

Static properties and spin dynamics of the ferromagnetic spin-1 Bose gas in a magnetic field

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The properties of spin-1 Bose gases with ferromagnetic interactions in the presence of a nonzero magnetic field are studied. The equation of state and thermodynamic quantities are worked out with the help of a mean-field approximation. The phase diagram besides Bose-Einstein condensation contains a first-order transition where two values of the magnetization coexist. The dynamics is investigated with the help of the random phase approximation. The soft mode corresponding to the critical point of the magnetic phase transition is found to behave like in conventional theory.

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I. INTRODUCTION

Atomic Bose gases consisting of atoms with spin 1 can exhibit a spinor condensate, which has attracted considerable attention in recent years [1–16]. Such gases have interesting properties also before the Bose-Einstein condensation (BEC) sets in. This is particularly true when the coupling between the spin degrees of freedom prefers ferromagnetic ordering. Such a system can be realized by the gas of ^{87}Rb atoms. A ^{87}Rb atom has a nuclear spin of $j=3/2$ and an electron spin of $s=1/2$; therefore, its net spin can be $F=1$ or $F=2$. Since the energy of the $F=1$ multiplet is smaller than that of the $F=2$, the population in the $F=2$ multiplet dwindles at sufficiently low temperatures, resulting in a gas of purely spin-1 (three-component) bosons [6,7].

At zero external magnetic field it has been found that when lowering the temperature a transition to the ferromagnetic state can occur first which can be first or second order as well depending on the strength of the spin-spin interaction [17,18]. The transition to the Bose condensed phase can also be first or second order according to mean-field theory results. Note that the tendency towards ferromagnetic ordering is present in the Bose gas formed by atoms with nonzero spin even in the case when only a spin-independent interaction acts between the atoms (or the gas is ideal) [19–22]. The effects of an external magnetic field have been studied for the free Bose gas in Ref. [22]. In the present paper a gas of spin-1 bosons is investigated in the presence of an interaction of ferromagnetic type and a nonzero magnetic field.

The system is supposed to be translationally invariant with a homogeneous magnetic field pointing to the z direction. The Hamiltonian takes the following form:

$$\begin{aligned} \mathcal{H} = & \sum_{\mathbf{k}} [(e_{\mathbf{k}} - \mu) \delta_{rs} - g \mu_B B(F_z)_{rs}] a_r^\dagger(\mathbf{k}) a_s(\mathbf{k}) \\ & + \frac{1}{2V} \sum_{\mathbf{k}_1 + \mathbf{k}_2 = \mathbf{k}_3 + \mathbf{k}_4} a_{r'}^\dagger(\mathbf{k}_1) a_r^\dagger(\mathbf{k}_2) V_{rs}^{r's'} a_s(\mathbf{k}_3) a_{s'}(\mathbf{k}_4), \end{aligned} \quad (1)$$

where $a_r^\dagger(\mathbf{k})$ and $a_r(\mathbf{k})$ create and destroy one-particle plane-wave states with momentum \mathbf{k} and spin projection r . The spin index r refers to the eigenvalue of the z component of the spin operator and can take values from $+$, 0 , $-$. In this basis the spin operators are given by

$$\begin{aligned} F_x = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}, \quad F_y = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{bmatrix}, \\ F_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}. \end{aligned} \quad (2)$$

In Eq. (1), $e_{\mathbf{k}} = \hbar^2 k^2 / 2M$ refers to the kinetic energy of an atom (M is the mass of an atom), μ to the chemical potential, g to the gyromagnetic ratio, μ_B to the Bohr magneton, B to the modulus of the homogeneous magnetic field, V is the volume of the system, and $V_{rs}^{r's'}$ the Fourier transform of the two-particle interaction potential, which for the low-temperature, dilute gas can be modeled by the momentum-independent s -wave scattering amplitude given for spin-1 bosons by [5–7,23,24]

$$V_{rs}^{r's'} = c_n \delta_{rs} \delta_{r's'} + c_s(\mathbf{F})_{rs}(\mathbf{F})_{r's'}, \quad (3)$$

with parameters

$$c_n = \frac{4\pi\hbar^2 a_0 + 2a_2}{M \cdot 3}, \quad (4a)$$

$$c_s = \frac{4\pi\hbar^2 a_2 - a_0}{M \cdot 3}. \quad (4b)$$

The parameters $a_0 > 0$ and $a_2 > 0$ are the scattering length in the total hyperfine spin channels 0 and 2, respectively. Note that $c_s < 0$ for the gas of ^{87}Rb atoms [25]. For such a system it is energetically favorable to align the spins along one direction; i.e., the system has a ferromagnetic coupling [6,7]. In this paper we assume such a system.

The outline of the paper is as follows. In Sec. II the Hartree equation of state of the dilute and low-temperature, interacting spin-1 Bose gas is given in the presence of a non-zero magnetic field. In Sec. III the magnetic susceptibility of the system is investigated in the uncondensed phase. Section IV is devoted to the determination of correlation functions of generalized density operators, which are used in Sec. V to express the linear response functions of the system. With the help of the response functions further static properties and the spin dynamics of the system are also investigated. In Sec. VI the results are summarized.

II. EQUATION OF STATE

For the spin-1 Bose gas the Hartree approximation [26] yields a plausible set of equations, which form the equation of state of the system. As a matter of fact, as we will see, this leads to a magnetic mean-field approach. The first equation in the set expresses the total density as the sum of the density of the condensate and that of the different spin projections of the noncondensate and reads as

$$n = n_0 + n'_+ + n'_0 + n'_-, \quad (5)$$

where $n = N/V$ the total density of atoms in the gas, $n_0 = N_0/V$ the density of the Bose-Einstein condensed atoms, and

$$n'_r = \sum_{\mathbf{k}} n'_{\mathbf{k},r} \quad (6a)$$

is the density of the noncondensed atoms with spin projection r , where

$$n'_{\mathbf{k},r} = \frac{1}{e^{\beta\varepsilon_{\mathbf{k},r}^H} - 1}, \quad (6b)$$

$$\varepsilon_{\mathbf{k},r}^H = \varepsilon_{\mathbf{k}} - \mu + c_n n + r(mc_s - g\mu_B B). \quad (6c)$$

In the last equation m is the magnetization density of the system (see below) and $\beta = 1/k_B T$ is the inverse temperature. The term rmc_s can be interpreted as the energy shift of the internal state r arising from a “molecular field.” The formula is quite plausible and can be derived from a self-consistent Hartree approximation in the Green’s function technique.

The next equation of the set is the expression of the magnetization density m , and it takes the following form:

$$m = n_0 + n'_+ - n'_-, \quad (7)$$

since the condensate spinor points to the z direction. In the case, when $n_0 = 0$ —i.e., the system is not Bose-Einstein condensed—Eqs. (5) and (7) together with expressions (6) form a closed set of equations, and with knowledge of the temperature, the magnetic field and particle density can be solved for the chemical potential and magnetization density. However, with lowering the temperature, one arrives at a point when the lowest bound of the energy expression will be zero: $\varepsilon_{0,+}^H = 0$; i.e., the chemical potential will reach the value of $\mu = c_n n + c_s m - g\mu_B B$, which means that $n'_{\mathbf{k},+} = [\exp(\beta\varepsilon_{\mathbf{k}}) - 1]^{-1}$, so the system undergoes Bose-Einstein condensation. The expression for μ remains true at lower temperatures; i.e.,

$$0 = n_0[-\mu + c_n n + c_s m - g\mu_B B] \quad (8)$$

holds. The multiplicative factor n_0 is used to make the equation valid for the high-temperature phases as well, where $n_0 = 0$. In conclusion Eqs. (5), (7), and (8) together with expressions (6) form a closed set of equations for all possible temperature values, which is considered as the equation of state of the spin-1 Bose gas with ferromagnetic interactions in the presence of a magnetic field. Our equation of state compares for zero magnetic field with that obtained by Gu and Klemm [17] in a completely different approach, while for $c_s = 0$ it becomes similar to that of the free Bose gas treated in a nonzero magnetic field by Simkin and Cohen [22].

For the solution of the equation of state let us restrict ourselves to the case with fixed particle density, magnetic field, and temperature; i.e., Eqs. (5), (7), and (8) are solved for (μ, m, n_0) with (n, B, T) fixed. It is important to note that with introducing $\mu' = \mu - c_n n$ the effect of $c_n n$ can be incorporated into the chemical potential for a fixed particle density. Detailed investigations show that the magnetic separation found is accompanied by the separation of density. The density difference, however, between the phases is smaller by a factor of the order of $|c_s|/c_n$ than the density itself. To concentrate to the magnetic properties alone we disregard the phase separation in the density. The phase diagram including phase separation will be published elsewhere [27].

The BEC transition temperature of the homogeneous spin-1 Bose gas is given by

$$T_0 = \frac{2\pi\hbar^2}{k_B M} \left[\frac{n}{3\zeta\left(\frac{3}{2}\right)} \right]^{2/3}, \quad (9)$$

and by taking T_0 to be, e.g., 200 nK (as is typical in experiments [28,29]) the particle density is given by fundamental constants (apart from the mass of the atoms in the gas). For the case of ^{87}Rb atoms, with $T_0 = 200$ nK the particle density by Eq. (9) is $n = 10^{20} \text{ m}^{-3}$ to a very good approximation. It is convenient to introduce the following dimensionless parameter:

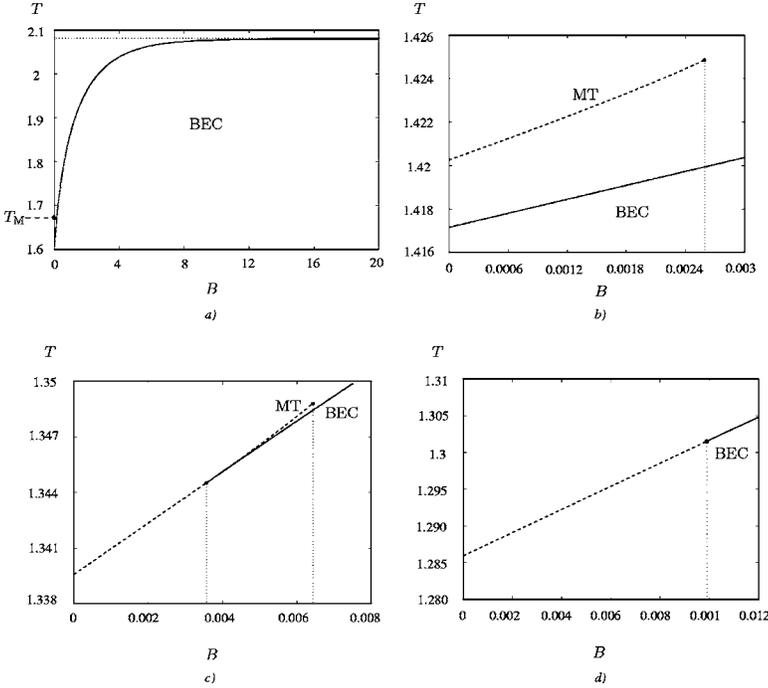


FIG. 1. Possible phase diagrams of the system: (a) for $\epsilon_s > \epsilon_s^{(1)}$, (b) for $\epsilon_s^{(2)} < \epsilon_s < \epsilon_s^{(1)}$, (c) for $\epsilon_s^{(3)} < \epsilon_s < \epsilon_s^{(2)}$, and (d) for $\epsilon_s \leq \epsilon_s^{(3)}$. The dashed line symbolizes a first-order phase transition, while the solid line refers to a continuous phase transition. The temperature is measured in units of T_0 , while the magnetic field is given in units of $k_B T_0 / g \mu_B$.

$$\epsilon_s = \frac{n|c_s|}{k_B T_0}, \quad (10)$$

which can be interpreted as a sort of mean-field energy in units of $k_B T_0$.

By solving the equation of state the domain of ϵ_s can be divided into four parts according to the character of the occurring magnetic and BEC phase transitions. In the first region, when ϵ_s is greater than a certain value ($\epsilon_s > \epsilon_s^{(1)} \approx 1.22$) there exists a paramagnetic-ferromagnetic transition for $B=0$ at $T=T_M$ above the BEC transition T_{BEC} . Such a phase diagram is depicted in Fig. 1(a) for $\epsilon_s=1.4$. Both transitions are continuous for these values of ϵ_s ; the magnetic transition exists only in the absence of a magnetic field and its critical temperature is higher than the BEC transition temperature. At this point we note that in case of zero external magnetic field the magnetic transition and its relation to the BEC have been investigated previously in detail with the help of a magnetic mean-field theory [17] and in the framework of a Landau theory [18].

If the value of ϵ_s is smaller than $\epsilon_s^{(1)}$, the magnetic transition at $B=0$ becomes a first-order one. Therefore the point ($\epsilon_s = \epsilon_s^{(1)}, B=0$) can be understood as a tricritical point for the magnetic transition, since it separates the regions of first-order and continuous transitions. The first-order transition survives even in the presence of a small magnetic field, leading to the coexistence of two phases with different magnetizations. The transition, called the magnetic transition (MT) in the following, ends in a magnetic critical point (MCP), specified by the critical value of the temperature T_c and that of the magnetic field B_c for fixed ϵ_s . Note that a first-order phase transition due to an external field coupled to the order parameter was observed in the ferroelectric BaTiO₃ already in 1953 [30,31]. If at the same time $\epsilon_s > \epsilon_s^{(2)} \approx 0.78$, BEC remains a continuous phase transition and the phase diagram

of this region looks like plotted in Fig. 1(b) for $\epsilon_s=0.9$.

If ϵ_s becomes smaller than $\epsilon_s^{(2)}$, BEC becomes also of first order at $B=0$. However, for $g \mu_B B / k_B T_0 \gg 1$ the system behaves like the gas of noninteracting scalar particles with a continuous BEC phase transition at $3^{2/3} T_0$; therefore, there must be a critical magnetic field value $B_c^{(1)}$ which is also a tricritical point, but in the sense of the BEC transition, which separates the first-order BEC in a small magnetic field from the continuous BEC in a strong magnetic field. Such a phase diagram is plotted in Fig. 1(c) for $\epsilon_s=0.72$. As long as $\epsilon_s > \epsilon_s^{(3)} \approx 0.62$ there exists another critical magnetic field value ($B_c^{(2)}$) above which there is no magnetic transition (magnetization behaves analytically).

For $\epsilon_s \leq \epsilon_s^{(3)}$ the two critical magnetic field values are equal ($B_c^{(1)} = B_c^{(2)}$). A phase diagram for this situation is shown in Fig. 1(d) for $\epsilon_s=0.6$.

After discussing the above four possible situations (according to the value of ϵ_s), it is worthwhile to plot the full phase diagram of the system, where ϵ_s is also considered as a variable besides T and B . It can be seen in Fig. 2. The above four figures can be obtained as sections of Fig. 2 made with a fixed ϵ_s . It is important to note that inside the simply hatched region on the (ϵ_s, B) plane of Fig. 2 the magnetic transition is of first order and its transition temperature is higher than that of the continuous BEC (of the same ϵ_s and B values).

As far as the equation of state is concerned one can regard our calculation as an extension of the work of Gu and Klemm [17] to the presence of a nonzero external magnetic field. At $B=0$ our results are in agreement with those of Gu and Klemm in the region $\epsilon_s > \epsilon_s^{(2)}$. Note that for $\epsilon_s < \epsilon_s^{(2)}$ the BEC becomes a first-order transition; i.e., $\epsilon_s^{(2)}$ corresponds to the value I_c of the reduced ferromagnetic coupling I in their paper. There is a slight difference between our and their results if $\epsilon_s < \epsilon_s^{(2)}$. Namely, we have found that the two first-

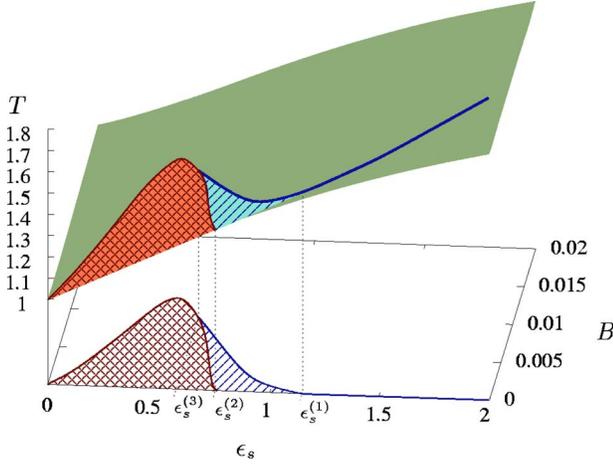


FIG. 2. (Color online) The phase diagram of the spin-1 Bose gas in the space of (ϵ_s, B, T) . The temperature is measured in units of T_0 , while the magnetic field is given in units of $k_B T_0 / g \mu_B$. The solid surface indicates a continuous BEC transition, except in the crosshatched region, where BEC is of first order. The simply hatched region, outside the region of first-order BEC, refers to the first-order magnetic transition and is lifted slightly from the surface of continuous BEC. At the heavy curve the magnetic transition is continuous, and its transition temperature is above that of the BEC. For $\epsilon_s > \epsilon_s^{(1)}$ this curve lies in the $B=0$ surface. The surfaces of first-order transitions and the curve of the continuous magnetic transition are projected to the (ϵ_s, B) plane for transparency. The relevant ϵ_s values are also indicated [compare with Figs. 1(a)–1(d)].

order transitions (MT and BEC) coincide at least for small B values, including $B=0$, while they claim that the ferromagnetic transition occurs always first.

III. MAGNETIC SUSCEPTIBILITY IN THE UNCONDENSED PHASE

With differentiating the equations of state (5) and (7) with respect to the thermodynamic quantities T , B , and n one can obtain generalized susceptibilities of the system, such as $(\partial n / \partial \mu)_{T,B}$ or $(\partial m / \partial B)_{T,n}$, etc. (the subscripts are referring to variables kept constant during differentiation). Focusing on the magnetic transition here we restrict ourselves to the magnetic susceptibility of the system with fixed particle number—i.e., $(\partial m / \partial B)_{T,n}$. The region of interest in the (ϵ_s, B) plane is also restricted to the simply hatched region in Fig. 2 and to the heavy line with $(\epsilon_s > \epsilon_s^{(1)}, B=0)$ or, equivalently, to the situations depicted in Figs. 1(a)–1(c), where one can find a purely magnetic transition above the BEC transition temperature. The temperature is also restricted above $T_{\text{BEC}}(\epsilon_s, B)$.

For this purpose let us first cast the expression of the density of the noncondensed particles (6) to a more explicit form by performing the momentum integration

$$n_r' = \frac{\Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} F\left(\frac{3}{2}, \beta[-\mu + c_n n + r(mc_s - g\mu_B B)]\right), \quad (11)$$

where $\lambda = \hbar / \sqrt{2Mk_B T}$ is the thermal wavelength of the atom, $\Gamma(s)$ the gamma function, and $F(s, \gamma)$ is the Bose-Einstein integral with parameter s and argument γ , defined with the help of the polylogarithm function [32,33]:

$$F(s, \gamma) \equiv \text{Li}_s(e^{-\gamma}). \quad (12)$$

The derivative of Eq. (11) with respect to B can be easily evaluated with the result

$$\left(\frac{\partial n_r'}{\partial B}\right)_{T,n} = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} F\left(\frac{1}{2}, \beta[-\mu' + r(mc_s - g\mu_B B)]\right) \times \left\{ \left(\frac{\partial \mu}{\partial B}\right)_{T,n} + r \left[g\mu_B - c_s \left(\frac{\partial m}{\partial B}\right)_{T,n} \right] \right\}, \quad (13)$$

where $\mu' = \mu - c_n n$ was introduced for simpler notation and the relation $dF(s, x)/dx = -F(s-1, x)$ was used [32]. Differentiating Eqs. (5) and (7) with respect to B with n and T held fixed one arrives at a system of two equations for the quantities $(\partial m / \partial B)_{T,n}$ and $(\partial \mu / \partial B)_{T,n}$, from which the former one can be expressed as

$$\left(\frac{\partial m}{\partial B}\right)_{T,n} = g\mu_B \frac{(P+R)Q + 4PR}{P+Q+R+c_s[(P+R)Q+4PR]}, \quad (14)$$

with

$$P = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} F\left(\frac{1}{2}, \beta[-\mu' + (mc_s - g\mu_B B)]\right), \quad (15a)$$

$$Q = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} F\left(\frac{1}{2}, -\beta \mu'\right), \quad (15b)$$

$$R = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} F\left(\frac{1}{2}, \beta[-\mu' - (mc_s - g\mu_B B)]\right). \quad (15c)$$

The continuous magnetic transition is signaled by the divergence of the susceptibility (14) or, equivalently, by the vanishing of its denominator:

$$P+Q+R+c_s[(P+R)Q+4PR]=0, \quad (16)$$

which is fulfilled along the thick curve of Fig. 2. The magnetic susceptibility shows interesting properties also near the BEC. According to expression (14) $(\partial m / \partial B)_{T,n}$ develops a cusp at $T_{\text{BEC}}(B)$ similarly to the susceptibility of the free Bose gas [22] at a fixed number of particles.

IV. CORRELATION FUNCTIONS OF GENERALIZED DENSITY OPERATORS

Consider the following density operators:

$$n(\mathbf{k}) = \sum_{\mathbf{q}, r} a_r^\dagger(\mathbf{k} + \mathbf{q}) a_r(\mathbf{q}), \quad (17a)$$

$$\mathcal{F}_z(\mathbf{k}) = \sum_{\mathbf{q}, r, s} (F_z)_{r,s} a_r^\dagger(\mathbf{k} + \mathbf{q}) a_s(\mathbf{q}). \quad (17b)$$

The former one is the particle density operator, while the latter one is the longitudinal magnetization density operator. Other generalized density operators can be defined as well for the spin-1 Bose gas, as done, e.g., in Ref. [26], but for the purposes of this paper the above two are enough. The correlation functions of the generalized density operators (17) are defined (for $\mathbf{k} \neq 0$) as

$$D_{nn}(\mathbf{k}, \tau) = -\langle T_\tau [n(\mathbf{k}, \tau) n^\dagger(\mathbf{k}, 0)] \rangle, \quad (18a)$$

$$D_{zz}(\mathbf{k}, \tau) = -\langle T_\tau [\mathcal{F}_z(\mathbf{k}, \tau) \mathcal{F}_z^\dagger(\mathbf{k}, 0)] \rangle, \quad (18b)$$

$$D_{nz}(\mathbf{k}, \tau) = -\langle T_\tau [n(\mathbf{k}, \tau) \mathcal{F}_z^\dagger(\mathbf{k}, 0)] \rangle, \quad (18c)$$

with τ being the imaginary time and T_τ the τ ordering operator (see, e.g., Ref. [34]). After the usual Fourier transformation into the Matsubara frequency representation these correlation functions in general satisfy the following equations [26]:

$$D_{nn} = \hbar \Pi_{nn} + c_n \Pi_{nn} D_{nn} + c_s \Pi_{nz} D_{nz}, \quad (19a)$$

$$D_{zz} = \hbar \Pi_{zz} + c_n \Pi_{nz} D_{nz} + c_s \Pi_{zz} D_{zz}, \quad (19b)$$

$$D_{nz} = \hbar \Pi_{nz} + c_n \Pi_{nn} D_{nz} + c_s \Pi_{nz} D_{zz}, \quad (19c)$$

with the polarization functions

$$\Pi_{nn}(\mathbf{k}, i\omega_n) = \sum_{r,s} \Pi_{ss}^{rr}(\mathbf{k}, i\omega_n), \quad (20a)$$

$$\Pi_{zz}(\mathbf{k}, i\omega_n) = \sum_{r,s} rs \Pi_{ss}^{rr}(\mathbf{k}, i\omega_n), \quad (20b)$$

$$\Pi_{nz}(\mathbf{k}, i\omega_n) = \sum_{r,s} s \Pi_{ss}^{rr}(\mathbf{k}, i\omega_n). \quad (20c)$$

The polarization part $\Pi_{ss}^{rr}(\mathbf{k}, i\omega_n)$ is the contribution of interaction-line-irreducible Feynman diagrams, which can connect to an interaction line $V_{r,r}^{a,b}$ from the right and to an interaction line $V_{c,d}^{s,s}$ (a, b, c, d arbitrary spin indices) from the left [26]. The interaction with four indices is defined in Eq. (3). [All correlation functions and polarization functions in Eqs. (19) depend on the $(\mathbf{k}, i\omega_n)$ variables, which are omitted for the sake of brevity.] The solution of Eqs. (19) reads as

$$D_{nn} = \hbar \frac{\Pi_{nn}(1 - c_s \Pi_{zz}) + c_s \Pi_{nz}^2}{\det^0_{\underline{\underline{\xi}}}}, \quad (21a)$$

$$D_{nz} = \hbar \frac{\Pi_{nz}}{\det^0_{\underline{\underline{\xi}}}}, \quad (21b)$$

$$D_{zz} = \hbar \frac{\Pi_{zz}(1 - c_n \Pi_{nn}) + c_n \Pi_{nz}^2}{\det^0_{\underline{\underline{\xi}}}}, \quad (21c)$$

with the abbreviating notation

$$\det^0_{\underline{\underline{\xi}}} = (1 - c_n \Pi_{nn})(1 - c_s \Pi_{zz}) - c_n c_s \Pi_{nz}^2. \quad (21d)$$

Expressions (21) are quite general. They are valid both in the condensed and uncondensed phases and contain no approximations. Of course the choice of the actual form of the polarization functions Π_{ss}^{rr} selects between the different approximations and possible phases. The correlation functions are evaluated in the framework of the random phase approximation (RPA) and for the uncondensed phase ($n_0=0$), where the polarization function is taken as the contribution of the bubble graph [26], which (for \mathbf{k} and ω_n not simultaneously zero) reads as

$$\Pi_{ss}^{rr}(\mathbf{k}, i\omega_n) = -\frac{\delta_{r,s}}{\hbar} \int \frac{d^3q}{(2\pi)^3} \frac{n'_{\mathbf{k}+\mathbf{q},r} - n'_{\mathbf{q},r}}{i\omega_n - \hbar^{-1}(e_{\mathbf{k}+\mathbf{q}} - e_{\mathbf{k}})}. \quad (22)$$

The expressions for finite magnetic field are quite similar to those of zero magnetic field [26]. The effect of the magnetic field appears explicitly only in the contribution of the bubble graph (22) and only through $n'_{\mathbf{q},r}$; see Eq. (6).

V. PROPERTIES OF WAVE-NUMBER-DEPENDENT SUSCEPTIBILITIES

The dynamics of the system can be studied with the help of elementary excitations. Spin dynamics is related to longitudinal and transverse spin excitations. However, at the magnetic transition, where the susceptibility $(\partial m / \partial B)_{T,n}$ diverges, longitudinal spin dynamics plays the relevant role as the soft mode of the transition. The spectrum of elementary excitations is related to linear response functions of the system (see, e.g., Ref. [34]), which can be obtained from the correlation functions by analytical continuation in frequency through the real axis from above. From now on we shall deal with such retarded correlation functions (response functions). With the help of linear response theory the density and magnetization fluctuations of the system are related to the external potentials $\delta\mu(\mathbf{k}, \omega)$ and $\delta B(\mathbf{k}, \omega)$ by

$$\begin{aligned} \delta n(\mathbf{k}, \omega) &= -\hbar^{-1} D_{nn}(\mathbf{k}, \omega) \delta\mu(\mathbf{k}, \omega) \\ &\quad - g\mu_B \hbar^{-1} D_{nz}(\mathbf{k}, \omega) \delta B(\mathbf{k}, \omega), \end{aligned} \quad (23a)$$

$$\begin{aligned} \delta m(\mathbf{k}, \omega) &= -\hbar^{-1} D_{zn}(\mathbf{k}, \omega) \delta\mu(\mathbf{k}, \omega) \\ &\quad - g\mu_B \hbar^{-1} D_{zz}(\mathbf{k}, \omega) \delta B(\mathbf{k}, \omega). \end{aligned} \quad (23b)$$

From Eq. (23a),

$$\delta\mu(\mathbf{k}, \omega) = -g\mu_B \frac{D_{nz}(\mathbf{k}, \omega)}{D_{nn}(\mathbf{k}, \omega)} \delta B(\mathbf{k}, \omega) - \hbar \frac{\delta n(\mathbf{k}, \omega)}{D_{nn}(\mathbf{k}, \omega)}. \quad (24)$$

Substituting it into Eq. (23b) one obtains the equation

$$\begin{aligned} &-\frac{\hbar}{g\mu_B} \delta m(\mathbf{k}, \omega) \\ &= -\frac{\hbar}{g\mu_B} \frac{D_{nz}(\mathbf{k}, \omega)}{D_{nn}(\mathbf{k}, \omega)} \delta n(\mathbf{k}, \omega) \\ &\quad + \frac{D_{nn}(\mathbf{k}, \omega) D_{zz}(\mathbf{k}, \omega) - D_{nz}(\mathbf{k}, \omega) D_{zn}(\mathbf{k}, \omega)}{D_{nn}(\mathbf{k}, \omega)} \\ &\quad \times \delta B(\mathbf{k}, \omega). \end{aligned} \quad (25)$$

On this basis one can define

$$\begin{aligned}
& \hbar^{-1} D_{zz}^{(n)}(\mathbf{k}, \omega) \\
& := \hbar^{-1} \frac{D_{m\bar{m}}(\mathbf{k}, \omega) D_{z\bar{z}}(\mathbf{k}, \omega) - D_{n\bar{z}}(\mathbf{k}, \omega) D_{z\bar{n}}(\mathbf{k}, \omega)}{D_{m\bar{m}}(\mathbf{k}, \omega)} \\
& = \frac{\Pi_{m\bar{m}}(\mathbf{k}, \omega) \Pi_{z\bar{z}}(\mathbf{k}, \omega) - \Pi_{n\bar{z}}(\mathbf{k}, \omega) \Pi_{z\bar{n}}(\mathbf{k}, \omega)}{\Pi_{m\bar{m}}(\mathbf{k}, \omega) [1 - c_s \Pi_{z\bar{z}}(\mathbf{k}, \omega)] + c_s \Pi_{n\bar{z}}(\mathbf{k}, \omega) \Pi_{z\bar{n}}(\mathbf{k}, \omega)},
\end{aligned} \tag{26}$$

where Eqs. (21) were used to arrive at the last equation.

The magnetic susceptibility (14) can be expressed with the help of the response functions in the static limit ($\omega=0$), since

$$\left(\frac{\partial m}{\partial B} \right)_{T,n} = \lim_{\mathbf{k} \rightarrow 0} \lim_{\omega \rightarrow 0} \frac{\delta m(\mathbf{k}, \omega)}{\delta B(\mathbf{k}, \omega)}, \tag{27a}$$

$$\text{with } \lim_{\mathbf{k} \rightarrow 0} \lim_{\omega \rightarrow 0} \delta n(\mathbf{k}, \omega) = 0. \tag{27b}$$

In this limit the contribution to δm comes from the second term on the right-hand side (RHS) of Eq. (25). According to the definition (26) it means that

$$\left(\frac{\partial m}{\partial B} \right)_{T,n} = - \frac{g\mu_B}{\hbar} \lim_{\mathbf{k} \rightarrow 0} D_{zz}^{(n)}(\mathbf{k}, 0). \tag{28}$$

In the uncondensed phase the long-wavelength limit of the static polarization functions take the following forms in the RPA [26,35]:

$$\Pi_{++}^{(r)++}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -P, \tag{29a}$$

$$\Pi_{00}^{(r)00}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -Q, \tag{29b}$$

$$\Pi_{--}^{(r)--}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -R, \tag{29c}$$

where the quantities P , Q , and R are defined in Eqs. (15). Therefore $\Pi_{m\bar{m}}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -P - Q - R$, $\Pi_{n\bar{z}}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -P + R$ and $\Pi_{z\bar{z}}(\mathbf{k} \rightarrow \mathbf{0}, 0) = -P - R$. One can verify that the sum rule (28) is equivalent to Eq. (14).

When the density fluctuations are small the second term on the RHS of Eq. (25) will dominate for small \mathbf{k} , ω values. [Note that neglecting δn , then $\delta\mu$ and δB are related according to Eq. (23a).] Therefore we concentrate on the expression (26) of $D_{zz}^{(n)}$.

In the case when the momentum-independent part of the Hartree energies (6c) can be assumed to be small—i.e., $|\mu'| \ll k_B T$ and $|mc_s - g\mu_B B| \ll k_B T$, and the wave number is much smaller than the thermal wave number, $k\lambda \ll 1$ furthermore, the frequency is also sufficiently small: $\beta\omega \ll k\lambda$, the contribution of the bubble graph (22) can be approximated as [26,36]

$$\begin{aligned}
\Pi_{rr}^{rr}(u, \Omega) = & - \frac{\beta}{4\pi^2 \lambda^3} \left[\frac{\sqrt{\pi}}{2} F\left(\frac{1}{2}, \sigma_r\right) - \frac{\pi}{2\sqrt{\sigma_r}} + i\pi \frac{1}{\Omega u + i2\sqrt{\sigma_r}} \right. \\
& \left. + i\pi \frac{u^2}{3(\Omega u + i2\sqrt{\sigma_r})^3} \right],
\end{aligned} \tag{30a}$$

with

$$\sigma_r = -\beta[\mu' + r(mc_s - g\mu_B B)], \tag{30b}$$

$$u = k\lambda, \tag{30c}$$

$$\Omega = \frac{\hbar\omega}{e_{\mathbf{k}}} = \frac{\beta\hbar\omega}{u^2}. \tag{30d}$$

With these newly introduced notations the validity of the limiting form (30a) is equivalent to $\sigma_r \ll 1$, $|\Omega u| \ll 1$, and $|\Omega + i2\sqrt{\sigma_r}/u| \gg 1$. Expression (30a) is to be used in formulas (20) and (26) to obtain an explicit form for the response function $D_{zz}^{(n)}(\mathbf{k}, \omega)$.

In the static limit one can set $\Omega=0$ in expression (30a) safely with the result

$$\Pi_{rr}^{rr}(u, 0) = - \frac{\beta}{4\pi^2 \lambda^3} \left[\frac{\sqrt{\pi}}{2} F\left(\frac{1}{2}, \sigma_r\right) - \pi \frac{u^2}{24\sigma_r^{3/2}} \right], \tag{31}$$

which can be used in the polarization functions (20) to obtain

$$\Pi_{m\bar{m}} = -\tilde{P} - \tilde{Q} - \tilde{R}, \quad \tilde{P} = P - \tilde{p}u^2, \quad \tilde{p} = \frac{\beta}{96\pi\lambda^3} \frac{1}{\sigma_+^{3/2}},$$

$$\Pi_{n\bar{z}} = -\tilde{P} + \tilde{R}, \quad \tilde{Q} = Q - \tilde{q}u^2, \quad \tilde{q} = \frac{\beta}{96\pi\lambda^3} \frac{1}{\sigma_0^{3/2}},$$

$$\Pi_{z\bar{z}} = -\tilde{P} - \tilde{R}, \quad \tilde{R} = R - \tilde{r}u^2, \quad \tilde{r} = \frac{\beta}{96\pi\lambda^3} \frac{1}{\sigma_-^{3/2}},$$

up to the order of u^2 . Therefore the long-wavelength limit of the static susceptibility at $T=T_c$, where Eq. (16) holds, takes the following form:

$$\begin{aligned}
D_{zz}^{(n)}(k, \omega = 0) & = \frac{\hbar}{(k\lambda)^2} \\
& \times \frac{Q(P+R) + 4PR}{\tilde{p} + \tilde{q} + \tilde{r} + c_s [\tilde{q}(P+R) + Q(\tilde{p} + \tilde{r}) + 4(P\tilde{r} + \tilde{p}R)]}.
\end{aligned} \tag{32}$$

From Eq. (32) one can see that the critical exponent η , defined as $C(k) \propto k^{-2+\eta}$ at the critical temperature for the correlation function C of the order parameter, is zero ($\eta=0$).

To obtain the spectrum of the longitudinal spin fluctuations one has to look for the poles of the response function (26) or, equivalently, look for the zeros of its denominator. The resulting equation is as follows:

$$\Pi_{m\bar{m}}(\mathbf{k}, \omega) [1 - c_s \Pi_{z\bar{z}}(\mathbf{k}, \omega)] + c_s \Pi_{n\bar{z}}(\mathbf{k}, \omega) \Pi_{z\bar{n}}(\mathbf{k}, \omega) = 0. \tag{33}$$

With the help of the numerical approximation of the analytic continuation of the bubble graph (22) [36,37] and with the help of Eqs. (20), Eq. (33) can be solved directly. In the long-wavelength limit one finds a purely imaginary (over-damped) excitation spectrum depending linearly on wave number:

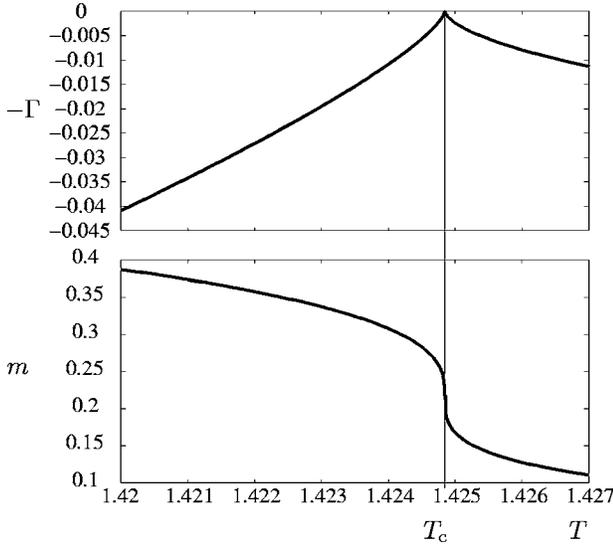


FIG. 3. The damping rate $-\Gamma$ (in units of $k_B T_0 \lambda_0 / \hbar$) of the longitudinal spin excitations (spin density fluctuations) as a function of the temperature T (in units of T_0) at $B=B_c$ and $\epsilon_s=0.9$ (upper panel). The magnetization density (in units of the particle density n) is plotted in the bottom panel for illustration.

$$\omega(k) = -i\Gamma k, \quad (34)$$

with Γ the velocity dimensional damping rate. The numeric values of Γ are given in Fig. 3 for $\epsilon_s=0.9$, $B=B_c$, and temperature values above that of the BEC.

One can clearly see the soft mode ($\Gamma=0$) at $B=B_c$ and $T=T_c$.

For analytical calculation at B_c and near T_c one can suppose that $|\Omega u| \ll 2\sqrt{\sigma_r}$ for all r , since the mode is soft and neither of the σ 's is zero. In this case Eq. (30a) can be further approximated. Keeping that only the first three terms from the expression and casting the last one into series of $\Omega u / 2\sqrt{\sigma_r}$, one arrives at

$$\Pi_{rr}^{rr}(u, \Omega) = -\frac{\beta}{4\pi^2 \lambda^3} \left[\frac{\sqrt{\pi}}{2} F\left(\frac{1}{2}, \sigma_r\right) + i \frac{\Omega u}{4\sigma_r} \right]. \quad (35)$$

Using Eqs. (30d) and (34) for Γ one can obtain

$$\Gamma = \frac{\lambda}{\beta \hbar} \frac{P + Q + R + c_s [Q(P + R) + 4PR]}{\hat{p} + \hat{q} + \hat{r} + c_s [\hat{q}(P + R) + Q(\hat{p} + \hat{r}) + 4(P\hat{r} + \hat{p}R)]}, \quad (36)$$

where P , Q , and R are given by Eqs. (15) and

$$\hat{p} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_+}, \quad (37a)$$

$$\hat{q} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_0}, \quad (37b)$$

$$\hat{r} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_-}. \quad (37c)$$

The numerator of the damping parameter (36) is equal to the denominator of the static, homogeneous susceptibility (14). Accordingly the damping rate Γ vanishes at $T=T_c$ (for $B=B_c$, where the transition is continuous) and Γ is proportional to the inverse of the susceptibility (14) for $T \approx T_c$, like in conventional theory.

VI. SUMMARY AND DISCUSSION

We have studied the statistical physics of the spin-1 Bose gas with ferromagnetic coupling in the presence of a magnetic field both from the static and dynamical points of view. The equation of state and the phase diagram of the system were investigated for both Bose-Einstein-condensed and -uncondensed phases. Near the transition we generalized to nonzero magnetic field the investigation made by Gu and Klemm [17]. The discussion of other static quantities and the dynamics is concentrated to the noncondensed phase, where the purely magnetic phase transition takes place, which occurs prior the Bose-Einstein condensation if the spin-flipping coupling constant ($|c_s|$) is large enough.

This magnetic transition was found to be of first order in general. There is always a critical magnetic field value where the magnetic transition is continuous, and above that there is no phase transition at all (magnetization behaves analytically). There is also a tricritical point (at $\epsilon_s = \epsilon_s^{(1)} \approx 1.22$, $T \approx 1.58$) when the critical magnetic field reaches zero. Above this value of ϵ_s the usual paramagnetic-ferromagnetic phase transition occurs in zero external magnetic field. The static susceptibility $(\partial m / \partial B)_{T,n}$ shows a divergence at the critical points of the continuous MT, while it has only a cusp at the point of the BEC.

The long-wavelength dynamics also exhibits features of the MT. The longitudinal spin excitation becomes a soft mode in accordance with the diverging susceptibility in the vicinity of the critical point of the MT. Moreover, the soft mode in the RPA behaves like in conventional theory; close to T_c the damping rate is proportional to the inverse of the susceptibility.

Some remarks are appropriate about our approach, which amounts to a magnetic mean-field theory. Mean-field theory in magnetism has been proved to be at least qualitatively correct in a wide range of magnetic systems. Moreover, the magnetic transitions we have been interested in are close to the Bose-Einstein condensation; the qualitatively correct description of the latter one is therefore mandatory for our purposes. The Hartree approximation, which is behind the magnetic mean-field theory at the atomic degrees of freedom, produces a continuous Bose-Einstein condensation in the absence of a spin-dependent interaction in contrast to the Hartree-Fock approach which leads to a first-order transition in this case [24,35,37,38].

The conservation of the total magnetization influences the behavior of the spinor Bose gas significantly [3,5,13–16]. The question arises as to how our results can be applied when keeping the magnetization fixed. For this purpose one

has to introduce a Lagrange multiplier, which appears in our equations in the same way as the external magnetic field. Consequently, one can conceive B in Eq. (1) as a linear combination of them. Keeping m fixed and changing the temperature, the parameter B is determined by the equation of state. Entering a two-phase region the system with homogeneous magnetization becomes unstable and a phase separation sets in. In suitable proportions the two stable magnetizations combine to produce the given total magnetization.

Though our purpose has been to further investigate the theoretically interesting problem—namely, the interplay between the magnetic properties of a spinor gas and the relevant Bose statistics—a few remarks are also in order about possible experimental observations of our findings. It has been shown [3,5] that one can investigate fine magnetic effects, because after a suitable transformation the Lagrange multiplier cancels the homogeneous magnetic field and what counts is a position-dependent magnetic field, which can be almost arbitrarily small. Our magnetic field might correspond to the local value of this magnetic field, and our cal-

culaton can be valid in the local density approximation. Note that in the experiment (since the sample was prepared to have zero magnetization) magnetic fields with opposite directions are always simultaneously present, ensuring in this way conservation of the total magnetization. If it were possible to carry out such an experiment, in which the magnetic field reaches the two-phase region, even double hysteresis could be detected, similarly as was done in the case of the ferroelectric system [30,31], by applying a time-dependent magnetic field gradient.

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