charged spin-0 Bose gas (which is diamagnetic when Bose-condensed). In our case they also have a profound effect and change the order of the transition from second to first. The previous discussion was of ideal Bose gas in an external magnetic field. As we argued, fields of the order of 0.1 Gs (which are also of the order of the magnetic field of the Earth) will dominate over exchange interactions, so the effect of the latter may not be observed. However, if the external field is screened down to \(10^{-4}\text{Gs}\) they may play a role. We shall now address the case of a Bose gas with ferromagnetic exchange interactions. Without ferromagnetic exchange the system undergoes a conventional Bose condensation, while without Bose statistics it undergoes a conventional ferromagnetic transition. This system is characterized by two parameters: the Bose condensation temperature \(T_{bc}\), when ferromagnetic exchange is neglected, and the ferromagnetic transition temperature \(T_f\), when the effects of the Bose statistics are neglected. The behaviour of the system will depend on the ratio \(\kappa = T_f/T_{bc}\). The details and the complete phase diagram will be reported in a future publications, here we shall give an essential result. If \(\kappa > \kappa_c\), where \(\kappa_c\) is close to 1, that is in the case of strong ferromagnetic
interactions, upon cooling, the system undergoes first a ferromagnetic transition and then at a lower temperature a Bose condensation. Both transitions are of second order. If $\kappa < \kappa_c$ then two transitions merge into a single Bose-ferromagnetic phase transition, which is of first order. Estimates show that for the condensates, experimentalists are currently working with, $\kappa << \kappa_c$.

A few final remarks. Since in a vanishing field the condensate carries magnetization while the normal component does not, superflow is accompanied by a transfer of the magnetization. In particular, second sound condensate carries magnetization while the normal component ferromagnets. Similarly, a charged Bose gas would undergo a Bose-Einstein condensation. Both transitions are of second order, upon cooling, the system undergoes first a transition to a magnetic state, followed by a transition to a superfluid state. The authors acknowledge helpful discussions with J.T. Liu, H.C. Ren and J. Stenger. This work was supported by the Department of Energy Contract No. DE-F602-88-ER13847.

APPENDIX:

From Eq. (13) one obtains:

$$\left( \frac{\partial m}{\partial t} \right)_b = - \frac{t}{\zeta(\frac{3}{2})} \left[ \frac{1}{2} F_{\frac{1}{2}}(a + y) + F_{\frac{3}{2}}(a + 2y) + \frac{y}{3} F_{\frac{1}{2}}(a + y) + 4F_{\frac{1}{2}}(a + 2y) - \frac{1}{3}(F_{\frac{1}{2}}(a + y) + 2F_{\frac{1}{2}}(a + 2y)) \right] \left( \frac{\partial a}{\partial t} \right)_b .$$ (A1)

Where $(\frac{\partial a}{\partial t})_b$ can be found from Eq. (10) to be:

$$t \left( \frac{\partial a}{\partial t} \right)_b = \left[ \frac{3}{2}(F_{\frac{1}{2}}(a) + F_{\frac{3}{2}}(a + y) + F_{\frac{1}{2}}(a + 2y)) + y(F_{\frac{1}{2}}(a + y) + 2F_{\frac{1}{2}}(a + 2y)) \right]^{-1} .$$ (A2)

Now $(\frac{\partial m}{\partial t})_b$ can be found numerically from Eqs. (A1), (A2), with $a$ from Eq. (10). To find the discontinuity in the $\frac{\partial^2 m}{\partial t^2}$ at the phase transition we note that when $a = 0$: $(\frac{\partial^2 m}{\partial t^2})_b = 0$ (Cf. Eq. (A2), taking into account that $F_{\frac{1}{2}}(0) = \infty$). Therefore the discontinuity comes only from the second derivative of $a$. We find for the jump:

$$\Delta \frac{\partial^2 m}{\partial t^2} = \frac{1}{6\pi \zeta(\frac{5}{2})} \left[ \frac{3}{2} \zeta(\frac{3}{2}) + F_{\frac{1}{2}}(y) + F_{\frac{3}{2}}(2y) \right] \left( \frac{\partial a}{\partial t} \right)_b .$$ (A3)

This has asymptotics $\Delta \frac{\partial^2 m}{\partial t^2} \sim b^{-\frac{1}{2}}$ for $b \ll 1$ and $\Delta \frac{\partial^2 m}{\partial t^2} \sim \exp(-b/3)\frac{t}{\zeta(\frac{5}{2})}$ for $b \gg 1$.

Derivatives with regard to the magnetic field can be done analogously, leading to:

$$\left( \frac{\partial m}{\partial b} \right)_t = - \frac{t}{3\zeta(\frac{5}{2})} \left[ F_{\frac{1}{2}}(a + y) + 4F_{\frac{1}{2}}(a + 2y) \right] + (F_{\frac{1}{2}}(a + y) + 2F_{\frac{1}{2}}(a + 2y)) \left( \frac{\partial a}{\partial b} \right)_t .$$ (A4)

$$t \left( \frac{\partial a}{\partial b} \right)_t = - \frac{F_{\frac{1}{2}}(a + y) + 2F_{\frac{1}{2}}(a + 2y)}{F_{\frac{1}{2}}(a) + F_{\frac{1}{2}}(a + y) + F_{\frac{1}{2}}(a + 2y)} .$$ (A5)

$$\Delta \frac{\partial^2 m}{\partial b^2} = \frac{1}{6\pi \zeta(\frac{5}{2})} \left[ F_{\frac{1}{2}}(y) + 2F_{\frac{1}{2}}(2y) \right] \left( \frac{\partial a}{\partial b} \right)_t .$$ (A6)

This has asymptotics $\Delta \frac{\partial^2 m}{\partial b^2} \sim -\frac{1}{(t-1)^2}$ for $t - 1 \ll 1$ and $\Delta \frac{\partial^2 m}{\partial b^2} \sim -(3\frac{t}{\zeta(\frac{5}{2})} - t)^3$ for $3\frac{t}{\zeta(\frac{5}{2})} - t \ll 1$.

One can show similarly that $\frac{\partial^2 m}{\partial ab}$ is also discontinuous along the phase boundary.

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