Ferromagnetic phase transition and Bose-Einstein condensation in spinor Bose gases

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(Dated: March 22, 2022)

Phase transitions in spinor Bose gases with ferromagnetic (FM) couplings are studied via mean-field theory. We show that an infinitesimal value of the coupling can induce a FM phase transition at a finite temperature always above the critical temperature of Bose-Einstein condensation. This contrasts sharply with the case of Fermi gases, in which the Stoner coupling $I_s$ can not lead to a FM phase transition unless it is larger than a threshold value $I_0$. The FM coupling also increases the critical temperatures of both the ferromagnetic transition and the Bose-Einstein condensation.

PACS numbers: 05.30.Jp, 03.75.Mn, 75.10.Lp, 75.30.Kz

The magnetism of Fermi (electron) gases has long been a research topic in solid state physics. Although many open questions remain, the magnetic properties of Fermi gases have been well understood. The Fermi surface plays an important role in determining their magnetism. For example, a magnetization density $M$ in Fermi gases increases the band energy by splitting the Fermi surfaces for spin-up and spin-down particles. As a result, Fermi gases mainly behave as Pauli paramagnets in the absence of an exchange interaction. If an effective ferromagnetic (FM) exchange $I_s$ is present, electron gases can exhibit ferromagnetism. Within the framework of the Stoner theory, $I_s$ results in a negative molecular field energy when $M$ is finite. If $I_s > I_0$, the Stoner threshold, the value of the molecular field energy becomes larger than that of the increase of the band energy induced by $M$, and then a FM ground state is energetically favored.

The magnetism of Bose gases has been less studied. But since the realization of Bose-Einstein condensation (BEC) in ultracold atomic gases, more and more attention has been attracted to this topic, because the constituent atoms, such as $^{87}$Rb, $^{23}$Na, and $^7$Li usually have (hyperfine) spin degrees of freedom and thus a magnetic moment $m$. $m$ can be large in atoms such as $^{52}$Cr, for which $m = 6\mu_B$, where $\mu_B$ is the Bohr magneton. Since 1998, atomic gases can be confined and cooled in purely optical traps in which their spin degrees of freedom remain active, and therefore investigating their magnetic properties becomes experimentally possible.

Ferromagnetism in spinor bosons without any spin-dependent interactions has already been theoretically studied. As opposed to the case of fermions, the ground states of spinor bosons are degenerate and a ferromagnetic state is among the ground states. Furthermore, the spinor Bose gas is rather apt to be magnetized by an external magnetic field even at a finite temperature $T$, as long as $T < T_c$, the BEC critical temperature, regardless of the size of the coupling. This contrasts sharply with the case of fermions. Figure 1 shows schematically the relation between $T_F$ and $I_s$ for both Bose and Fermi gases. More recently, Isoshima et al. studied BEC in trapped $F = 1$ spinor bosons with FM couplings, but the FM transition was not considered.
The model.— Following the Stoner theory for fermion gases, a molecular field $H_m = I_s \overline{M}$ is introduced to describe the effective FM coupling between bosons, and the energy shift arising from the molecular field is

$$\epsilon_i^m = -H_m S_i^z = -I_s \overline{M} S_i^z. \quad (3)$$

The molecular field contains all the spin-dependent interactions. It can be derived from the exchange interactions via the mean-field approximation. In order to avoid the spin-spin interaction of a particle with itself, we treat the particles as being on some kind of “lattice”,

$$-\sum_{(ij)} S_i \cdot S_j \approx -\sum_{(ij)} (\langle S_i \rangle \cdot S_j + S_i \cdot (\langle S_j \rangle - \langle S_i \rangle)) = -Z \overline{M} \sum_i S_i^z + \frac{1}{2} Z N \overline{M}^2, \quad (4)$$

where $Z$ is the effective “coordination number”, which for a gas is an irrelevant dimensionless parameter of order unity, and $N$ is the number of sites. Therefore $I_s = Z I_H$ for the Hamiltonian in Eq. (2). $\overline{M} = \langle S_i \rangle$ serves as the ferromagnetic order parameter. We investigate a spinor Bose gas with hyperfine spin-$F$ and set the boson magnetic moment to unity. It is convenient to choose $\langle S_i \rangle = (0, 0, \overline{M})$ and $\overline{M}_i = \langle S_i^z \rangle = \sum_\sigma \sigma \langle \psi_i^\dagger \psi_i \rangle$ where $\psi_i$ annihilates a boson with spin quantum number $\sigma$ at site $i$. We take $\overline{M} = \overline{M}$ for a homogeneous boson gas.

Our main purpose is to show how the FM coupling affects the properties of spinor bosons. So we neglect spin-independent interactions for simplicity. Then the effective Hamiltonian for the grand canonical ensemble reads

$$H - N \mu = \sum_{k\sigma} [\epsilon_k - \mu - \sigma (H_m + H_e)] n_{k\sigma}, \quad (5)$$

where $\epsilon_k = \hbar^2 k^2 / 2m^*$ is the kinetic energy of free particles with mass $m^*$, $\mu$ is the chemical potential, and $H_e$ is the external magnetic field. Since the Hamiltonian is diagonal, we may calculate the grand thermodynamical potential

$$\Omega = -\frac{1}{\beta} \ln Z = -\frac{1}{\beta} \text{Tr} e^{-\beta (H - N \mu)}, \quad (6)$$

where $Z = \text{Tr} \{ \exp [-\beta (H - N \mu)] \}$ is the partition function, and $\beta = 1/(k_B T)$. The density of particles is

$$n = \frac{1}{V} \left( \frac{\partial \Omega}{\partial \mu} \right)_{T, V} = \frac{1}{V} \sum_{k\sigma} \langle n_{k\sigma} \rangle, \quad (7)$$

where $V$ is the volume of the system, $N$ is the total number of particles, and $\bar{n} = N/V$. $\overline{M}$ is determined self-consistently by

$$\overline{M} = -\frac{1}{V} \left( \frac{\partial \Omega}{\partial H_e} \right)_{T, V} = \frac{1}{V} \sum_{k\sigma} \sigma (n_{k\sigma}); \quad (8)$$

The external magnetic field $H_e$ is set to zero in the following calculations.

We now consider only $F = 1$ bosons. Eqs. (7) and (8) lead to the basic equations determining the phase diagram of the spin-1 boson system,

$$1 = n_0 + t^2 \left[ f_2(a) + f_2(a + b) + f_2(a + 2b) \right], \quad (9a)$$

$$M = n_0 + t^2 \left[ f_2(a) - f_2(a + 2b) \right], \quad (9b)$$

where $a = -\mu m / (k_B T)$, $b = H_m / (k_B T)$, the reduced temperature and coupling are given by $t = k_B T m^*/(2\hbar \pi^{2/3})$ and $I = I_s \overline{M}^2 / (2\pi \hbar^2)$, respectively. $n_0$ is the condensate density, $\overline{n} = n_0 / \overline{M}$ is the normalized magnetization, and $f_2(a)$ is the polylogarithm function defined as

$$f_2(a) \equiv \text{Li}_2(e^{-a}) = \sum_{p=1}^\infty \frac{(e^{-a})^p}{p^2}. \quad (10)$$

We note that $f_2(0) = \zeta(2)$, the Riemann zeta function.

Eq. (9a) is the standard formula for the density of bosons, by which the reduced BEC critical temperature $t_c$ can be determined. $a > 0$ for $t > t_c$ and $a \to 0$ as $t \to t_c$ from above. $\overline{n} > 0$ and $a = 0$ for $t < t_c$. In deriving Eq. (9b), we assume that only the spin-1 component of the bosons can condense. This assumption is discussed in the following.

Preliminary analyses.— Assuming a FM phase transition is induced by $I$ below the reduced transition temperature $t_F$, it is of special interest to determine the relation between $t_F$ and $I$. We first suppose $I$ is very large so that $t_F > t_c$. Provided that the FM transition is continuous, i.e., $b \to 0$ with $t \to t_F$, Eqs. (9) become

$$1 = 3t_F^2 f_2(a_F), \quad (11a)$$

$$1 = 2t_F^2 f_2(a_F). \quad (11b)$$
where $a_F = a(t_F)$. Equations (11) define a relation between $t_F$ and $I$. For a given $t_F$, $I$ is given by

$$I = \left[ \frac{3f_\frac{1}{2}(a_F)}{2f_\frac{3}{2}(a_F)} \right]^{\frac{1}{3}}.$$  \hfill (12)

$I$ is a monotonically decreasing function of $a_F$. As $a_F \to 0$, $f_\frac{1}{2}(a_F) \to \zeta(3/2) \approx 2.612$, and $f_\frac{3}{2}(a_F) \approx \sqrt{\pi/a_F}$. So for small values of $I$ and $a_F$ we have

$$a_F \approx 4\pi t_0 I^2,$$  \hfill (13)

where $t_0 = 1/[3\zeta(3/2)]^{2/3}$ is the reduced BEC critical temperature for the Bose gas with $I = 0$. Since $a_F$ is always larger than zero as long as $I$ is finite, Eq. (13) implies that an infinitesimal FM coupling can induce a FM phase transition at a finite temperature above the BEC critical temperature, because $a_F$ is finite only for $t > t_c$. We now calculate the asymptotic behavior of the relation between $t_F$ and $I$ for small couplings: $I \ll 1$. From Eqs. (11) we find

$$t_F \approx t_0 \left( 1 + \frac{8\pi^2}{3} I \right).$$  \hfill (14)

This equation shows that the FM transition temperature increases with the FM coupling.

By decreasing $t$ further, the Bose gas will undergo BEC. Due to the molecular field, the spin-1 bosons have the lowest free energy. So the condensate contains only the spin-1 component and the other two boson spin components remain in their excited states. Since $n_0 = 0$ at the BEC critical temperature, the self-consistent Eqs. (9) reduce to

$$1 = t_F^c \left[ \zeta(3/2) + f_\frac{1}{2}(b_c) + f_\frac{3}{2}(2b_c) \right],$$  \hfill (15a)

$$b_c^c = t_F^c \left[ \zeta(3/2) - f_\frac{3}{2}(2b_c) \right],$$  \hfill (15b)

where $b_c = b(t_c)$. These equations define the relation between $t_c$ and $I$. Since the FM phase transition occurs above $t_c$, the system has a finite magnetization at $t_c$. When $I < 1$ and $b_c$ is very small, Eq. (15a) leads to

$$t_c \approx 1 + \frac{4(1 + \sqrt{2})\sqrt{\pi b_c}}{9\zeta(\frac{3}{2})}.$$  \hfill (16)

Equation (16) is similar to the expression of the BEC critical temperature in an external magnetic field, but here $b_c \approx 8\pi t_0 I^2$ is not the external field, but is a self-consistently determined quantity proportional to the spontaneous magnetization. Substituting $b_c$ into Eq. (16), we find

$$t_c \approx 1 + \frac{8}{3} \left( 2 + \sqrt{2} \right) \pi t_0 I.$$  \hfill (17)

This equation indicates that the FM coupling also increases the BEC critical temperature.

Numerical results.– Comparing Eqs. (14) and (17), we see that $t_F$ is slightly smaller than $t_c$ for small FM couplings. This is unphysical and might be attributed to the assumption that the FM transition is continuous. To investigate this point, we solved the self-consistent Eqs. (9) numerically. The results obtained indicate that both the FM transition and the BEC become discontinuous if the FM coupling is sufficiently small.

Fig. 2 shows the phase diagram of spin-1 Bose gases. We first discuss the Bose-Einstein condensation. For
I \gtrsim I_c \approx 0.2$, $t_c = t_c^*$, as shown in the left inset, and both $a$ and $\pi_0$ are exactly determined to be zero at $t_c$, while $M$ has a finite value: $M(t_c) = M_c$. In this case, the results from Eqs. (15) agree perfectly with those obtained from Eqs. (9). With increasing $I$, $t_c(t_c^*)$ tends to the upper limit value $1/[\zeta(3/2)]^{2/3}$ which is the reduced BEC critical temperature of scalar bosons. Nevertheless, when $I < I_c$, the BEC becomes a discontinuous phase transition: $\pi_0$ has a small but nonzero value at $t_c^*$. In this case, $t_c^*$ is slightly larger than $t_c$, as the left inset shows. The fact that the Bose gas has a finite magnetization at $t_c(t_c^*)$ implies that a FM transition has taken place at a higher temperature as stated above. Fig. 3 shows the normalized magnetization $M_c$ at $t_c(t_c^*)$ versus the reduced FM coupling $I$.

Fig. 4 plots the order parameters of both phases. The normalized magnetization $M$ drops quickly with $t$ increasing above $t_c(t_c^*)$, and tends to zero at the reduced FM transition temperature $t_F^*$. $t_F^* = t_F$ when $I \gtrsim I_F \approx 0.35$, as shown in the right inset of Fig. 2. The smaller $I$ is, the more quickly the magnetization drops. When $I < I_F$, $M$ does not disappear continuously but drops from a finite value $M_F = M(t_F^*) \neq 0$ to zero abruptly at $t_F^*$, with $t_F^* > t_F$ as shown in the right inset of Fig. 2. This signals that the FM transition becomes first order. $M_F \approx 0.11$ for $I = 0.3$. In this case Eqs. (11) no longer hold. We determine $t_F^*$ for the coupling down to $I = 0.22$ and the results show that $t_F^* > t_c$, although $t_F < t_c$ when $I \lesssim 0.24$, as shown in the inset of Fig. 3. Hence the FM transition occurs at a higher temperature than the BEC. However, for small $I$, $t_F^*$ is so close to $t_c^*$ that it is very difficult to solve Eqs. (9) for the FM normal phase.

It is worth noting that the FM transition is continuous for large couplings. This point is consistent with the Weiss molecular field theory for classical particles, in which the FM transition is continuous. Because for large couplings, the FM transition occurs at a relatively high temperature, when the Bose statistics reduces to Boltzmann statistics.

In conclusion, we studied the ferromagnetic phase transition and Bose-Einstein condensation in spinor Bose gases with ferromagnetic couplings via mean-field theory. We showed that the coupling, regardless of its magnitude, induces a ferromagnetic phase transition at a temperature always above the critical temperature of Bose-Einstein condensation. Moreover, the ferromagnetic coupling also increases the critical temperatures of both phase transitions.

R.A.K. acknowledges partial support from the Max-Planck-Institut für Chemische Physik fester Stoffe.