Thermodynamic properties of the itinerant-boson ferromagnet

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Thermodynamics of a spin-1 Bose gas with ferromagnetic interactions are investigated via the mean-field theory. It is apparently shown in the specific heat curve that the system undergoes two phase transitions, the ferromagnetic transition and the Bose-Einstein condensation, with the Curie point above the condensation temperature. Above the Curie point, the susceptibility fits the Curie-Weiss law perfectly. At a fixed temperature, the reciprocal susceptibility is also in a good linear relationship with the ferromagnetic interaction.

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I. INTRODUCTION

The realization of spinor Bose-Einstein condensation in optical traps has stimulated enormous interest in optical properties of quantum Bose gases. In optical traps, the hyperfine degree of freedom of confined atoms, such as $^{87}$Rb, is released and therefore the atom can exhibit magnetism. More intriguingly, an exchange-like spin-spin interaction can be present between atoms. In the $F = 1$ $^{87}$Rb atoms, the interaction is ferromagnetic, so the $^{87}$Rb gas appears to be a prototype of itinerant-boson ferromagnet.

Ferromagnetism is one of the central research themes in condensed matter physics. Two types of ferromagnetism have already been intensively studied: local-moment ferromagnetism and itinerant-electron ferromagnetism. Although particles in these two systems obey different statistics, they both share some common features. For example, both ferromagnets have a Curie point, above which the susceptibility conforms to Curie-Weiss law. Nonetheless, from the theoretical point of view, the origin of Curie-Weiss law is quite different for these two systems. In insulators, it is due to local thermal spin fluctuations and can be easily explained in the mean-field approximation. On the other hand, in itinerant-electron ferromagnets the Curie-Weiss law may be caused by the mode-mode coupling between spin fluctuations and the theoretical treatment is much more complicated. An appropriate theory is the self-consistent renormalization (SCR) theory, which goes beyond the Hartree-Fock approximation and the random-phase approximation. TheSCR theory succeeds in explaining various magnetic properties of itinerant-electron ferromagnets and is also extended to treat the specific heat.

The $^{87}$Rb gas provides opportunity to study the third type of ferromagnetism. Hao, Ohmi and Machida have studied its ground state properties and the spin-wave spectrum. The long wavelength spectrum is linear in $k$, the wave vector, as in the two former cases. In our previous papers, we have investigated the finite-temperature properties, especially the Curie point. We suggest that the phase diagram in itinerant bosons should be more complicated than the other two ferromagnets, because the Bose system has an intrinsic phase transition, other than the ferromagnetic transition. An interesting conclusion we arrived is that its Curie point, $T_F$, is never below the Bose-Einstein condensation temperature, $T_C$, regardless of the magnitude of the ferromagnetic coupling. Kis-Szabo et al got the same point later. However, thermodynamics of the itinerant-boson ferromagnet has not yet been investigated systematically so far.

The purpose of this paper is to calculate the thermodynamic quantities of ferromagnetic bosons. As in the fermion case, the specific heat and magnetic susceptibility are of the most interest. In Section 2, we introduce the mean-field approximation to deal with ferromagnetic interaction, taking the spin-1 Bose gas as an example. In Section 3, phase transitions are discussed by calculating the free energy and specific heat. In Section 4, the susceptibility above the Curie point is calculated. A summary is given in the last section.

II. THE MEAN-FIELD APPROXIMATION

The spin-1 Bose gas with ferromagnetic couplings is described by the following Hamiltonian,

$$
\hat{H} = \sum_\sigma \int d\mathbf{r} \hat{\psi}_\sigma^\dagger (\mathbf{r}) \left( \frac{1}{2m} \nabla^2 - \sigma \hat{h}_c \right) \hat{\psi}_\sigma (\mathbf{r}) - \frac{1}{2} I_s \int d\mathbf{r} \mathbf{S}(\mathbf{r}) \cdot \mathbf{S}(\mathbf{r}),
$$

(1)

where $\hat{\psi}_\sigma (\mathbf{r})$ is the quantum field operator for annihilating an atom in spin state $| \sigma \rangle$ at site $\mathbf{r}$. For a spin-1 gas, $\sigma = +1, 0, -1$. The parameter $\hat{h}_c$ denotes the external magnetic field. The last term represents the ferromagnetic exchange between two different bosons meeting at site $\mathbf{r}$ and $I_s (> 0)$ is the exchange constant.

$\mathbf{S} = \{ \hat{S}^x, \hat{S}^y, \hat{S}^z \}$ are the spin operators, which can be expressed via the $3 \times 3$ Pauli matrices, for example,

$$
\hat{S}^z = \begin{pmatrix}
\hat{\psi}_{+1}^\dagger & \hat{\psi}_0^\dagger & \hat{\psi}_{-1}^\dagger
\end{pmatrix} \begin{pmatrix}
1 & 0 & 0 \\
0 & 0 & 0 \\
0 & 0 & -1
\end{pmatrix} \begin{pmatrix}
\hat{\psi}_{+1} \\
\hat{\psi}_0 \\
\hat{\psi}_{-1}
\end{pmatrix}.
$$

(2)

Within the mean-field approximation, we treat the spin-dependent interactions as a molecular field except of a
particle with itself,
\[ -\frac{1}{2} \mathbf{S} \cdot \mathbf{S} \approx -\langle \mathbf{S} \rangle \cdot \mathbf{S} + \frac{1}{2} \langle \mathbf{S} \rangle \cdot \langle \mathbf{S} \rangle = -\mathcal{M} \mathbf{S}^2 + \frac{1}{2} \mathcal{M}^2, \]
where \( \mathcal{M} = \langle \mathbf{S}^2 \rangle \) is the ferromagnetic order parameter. Then the effective Hamiltonian for the grand canonical ensemble reads,
\[ \hat{H} - \hat{N} \mu = \sum_{k\sigma} [\epsilon_k - \mu - \sigma (h_m + h_e)] \hat{n}_{k\sigma} + \frac{1}{2} \mathcal{M}^2 I_s N, \]
where \( \epsilon_k \) is the kinetic energy for free particles, \( h_m = I_s \mathcal{M} \) is called the molecular field, similar to the Stoner theory for ferromagnetism, \( \mu \) is the chemical potential; \( N \) is the total particle number. The grand thermodynamic potential can be worked out in a standard way,
\[ \Omega = -k_B T \ln \mathcal{T} \exp \left[ \frac{\hat{H} - \hat{N} \mu}{k_B T} \right] \]
\[ = -\frac{(k_B T)^2 V m^2}{(2\pi \hbar^2)^2} \sum_\sigma f_{\frac{1}{2}} \left( \frac{\mu + \sigma h}{k_B T} \right) + \frac{1}{2} \mathcal{M}^2 I_s N, \]
where \( h = h_m + h_e, \) \( m \) is the mass of particle, and \( f \) is the polylogarithm function defined by
\[ f_n(x) \equiv \sum_{k=1}^\infty \frac{(ex)^k}{k^n}, \]
where \( x \leq 0. \) The mean-field self-consistent equations are derived from the grand thermodynamic potential,
\[ n = -\frac{1}{V} \left( \frac{\partial \Omega}{\partial \mu} \right)_{T,V} + n_0 \]
\[ = \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \sum_\sigma f_{\frac{1}{2}} \left( \frac{\mu + \sigma h}{k_B T} \right) + n_0; \quad (7a) \]
\[ M = -\frac{1}{V} \left( \frac{\partial \Omega}{\partial h} \right)_{T,V} + n_0 \]
\[ = \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \left[ f_{\frac{1}{2}} \left( \frac{\mu + h}{k_B T} \right) - f_{\frac{1}{2}} \left( \frac{\mu - h}{k_B T} \right) \right] + n_0; \quad (7b) \]
where \( n \) is the density of particles, \( n_0 \) is the density of condensed one and \( M \equiv \frac{\mathcal{M}}{N} \) is the magnetization. \( n_0 \) is zero unless the temperature is below the BEC point \( T_c. \)

III. THE FREE ENERGY AND SPECIFIC HEAT

In our previous investigations, we showed that the system exhibits two phase transitions, the Bose-Einstein condensation (BEC) and the ferromagnetic transition.\(^{18,19}\) The condensation temperature \( T_c \) and the Curie temperature \( T_F \) are calculated by solving the self-consistent equations. We find that \( T_F \) is never below \( T_c \) for all systems with a finite ferromagnetic exchange \((I_s \neq 0)\).

However, one can get another solution to the Eqs. (7), with \( M = 0 \) at all temperatures. It means the system does not undergo a ferromagnetic transition at all, but remains in paramagnetic (PM) state at low temperatures. Actually, whether there exists a Curie point in the ferromagnetic Bose gases is still a controversial question. Some researchers suppose that the Bose gas can not be magnetized spontaneously at low temperatures even if the ferromagnetic exchange is present.\(^{20}\)

In order to single out the physically correct solution, one has to compare the free energy of the the ferromagnetic (FM) state and the PM state. The relation between the free energy and the grand thermodynamic potential has the form:
\[ F = \Omega + N \mu. \]

For computational convenience, the temperature \( T \) and exchange interaction \( I_s \) are re-scaled, as did in Ref. [8], by the following formula: \( t = [3 \zeta(\frac{3}{2})]^{-\frac{3}{2}} T / T_0 \) and \( I = [3 \zeta(\frac{3}{2})]^{-\frac{3}{2}} I_s / (k_B T_0) \), where
\[ T_0 = \frac{1}{k_B} \left( \frac{n}{3 \zeta(\frac{3}{2})} \right)^{\frac{3}{2}} \left( \frac{2\pi \hbar^2}{m} \right) \]
is the condensation temperature of ideal spin-1 Bose gas. Hereinafter, all the numerical results are obtained by setting \( n = k_B = \frac{2\pi \hbar^2}{m} = 1. \) Figure 1 shows the free energy of unit volume for the gas with \( I = 1.0. \) It shows clearly that the free energy of FM state is lower than that of the PM state at the low temperature region, which demonstrates that the FM state should be more stable than PM state. Therefore, the low temperature state has a spontaneous magnetization. In experiments, the total spin of the ferromagnetic spinor condensate is observed to be conserved, which is called the spin conservation rule in some literatures.\(^{13,14}\) However, the spin conservation rule holds only globally, not locally. In the theoretical
IV. THE CURIE-WEISS LAW

For a ferromagnet, the susceptibility above the Curie point is of special interest. As already studied, the susceptibility is well described by Curie-Weiss law both in the insulating ferromagnet and the itinerant-electron ferromagnet. In this section we calculate the susceptibility for the itinerant-boson ferromagnet.

The susceptibility can be derived from Eqs. (7). Differentiating both sides of the two equations and removing the term \( d\mu \), the following equation are deduced,

\[
dM = f d\left( \frac{I_s M + h_e}{k_B T} \right),
\]

where

\[
f = \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \left[ f_+^{\frac{1}{2}} \left( \frac{\mu + h}{k_B T} \right) + f_-^{\frac{1}{2}} \left( \frac{\mu - h}{k_B T} \right) \right] - \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \left[ f_+^{1} \left( \frac{\mu + h}{k_B T} \right) - f_-^{1} \left( \frac{\mu - h}{k_B T} \right) \right]^2
to\sum_{\sigma} f_+^{\frac{1}{2}} \left( \frac{\mu + h_e}{k_B T} \right) .
\]

Above the Curie point, the magnetization \( M \) (then \( h = I_s M + h_e \)) diminishes correspondingly when the external field \( h_e \) tends to zero. So the second term in the above equation is omitted and then \( f \) has a simple form:

\[
f \approx 2 \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} f_+^{1} \left( \frac{\mu}{k_B T} \right) .
\]

Thus the zero-field susceptibility of unit volume is given by

\[
\chi = \left( \frac{\partial M}{\partial h} \right)_{T,V} = \frac{1}{k_B T f^{-1} - n^{-1} I_s} .
\]

The susceptibility \( \chi \) is a function of the coupling \( I_s \) and temperature \( T \). Figure 3 shows \( 1/\chi \) and \( \chi \) versus \( I_s \) at different given temperatures. As shown in the inset of Fig. 3, the susceptibility becomes larger as the coupling \( I \) increasing. It is physically reasonable since the the system with larger \( I \) can be magnetized more easily. At a given temperature, \( \chi \) diverges as \( I \) approaches a critical value. It is worth noting that the inverse of the susceptibility is in a good linear relationship with the coupling.

The susceptibility versus temperature is shown in Fig. 4. One can immediately find that the susceptibility meet quite well with the Curie-Weiss law in a very large temperature region. Seeing that the Curie-Weiss law is very difficult to be derived for the itinerant-fermion ferromagnet, it is really surprising that we get it for the itinerant-boson ferromagnet just based on the mean-field approximation.

In order to discuss the Curie-Weiss law in a more explicit way, we proceed to carry out a semi-analytical calculation to deduce the linear dependence of \( 1/\chi \) on the
temperature. The first step is to analyze the temperature dependence of $f$. It is quite complicated, because the chemical potential $\mu$ is an implicit function of the temperature. We consider a limit case that the parameter $I_s$ is quite small, when $T_f$ is close to $T_c$. So $\mu$ is close to zero in the vicinity of $T_f$. According to the asymptotic behavior of the polylogarithm function: $f_{\frac{1}{2}}(x) \approx \zeta(\frac{1}{2}) - 2\sqrt{x}$ and $f_{\frac{1}{2}}(x) \approx \sqrt{x}$ as $x \to 0^-$, we get the following equations from Eqs. (7a) and (13) respectively,

$$n \approx 3 \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \left[ f_{\frac{1}{2}}(0) - 2\sqrt{\frac{\pi \mu}{k_B T}} \right].$$

and

$$f \approx 2 \left( \frac{k_B T m}{2\pi \hbar^2} \right)^{\frac{3}{2}} \sqrt{-\frac{k_B T \pi}{\mu}}.$$  

Substitute Eqs. (15) and (16) into Eq. (14), we get

$$\chi^{-1} = \frac{nk_B^2}{12\pi} \left( \frac{m}{2\pi \hbar^2} \right)^{\frac{3}{2}} T^{-\frac{1}{2}} \left( T_0^{-\frac{3}{2}} - T^{-\frac{3}{2}} \right) - n^{-1}I_s.$$  

In the vicinity of $T_F$ which is only slightly larger than $T_0$, Eq. (17) could be further simplified to

$$\chi^{-1} \approx \frac{nk_B^2}{8\pi} \left( \frac{m}{2\pi \hbar^2} \right)^{\frac{3}{2}} T_0^{-3} (T - T_0) - n^{-1}I_s$$

$$= \frac{9\zeta(\frac{3}{2})}{8\pi} n^{-1}k_B \left[ T - \left( T_0 + \frac{8\pi}{9\zeta(\frac{3}{2})k_B} I_s \right) \right].$$

Thus the effective FM transition temperature is defined as

$$T_f = T_0 + \frac{8\pi}{9\zeta(\frac{3}{2})k_B} I_s.$$  

So far the Curie-Weiss law is derived. We note that the derivation is only valid in small $I_s$ cases.

In the high temperature limit, one can also easily prove that $\chi^{-1}$ is linearly dependant on $T$. In this case, $-\frac{\mu}{k_B T}$ has a quite large value, so that

$$f_{\frac{1}{2}} \left( \frac{\mu}{k_B T} \right) \approx f_{\frac{1}{2}} \left( \frac{\mu}{k_B T} \right) \approx e^{\frac{\mu}{k_B T}}$$

according to Eq. (6). Combining Eqs. (7a), (13) and (14), it yields

$$\chi^{-1} = n^{-1}(k_B T - I_s).$$

We estimate this equation holds in the range of $t \gtrsim 10$.

V. SUMMARY

In summary, we calculate thermodynamic quantities of the spinor Bose gas with ferromagnetic interactions. Such kind of investigations has already been performed intensively for the ferromagnetic fermions, while few as yet for bosons. Based on a mean-field approximation, we show that the system undergoes a ferromagnetic phase transition first, then the Bose-Einstein condensation with the temperature decreasing. The specific heat shows a jump discontinuity at the Curie point and a bend at the Bose-Einstein condensation temperature, indicating that critical behaviors are different near the two transition. The more surprising result is that the mean-field theory yield the magnetic susceptibility which satisfies perfectly the Curie-Weiss law over a wide range of temperature.

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