Thermodynamic properties of the itinerant-boson ferromagnet

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Thermodynamics of a spin-1 Bose gas with ferromagnetic interactions is 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 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 (BEC) in optical traps[1,2] has stimulated enormous interest in magnetic properties of quantum Bose gases.[3–15] 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 exchangelike spin-spin interaction can be present between atoms. In the $F=1$ ^{87}Rb atoms, the interaction is ferromagnetic (FM),[3] so the ^{87}Rb gas appears to be a prototype of itinerant-boson ferromagnets.[4–8]

Ferromagnetism is one of the central research themes in condensed-matter physics.[16,17] 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 the Curie-Weiss law. Nonetheless, from the theoretical point of view, the origin of the 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.[17] An appropriate theory is the self-consistent renormalization (SCR) theory[18] which goes beyond the Hartree-Fock approximation and the random-phase approximation. The SCR theory succeeds in explaining various magnetic properties of itinerant-electron ferromagnets and is also extended to treat the specific heat.[19]

The ^{87}Rb gas provides the opportunity to study the third type of ferromagnetism. Ho[4] and Ohmi and Machida[5] studied its ground-state properties and the spin-wave spectrum. The long-wavelength spectrum is linear in $\mathbf{k}$, the wave vector, as in the two former cases. In our previous papers, we have investigated the finite-temperature properties, especially the Curie point.[8] 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. We arrived at the interesting conclusion that its Curie point, T_F, is never below the Bose-Einstein condensation temperature, T_C, regardless of the magnitude of the ferromagnetic coupling.[8] Kis-Szabo *et al.*[9] 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 Sec. II, we introduce the mean-field approximation to deal with ferromagnetic interaction, taking the spin-1 Bose gas as an example. In Sec. III, phase transitions are discussed by calculating the free energy and specific heat. In Sec. IV, the susceptibility above the Curie point is calculated. A summary is given in Sec. V.

II. MEAN-FIELD APPROXIMATION

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

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

where $\hat{\psi}_{\sigma}(\mathbf{r})$ is the quantum field operator for annihilating an atom in spin state $|\sigma\rangle$ at site r. For a spin-1 gas, $\sigma=+1,0,-1$. The parameter h_e denotes the external magnetic field. The last term represents the ferromagnetic exchange between two different bosons meeting at site r and $I_s(>0)$ is the exchange constant. $\hat{\mathbf{S}}=\{\hat{S}^x,\hat{S}^y,\hat{S}^z\}$ are the spin operators, which can be expressed via the 3×3 Pauli matrices, for example,

$$\hat{S}^z=(\hat{\psi}_{+1}^{\dagger}\quad\hat{\psi}_{0}^{\dagger}\quad\hat{\psi}_{-1}^{\dagger})\begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}\begin{pmatrix}\hat{\psi}_{+1}\\\hat{\psi}_{0}\\\hat{\psi}_{-1}\end{pmatrix}. \tag{2}$$

Within the mean-field approximation, we treat the spin-dependent interactions as a molecular field except of a particle with itself,

$$-\frac{1}{2}\hat{\mathbf{S}}\cdot\hat{\mathbf{S}}\approx-\langle\hat{\mathbf{S}}\rangle\cdot\hat{\mathbf{S}}+\frac{1}{2}\langle\hat{\mathbf{S}}\rangle\cdot\langle\hat{\mathbf{S}}\rangle=-\bar{M}\hat{S}^z+\frac{1}{2}\bar{M}^2, \tag{3}$$

where $\bar{M}=\langle\hat{S}^z\rangle$ is the ferromagnetic order parameter. Then the effective Hamiltonian for the grand canonical ensemble reads

$$\hat{H} - \hat{N}\mu = \sum_{\mathbf{k}\sigma} [\epsilon_{\mathbf{k}} - \mu - \sigma(h_m + h_e)]\hat{n}_{\mathbf{k}\sigma} + \frac{1}{2}\bar{M}^2 I_s N, \quad (4)$$

where $\epsilon_{\mathbf{k}}$ is the kinetic energy for free particles, $h_m = I_s\bar{M}$ is called the molecular field, similar to the Stoner theory for fermion gases,[16] μ is the chemical potential, and N is the total particle number. The grand thermodynamic potential can be worked out in a standard way,

$$\Omega = -k_B T \ln \mathrm{Tr}\exp\left[-\frac{\hat{H} - \hat{N}\mu}{k_B T}\right] = -\frac{(k_B T)^{5/2} V m^{3/2}}{(2\pi\hbar^2)^{3/2}} \sum_{\sigma} f_{5/2}\left(\frac{\mu + \sigma h}{k_B T}\right) + \frac{1}{2}\bar{M}^2 I_s N, \quad (5)$$

where $h = h_m + h_e$, m is the mass of particle, and f is the polylogarithm function defined by

$$f_n(x) \equiv \sum_{k=1}^{\infty} \frac{(e^x)^k}{k^n}, \quad (6)$$

where $x \le 0$. The mean-field self-consistent equations are derived from the grand thermodynamic potential,

$$n = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial\mu}\right)_{T,V} + n_0 = \left(\frac{k_B T m}{2\pi\hbar^2}\right)^{3/2} \sum_{\sigma} f_{3/2}\left(\frac{\mu + \sigma h}{k_B T}\right) + n_0, \quad (7a)$$

$$M = -\frac{1}{V}\left(\frac{\partial\Omega}{\partial h_e}\right)_{T,V} + n_0 = \left(\frac{k_B T m}{2\pi\hbar^2}\right)^{3/2} \left[f_{3/2}\left(\frac{\mu + h}{k_B T}\right) - f_{3/2}\left(\frac{\mu - h}{k_B T}\right)\right] + n_0, \quad (7b)$$

where n is the density of particles, n_0 is the density of the condensed one, and $M \equiv \frac{N\bar{M}}{V}$ is the magnetization. n_0 is zero unless the temperature is below the BEC point T_C.

III. FREE ENERGY AND SPECIFIC HEAT

In our previous investigations, we showed that the system exhibits the two phase transitions, the BEC and the ferromagnetic transition.[8] 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 Eqs. (7a) and (7b), with $M=0$ at all temperatures. It means that the system does not undergo a ferromagnetic transition at all but remains in the 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 cannot 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 FM state and that of the PM state. The relation between the free energy and the grand thermodynamic potential has the form

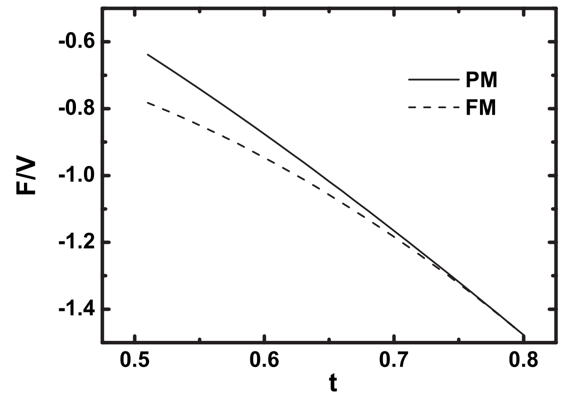

FIG. 1. Free energies of the FM and PM states with the ferromagnetic coupling $I=1$. The two curves cross at the temperature $t_F \approx 0.80$, which is just the FM transition point.

$$F = \Omega + N\mu. \quad (8)$$

For computational convenience, the temperature T and exchange interaction I_s are rescaled, as shown in Ref. 8, by the following formula: $t = [3\zeta(\frac{3}{2})]^{-2/3} T/T_0$ and $I = [3\zeta(\frac{3}{2})]^{-2/3} I_s/(k_B T_0)$, where

$$T_0 = \frac{1}{k_B}\left(\frac{n}{3\zeta\left(\frac{3}{2}\right)}\right)^{2/3}\left(\frac{2\pi\hbar^2}{m}\right)$$

is the condensation temperature of the 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 the 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 the 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 of the literature.[13,14] However, the spin conservation rule holds only globally but not locally. In the theoretical treatment in Ref. 20, the spin conservation rule is imposed by introducing a Lagrangian multiplier. It is overconstrained in some sense so that the spontaneous magnetization cannot be established. Recent experiments and theories indicate that some domain structures should be formed and each domain is magnetized,[11,12,15] where the conservation law for the total spin can be restored naturally.

The--> FM transition is induced by the FM coupling and the transition temperature is about $t_F \approx 0.8$ for the Bose gas with $I=1.0$. When the temperature goes down further, the BEC then occurs, which is the intrinsic phase transition of Bose gases. To demonstrate different features of the two transitions, we now calculate the specific heat of unit volume,

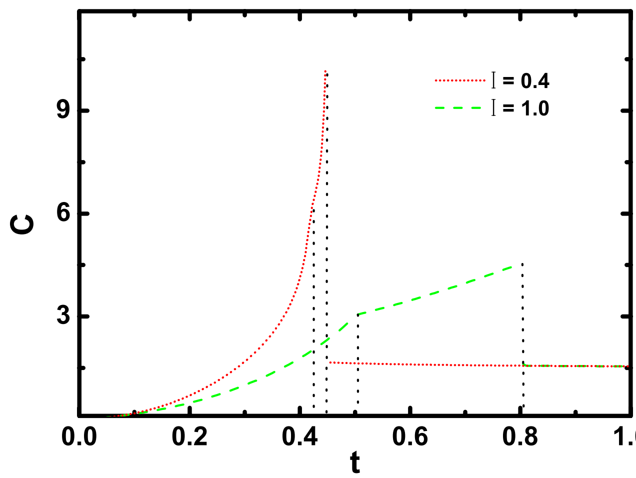

FIG. 2. (Color online) Specific heats of spinor Bose gases with the coupling $I=1.0$ and 0.4. The dotted vertical lines serve to guide the eyes to see the transition points.

$$C = \frac{1}{V}\left(\frac{\partial U}{\partial T}\right)_{B,V}, \tag{9}$$

where U is the internal energy,

$$U = F - TS = \Omega - T\left(\frac{\partial \Omega}{\partial T}\right) + N\mu$$
$$= \frac{3V(k_BT)^{5/2}m^{3/2}}{2(2\pi\hbar^2)^{3/2}}\sum_\sigma f_{3/2}\left(\frac{\mu+\sigma h}{k_BT}\right). \tag{10}$$

As shown in Fig. 2, for the system with $I=1.0$, the specific heat exhibits a jump discontinuity at $t_F\approx 0.8$ from the PM state to the FM state. This is a characteristic feature of the Landau type of second-order phase transition. Similar behaviors have been observed in the specific heat of ferromagnetic insulators or itinerant-fermion ferromagnets.[16,17] The BEC occurs at $t_C\approx 0.5$, where the specific heat exhibits a bend. But specific heat is continuous at the BEC point, similar to that of a free Bose gas. The results indicate that the critical behaviors are different at the two transition points on the mean-field level.

IV. 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 the 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. (7a) and (7b). Differentiating both sides of the two equations and removing the term $d\mu$, the following equations are deduced:

$$dM = fd\left(\frac{I_s\bar{M}+h_e}{k_BT}\right), \tag{11}$$

where

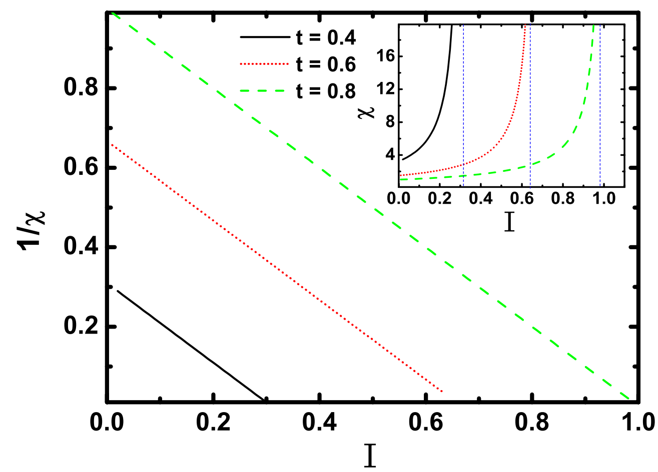

FIG. 3. (Color online) Magnetic susceptibilities versus ferromagnetic couplings of spinor Bose gases at temperature $t=0.4$, 0.6, and 0.8.

$$f = \left(\frac{k_BTm}{2\pi\hbar^2}\right)^{3/2}\left[f_{1/2}\left(\frac{\mu+h}{k_BT}\right)+f_{1/2}\left(\frac{\mu-h}{k_BT}\right)\right]$$
$$-\left(\frac{k_BTm}{2\pi\hbar^2}\right)^{3/2}\frac{\left[f_{1/2}\left(\frac{\mu+h}{k_BT}\right)-f_{1/2}\left(\frac{\mu-h}{k_BT}\right)\right]^2}{\sum_\sigma f_{1/2}\left(\frac{\mu+h\sigma}{k_BT}\right)}. \tag{12}$$

Above the Curie point, the magnetization M (then $h=I_s\bar{M}+h_e$) 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,

$$f \approx 2\left(\frac{k_BTm}{2\pi\hbar^2}\right)^{3/2} f_{1/2}\left(\frac{\mu}{k_BT}\right). \tag{13}$$

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

$$\chi = \left(\frac{\partial M}{\partial h_e}\right)_{T,V} = \frac{1}{k_BTf^{-1}-n^{-1}I_s}. \tag{14}$$

The susceptibility χ is a function of the coupling I_s and temperature T. Figure 3 shows $1/\chi$ and χ versus I at different given temperatures. As shown in the inset of Fig. 3, the susceptibility becomes larger as the coupling I increases. It is physically reasonable since the system with larger I can be magnetized more easily. At a given temperature, χ 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 meets 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.

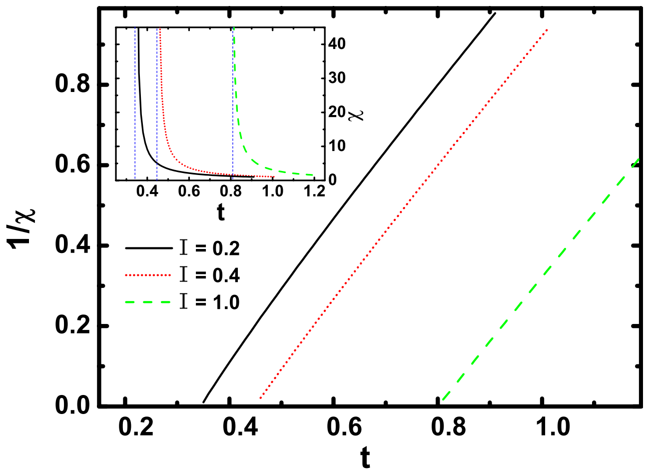

FIG. 4. (Color online) Magnetic susceptibilities versus temperatures of spinor Bose gases on coupling I=0.2, 0.4, and 1.0.

In order to discuss the Curie-Weiss law in a more explicit way, we proceed to carry out a semianalytical 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 μ is an implicit function of the temperature. We consider a limiting case that the parameter I_s is quite small when T_F is close to T_C. So μ is close to zero in the vicinity of T_F. According to the asymptotic behavior of the polylogarithm function, $f_{3/2}(x) \approx \zeta(\frac{3}{2}) - 2\sqrt{\pi x}$ and $f_{1/2}(x) \approx \sqrt{\pi/x}$ as $x \to 0^-$, we get the following equations from Eqs. (7a) and (13), respectively:

$$n \approx 3\left(\frac{k_B T m}{2\pi\hbar^2}\right)^{3/2}\left[f_{3/2}(0) - 2\sqrt{-\frac{\pi\mu}{k_B T}}\right] \tag{15}$$

and

$$f \approx 2\left(\frac{k_B T m}{2\pi\hbar^2}\right)^{3/2}\sqrt{-\frac{k_B T \pi}{\mu}}. \tag{16}$$

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

$$\chi^{-1} = \frac{n k_B^{-2}}{12\pi}\left(\frac{m}{2\pi\hbar^2}\right)^{-3} T^{-1/2}(T_0^{-3/2} - T^{-3/2}) - n^{-1} I_s. \tag{17}$$

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

$$\chi^{-1} \approx \frac{n k_B^{-2}}{8\pi}\left(\frac{m}{2\pi\hbar^2}\right)^{-3} T_0^{-3}(T - T_0) - n^{-1} I_s$$
$$= \frac{9\zeta^2\left(\frac{3}{2}\right)}{8\pi} n^{-1} k_B\left[T - \left(T_0 + \frac{8\pi}{9\zeta^2\left(\frac{3}{2}\right)k_B} I_s\right)\right]. \tag{18}$$

Thus the effective FM transition temperature is defined as

$$T_F = T_0 + \frac{8\pi}{9\zeta^2\left(\frac{3}{2}\right)k_B} I_s.$$

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 χ^{-1} is linearly dependent on T. In this case, $-\frac{\mu}{k_B T}$ has a quite large value, so that

$$f_{1/2}\left(\frac{\mu}{k_B T}\right) \approx f_{3/2}\left(\frac{\mu}{k_B T}\right) \approx e^{\mu/k_B T}$$

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

$$\chi^{-1} = n^{-1}(k_B T - I_s). \tag{19}$$

We estimate that 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 decreasing temperature. 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 transitions. The more surprising result is that the mean-field theory yields the magnetic susceptibility which satisfies perfectly the Curie-Weiss law over a wide range of temperature.

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