Phase separation of ferromagnetic spin-1 Bose gases in non-zero magnetic field

G. Szirmai^{1,a}, K. Kis-Szabó², and P. Szépfalusy^{2,3}

- Research Group for Statistical Physics of the Hungarian Academy of Sciences, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary

² Department of Physics of Complex Systems, Roland Eötvös University, Pázmány Péter sétány 1/A, 1117 Budapest, Hungary

³ Research Institute for Solid State Physics and Optics of the Hungarian
-

1525 Budapest, Hungary

Received 28 February 2005 / Received in final form 31 May 2005 Published online 9 August 2005 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2005

Abstract. Properties of ferromagnetic spin-1 Bose gases above and at the temperature of Bose-Einstein condensation are studied in the presence of a magnetic field. The equation of state is given in a mean-field approximation. It is found that there exists a critical magnetic field and below that two phases coexist with different particle densities. The stability of the system is also investigated with the help of the susceptibility matrix. The dynamics of the system is worked out in the Random Phase Approximation and the soft mode corresponding to the critical point is given.

PACS. 03.75.Mn Multicomponent condensates; spinor condensates – 03.75.Hh Static properties of condensates; thermodynamical, statistical and structural properties – 67.40.Db Quantum statistical theory; ground state, elementary excitations

1 Introduction

The realization of Bose-Einstein condensation (BEC) in magnetic traps of dilute, alkali metal atoms [1,2] has given new motivations to the investigation of the properties of many-particle Bose systems. With the appearance of optical trapping methods [3–7] it became possible to confine simultaneously all the $m_f \in \{-f \dots f\}$ Zeeman sublevels of the (hyperfine) spin-f atom, which initiated the experimental studies of the magnetic properties of dilute, spinor Bose gases. The scope of the theoretical investigation of the properties of spinor Bose gases is rather wide-ranging, aiming at a lot of novel and interesting phenomena, such as the topological structure of the condensate wavefunction [8,9], the multiple condensation due to the conservation of the total magnetization [10,11], the properties of elementary excitations [12–14], and a lot more.

Another interesting question is the interplay between Bose statistics and the magnetic properties of the spinor gas [15–19], moreover since the tendency towards ferromagnetic ordering is already present in the case of the ideal Bose gas, due to quantum correlations alone. The subject of this paper is to further analyze this interplay for the homogeneous spin-1 Bose gas in external magnetic field and with a ferromagnetic pairwise interaction.

The magnetic transition before the Bose-Einstein condensation was studied already in the absence [15] and also in the presence [19] of an external magnetic field assuming a single valued density. We concentrate on the fact, that the appearance of a first order phase transition of the gas can result in a phase separation leading to two coexisting phases with different particle densities and magnetizations. The single valued, homogeneous density can be obtained only in the "rigid" limit, when the compressibility of the system is zero, and the coexisting phases have the same density. The analysis is carried out above and at the Bose-Einstein condensation temperature in a mean-field calculation. Our aim is to study the behavior of the system determined mutually by the density and spin degrees of freedom, both from the static and dynamical points of view for temperatures above and at the temperature of Bose-Einstein condensation as a function of the magnetic field.

The outline of the paper is as follows. In Section 2, the system is specified with the help of its Hamilton operator. In Section 3, the equation of state of the homogeneous, ferromagnetic spin-1 Bose gas in the framework of the Hartree approximation is revisited. The resulting set of equations are solved for the particle density, the magnetization density, while keeping constant the volume of the system and the intensive parameters, the temperature, the chemical potential and the magnetic field. The phase

e-mail: szirmai@complex.elte.hu

diagram is given for temperature values above and at the Bose-Einstein condensation temperature. The found rich structure of the phase diagram is analyzed and its special points are discussed. In Section 4, a stability analysis is performed. Section 5, discusses the phase separation during the first order transition. In Section 6, the collective dynamics of the system is studied in the framework of the Random Phase Approximation. Finally Section 7, is devoted for further discussions.

2 The model

The Hamilton operator of the low temperature, homogeneous, dilute, spin-1 Bose gas in magnetic field takes the following form [8,9]:

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

where $e_k = \hbar^2 k^2 / 2M$ is the kinetic energy of an atom (with M the mass of an atom), μ is the chemical potential, g is the gyromagnetic ratio, μ_B is the Bohr magneton, and B is the modulus of the homogeneous magnetic field pointing towards the direction of the *z* -axis, V is the volume of the system. The operators $a_r^{\dagger}(\mathbf{k})$ and $a_r(\mathbf{k})$ create and destroy one-particle plane wave states with momentum **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:

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

$$
F_z = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{bmatrix}.
$$
 (2)

In equation (1) the pairwise interaction is given by momentum independent s-wave scattering, with the following tensorial structure:

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

where c_n and c_s are coupling constants related to the s-wave scattering lengths, a_0 and a_2 , in the total spin channel 0 and 2, respectively, in the following way:

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

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

In a so-called ferromagnetic system, such as studied here, $a_0 > a_2$, and correspondingly $c_s < 0$. For such a system ferromagnetic ordering is favored at low enough temperatures even in the absence of a magnetic field [8,9].

The Hamiltonian (1) has an $U(1) \times SO(3)$ symmetry and therefore the total particle number and the total spin are conserved. However it is practical to carry out calculations in the grand-canonical ensemble while ensuring the conservation of the above quantities with the introduction of two Lagrange multipliers, namely the chemical potential μ , already incorporated in equation (1) and the multiplier η , which shows up in the modified Hamiltonian as $\eta \sum_{\mathbf{k}} (F_z)_{rs} a_r^{\dagger}(\mathbf{k}) a_s(\mathbf{k})$ [7]. The terms containing η and B can be added to a modified magnetic field $B' = B + \eta/g\mu_B$. We consider the magnetic field in equation (1) in this sense and omit the prime for notational simplicity.

3 Equation of state

The equation of state of the spin-1 Bose gas can be obtained in different approximations. The Hartree approximation [12,19] gives a set of equations for the particle and magnetization density of atoms in the gas and it is equivalent with a mean-field theory in a "molecular field" approach.

The first equation gives the particle density

$$
n = n'_{+} + n'_{0} + n'_{-}, \tag{5}
$$

where $n = N/V$ is the density of the particles in the gas,

$$
n'_{r} = \sum_{\mathbf{k}} n'_{\mathbf{k},r} \tag{6a}
$$

is the density of non-condensed atoms in spin projections $r = +, 0, -$ and

$$
n'_{\mathbf{k},r} = \frac{1}{e^{\beta \epsilon_{\mathbf{k},r}^{\mathrm{H}}} - 1},\tag{6b}
$$

$$
\epsilon_{\mathbf{k},r}^{\mathrm{H}} = e_{\mathbf{k}} - \mu + c_n n + r(c_s m - g\mu_B B). \tag{6c}
$$

The density of condensed atoms is assumed zero throughout this paper. In equation (6c) m is the magnetization density [see Eq. (7)] and $\beta = 1/k_BT$ is the inverse temperature. The term rc_sm plays the same role as the "molecular field" in conventional ferromagnetic theories. The closing equation is written for the magnetization density, expressed in the following form:

$$
m = n'_{+} - n'_{-}.
$$
 (7)

Equations (5), (6) and (7) form a closed set of equations, which can be solved self-consistently to the particle and magnetization density in knowledge of the temperature, magnetic field and chemical potential.

Fig. 1. Figures (a) and (c) show the particle density and magnetization density as functions of the chemical potential for several values of the magnetic field, while figures (b) and (d) show the same quantities as functions of the magnetic field for several values of the chemical potential. Particle density and magnetization density are given in units of $n_c^{\text{(id)}}$, the chemical poten-
tial in units of $k_B T_0$ and tial in units of k_BT_0 and the magnetic field in units of $k_{\rm B}T_0/q\mu_{\rm B}$. The figures are plotted for $\epsilon_n = 90$ and $\epsilon_s = 0.9$.

It can be easily seen that under the scale transformation

$$
T = \gamma T,\tag{8a}
$$

$$
B = \gamma B,\tag{8b}
$$

$$
\widetilde{\mu} = \gamma \mu,
$$
\n(8c)\n
$$
\widetilde{n} = \gamma^{\frac{3}{2}} n,
$$
\n(8d)

$$
\widetilde{m} = \gamma^{\frac{3}{2}} m,\tag{8e}
$$

$$
\widetilde{c_n} = \gamma^{-\frac{1}{2}} c_n,\tag{8f}
$$

$$
\widetilde{c_s} = \gamma^{-\frac{1}{2}} c_s. \tag{8g}
$$

the equations of state (5) , (6) , (7) are invariant. A scaling parameter T_0 can be introduced, defined for temperature T by the expression

$$
T = 1.425 T_0. \t\t(9)
$$

The numerical factor has been chosen such a way that $n = n_c^{(\text{id})}$ line be at about the middle of the Figure 1a. This choice is also motivated by a later discussion in Section 5. Here $n_c^{(id)}$ is the critical density of the spin-1 ideal Bose gas at zero magnetic field, as given by

$$
n_c^{\text{(id)}} = \frac{3\Gamma\left(\frac{3}{2}\right)\zeta\left(\frac{3}{2}\right)}{(2\pi)^2\lambda_0^3},\tag{10}
$$

where $\Gamma(s)$ is the standard gamma-function and λ_0 is dewhere **1** (s) is the standard gamma-function and λ_0 is defined through the thermal wavelength $\lambda(T) = \hbar / \sqrt{2Mk_BT}$ with $\lambda_0 = \lambda(T_0)$.

It is convenient to define the following dimensionless parameters

$$
\epsilon_n = \frac{c_n n_c^{\text{(id)}}}{k_B T_0},\tag{11a}
$$

$$
\epsilon_s = \frac{|c_s| n_c^{\text{(id)}}}{k_B T_0}.\tag{11b}
$$

Solutions of the equations of state $(5-7)$ are shown Figure 1 for $\epsilon_n = 90$, $\epsilon_s = 0.9$. In Figures 1a and 1c the particle density and magnetization density are plotted versus the chemical potential for several values of magnetic field. For relative high magnetic fields there is only one value of the particle density and the magnetization density for a given value of the chemical potential. By decreasing the magnitude of the magnetic field a critical point shows up at B_c and μ_c . If B is smaller then B_c there is a region of the chemical potential, where equations of state give more than one solution for particle density and magnetization, representing a first order transition.

One can make a similar discussion regarding Figures 1b and 1d with reversing the roles of the chemical potential and magnetic field. The critical point is of course the same and the first order transition will occur if the chemical potential is larger than its critical value.

By solving the equations of state, one can find the full phase diagram of the system in the (μ, B, T) space, which is plotted in Figure 2 for $c_n/|c_s| \approx 151.5$ in arbitrary units. The magnetic transition is of first-order in the shaded surface and the blue line indicates the magnetic

Fig. 2. The phase diagram of the spin-1 Bose gas performed in the (μ, B, T) space for $c_n/|c_s| \approx 151.5$. The quantities μ , T, B are given in arbitrary units. The magnetic transition is first-order in the shaded surface and the blue line indicates the magnetic critical points. The red surface is related to BEC and the red line locates the tricritical points of the BEC. Between the points $(\mu = 0, B = 0, T = 0)$ and $(\mu^{(3)}, B^{(3)}, T^{(3)})$ the red and blue lines run together. In the region bounded by the red line and $B = 0$ line the BEC is first-order, while outside it is continuous. The tricritical point of the magnetic transition is at $(\mu^{(1)}, B = 0, T^{(1)})$.

critical points. There is another surface colored to red, which is related to BEC. The red line locates the tricritical points of the BEC and is common for the two surfaces. Moreover between the points $(\mu = 0, B = 0, T = 0)$ and $(\mu^{(3)}, B^{(3)}, T^{(3)})$ the red and blue lines run together. The region bounded by the red line and $B = 0$ line is common for the two surfaces and the BEC is of first-order (as the magnetic transition). Outside this region the two surfaces separate and the red one is the location of the continuous BEC-s. The magnetic transition also has a tricritical point at $(\mu^{(1)}, B = 0, T^{(1)})$. For $\mu > \mu^{(1)}$ the blue line indicates the points of the continuous magnetic transitions.

The calculations were carried out in a simple meanfield theory, where $c_s m$ can be conceived as a molecular field. Starting, however, with a Hartree–Fock theory the model cannot be formulated as a magnetic molecular field theory. The arising most important difficulty is that it leads to a first-order BEC even if it is believed to be continuous as in the scalar Bose gas.

4 Thermodynamical derivatives and the stability matrix

After discussing the possible phases of the system, one should raise a question concerning their stability. Investigating this point it is convenient to introduce the following matrix:

$$
\chi = \begin{bmatrix} \left(\frac{\partial n}{\partial \mu}\right)_{T,B} & \left(\frac{\partial n}{\partial B}\right)_{T,\mu} \\ \left(\frac{\partial m}{\partial \mu}\right)_{T,B} & \left(\frac{\partial m}{\partial B}\right)_{T,\mu} \end{bmatrix} . \tag{12}
$$

A lengthy but straightforward calculation leads to the expressions (13)

$$
\left(\frac{\partial n}{\partial \mu}\right)_{T,B} = \frac{P + Q + R + c_s[(P + R)Q + 4PR]}{[1 + c_n(P + Q + R)][1 + c_s(P + R)] - c_n c_s(P - R)^2}, \quad (13a)
$$

$$
\left(\frac{\partial n}{\partial B}\right)_{T,\mu} = g\mu_B \frac{P-Q}{[1+c_n(P+Q+R)][1+c_s(P+R)]-c_n c_s(P-R)^2},\tag{13b}
$$
\n
$$
\left(\frac{\partial m}{\partial \mu}\right)_{T,B} = \frac{P-Q}{[1+c_n(P+Q+R)][1+c_s(P+R)]-c_n c_s(P-R)^2},\tag{13c}
$$

$$
\left(\frac{\partial m}{\partial B}\right)_{T,\mu} = g\mu_B \frac{P + R + c_n[(P + R)Q + 4PR]}{[1 + c_n(P + Q + R)][1 + c_s(P + R)] - c_n c_s(P - R)^2},\tag{13d}
$$

where

$$
P = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} \mathcal{F}\left(\frac{1}{2}, \beta \left[c_n n - \mu + (c_s m - g \mu_B B)\right]\right),\tag{14a}
$$

$$
Q = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} \mathcal{F}\left(\frac{1}{2}, \beta[c_n n - \mu]\right),\tag{14b}
$$

$$
R = \frac{\beta \Gamma\left(\frac{3}{2}\right)}{(2\pi)^2 \lambda^3} \mathcal{F}\left(\frac{1}{2}, \beta[c_n n - \mu - (c_s m - g\mu_B B)]\right). \tag{14c}
$$

Here $F(s, \gamma)$ is the Bose-Einstein integral with parameter s and argument γ [20].

As it can be seen in Figure 1a, when B is large enough the derivative of the $n(\mu)$ curve is always positive. Decreasing the magnetic field below the critical value B_c the curves have some part, where the derivative becomes negative. For smaller magnetic fields the negative derivative of $n(\mu)$ passes into positive again in a small region of the unstable part, but at this time the system is still unstable. The stability is related to the eigenvalues of the susceptibility matrix, namely it requires that the eigenvalues be positive.

The eigenvalues ζ_1, ζ_2 of the inverse matrix of (12) are plotted in Figure 3 for the situation of Figures 1a and 1c. The figure shows clearly how the system becomes unstable. When the magnetic field goes to its critical value the eigenvalue ζ_2 becomes zero at the critical chemical potential μ_c . Below the critical magnetic field ζ_2 has three values in a chemical potential region, one of them is negative, which shows an instability. Meantime the other eigenvalue, ζ_1 is positive and barely changes. It demonstrates clearly, that the stability of the system cannot be determined by a thermodynamical derivative, but depends on the eigenvalues of the susceptibility matrix. To determine the stable phases one has to do a Maxwell construction, which is carried out in Section 5.

For later purpose we determine the derivative of the magnetization with respect to the magnetic field at fixed T and n. Carrying out a calculation similar to the one that leads to equations (13) one finds:

$$
\left(\frac{\partial m}{\partial B}\right)_{T,n} = g\mu_B \frac{(P+R)Q + 4PR}{P+Q+R+c_s[(P+R)Q+4PR]}.
$$
\n(15)

As long as the gas is uniform equation (15) is valid without restriction.

5 Phase transition at constant particle number

In this section we consider the situation, where the total particle number is fixed (besides the volume) and the strength of the magnetic field is varied (lowered from a relatively high starting value). Graphically this means that we cross the curves of constant magnetic fields with a horizontal line in Figure 1a. As long as the magnetic field is large enough only one phase exists, which is uniform and stable. Decreasing the magnetic field the behavior of the system depends on the value of the fixed n . If n is sufficiently larger or sufficiently smaller than $n = n_c^{(id)}$, we go through points representing stable states. Otherwise the horizontal line will intersect one or more curves at points representing metastable or unstable states. Physically this means that the system does not remain uniform, there will be two phases in equilibrium with each other and the fixed n means the average particle density. The Maxwell construction (keeping the magnetic field fixed) gives the value of the chemical potential and the particle densities n_1 and n_2 of the two phases. The average particle density can be written in the following form:

$$
n = \alpha n_1 + (1 - \alpha)n_2,\tag{16}
$$

which determines the parameter α . The densities n_1 , n_2 and the parameter α are functions of n, B and T. Denoting by m_i the magnetization density of the phase with particle density n_i , the average magnetization reads

$$
m = \alpha m_1 + (1 - \alpha)m_2. \tag{17}
$$

It is interesting to examine first, how the magnetization behaves when the temperature is specified through (9), (10) in such a manner that the prescribed density is equal to $n_c^{(\text{id})}$. With the procedure described above one can get the magnetization as a function of the magnetic field. In Figure 4 it is given at different values of ϵ_n . As long as $c_n/|c_s|$ is finite there are two phases with different magnetization and the average magnetization density is given by equation (17). If $c_n/|c_s|$ goes to infinity the system remains homogeneous. Furthermore a critical point shows up in this limit, where $(\partial m/\partial B)_{T,n}$ diverges [see Eq. (15)]. We denote the temperature by $T^{(c)}$ **Fig. 3.** Eigenvalues, ζ_1, ζ_2 of the inverse of the susceptibility matrix, χ as functions of the chemical potential for several values of the magnetic field. The figure is plotted for $c_n/|c_s| \approx 151.5$.

Fig. 4. Magnetization as a function of the magnetic field for several values of ϵ_n at the value of $\epsilon_s = 0.9$. The average density is fixed to $n = n_c^{\text{(id)}}$.

Fig. 5. Magnetization as a function of the magnetic field for several values of the temperature for $c_n/|c_s|\to\infty$ at fixed density, n.

for this reason. (Note that to have the location of the critical point at these parameter settings motivates the choice of the numerical factor in Eq. (9).) At the critical point $m = m^{(c)}$ and $B = B^{(c)}$. It can be seen, that the compressibility vanishes in the limit $c_n/|c_s|\to\infty$, which means that the system is rigid, the density is constant and the dynamical features are determined solely by the dynamics of spin degrees of freedom. The system can be also imagined as if the atoms were localized on some kind of a "lattice" [15].

In Figure 5 the magnetization is plotted for the same value of the particle density, n as in Figure 4 for

 $c_n/|c_s|\to\infty$ at different temperatures. If the temperature is above the critical value, $T^{(c)}$ the system is uniform. Below the critical temperature a phase separation takes place for the magnetization but the particle density remains homogeneous. In this limit one gets back the model with homogeneous particle density introduced in [19].

6 Spectrum of longitudinal spin fluctuations

The dynamics of the system can be studied with the help of correlation functions of the following density operators

$$
n(\mathbf{k}) = \sum_{\mathbf{q},r} a_r^{\dagger}(\mathbf{k} + \mathbf{q}) a_r(\mathbf{q}), \qquad (18a)
$$

$$
\mathcal{F}_z(\mathbf{k}) = \sum_{\mathbf{q},r,s} (F_z)_{rs} a_r^{\dagger}(\mathbf{k} + \mathbf{q}) a_s(\mathbf{q}) \tag{18b}
$$

where $n(\mathbf{k})$ and $\mathcal{F}_z(\mathbf{k})$ denotes the particle density operator and the magnetization density operator. From these operators one can build correlation functions, which take the following forms (for $\mathbf{k} \neq 0$):

$$
D_{nn}(\mathbf{k},\tau) = -\left\langle T_{\tau}\left[n(\mathbf{k},\tau)n^{\dagger}(\mathbf{k},0)\right]\right\rangle, \tag{19a}
$$

$$
D_{zz}(\mathbf{k},\tau) = -\left\langle T_{\tau} \left[\mathcal{F}_z(\mathbf{k},\tau) \mathcal{F}_z^{\dagger}(\mathbf{k},0) \right] \right\rangle, \tag{19b}
$$

$$
D_{nz}(\mathbf{k},\tau) = -\left\langle T_{\tau}\left[n(\mathbf{k},\tau)\mathcal{F}_{z}^{\dagger}(\mathbf{k},0)\right]\right\rangle. \tag{19c}
$$

Going over to the Matsubara representation the spectrum of the collective excitations is given by the analytical continuation of the correlation functions through the real axis to the lower half complex plane.

Applying the general theory one finds the relationships between the correlation functions and the thermodynamic derivatives

$$
\left(\frac{\partial n}{\partial \mu}\right)_{T,B} = -\frac{1}{\hbar} \lim_{\mathbf{k}\to 0} D_{nn}(\mathbf{k}, 0),\tag{20a}
$$

$$
\left(\frac{\partial m}{\partial B}\right)_{T,\mu} = -\frac{g\mu}{\hbar} \lim_{\mathbf{k}\to 0} D_{zz}(\mathbf{k}, 0),\tag{20b}
$$

$$
\left(\frac{\partial n}{\partial B}\right)_{T,\mu} = -\frac{g\mu}{\hbar} \lim_{\mathbf{k}\to 0} D_{nz}(\mathbf{k}, 0),\tag{20c}
$$

which represent sum-rules. To be consistent with the applied mean-field theory we calculate the correlation functions in the Random Phase Approximation. We do not give the details of the derivation here since the basic structures remain the same as at $B = 0$, the situation investigated in [12]. Namely the polarization contribution has the same form

$$
\Pi_{rs}^{sr}(\mathbf{k}, i\omega_n) = -\frac{\delta_{rs}}{\hbar} \int \frac{\mathrm{d}^3 q}{(2\pi)^3} \frac{n_r'(\mathbf{k} + \mathbf{q}) - n_r'(\mathbf{q})}{i\omega_n - \hbar^{-1}(e_{\mathbf{k} + \mathbf{q}} - e_{\mathbf{q}})},\tag{21}
$$

where n'_r is given by equations (6). Note that the magnetic field appears only through n'_r . The correlation functions (19) in Matsubara representation can be obtained formally by the following substitutions in equations (13)

$$
P \to -\Pi_{++}^{++}(\mathbf{k}, i\omega_n),\tag{22a}
$$

$$
Q \to -\Pi_{00}^{00}(\mathbf{k}, i\omega_n), \tag{22b}
$$

$$
R \to -\Pi^{--}_{--}(\mathbf{k}, i\omega_n). \tag{22c}
$$

The correspondence is also suggested by the sumrules (20).

If the following conditions are met:

$$
\sigma_r \equiv \beta \left[c_n n - \mu - r(c_s m - g\mu_B B) \right] \ll 1, \qquad (23)
$$

 $k\lambda \ll 1, |\beta\hbar\omega| \ll k\lambda$ and $|\beta\hbar\omega| \ll 2\sqrt{\sigma_r}k\lambda$, then the contribution of (21) can be approximated as

$$
\Pi_{rr}^{rr}(k,\omega) = -\frac{\beta}{4\pi^2\lambda^3} \left[\frac{\sqrt{\pi}}{2} F\left(\frac{1}{2},\sigma_r\right) + i\pi \frac{1}{4\sigma_r} \frac{\beta \hbar \omega}{k\lambda} \right].
$$
\n(24)

This approximation assumes the frequency to be small, which is fulfilled sufficiently close to the critical point.

The magnetic transition is connected to longitudinal spin dynamics, which is however coupled to density fluctuations (as long as c_n/c_s is finite). The Fourier transform of the correlation functions (19) have the same denominators as it follows from equations (13), (20) and the discussion above. The corresponding spectrum is given by the zeroes of this common denominator. In the long wavelength limit the frequency of the excitation is purely imaginary and linear in the wavenumber:

$$
\omega(k) = -i\Gamma k.\tag{25}
$$

Using Eq. (24) one can obtain the expression of Γ :

$$
\Gamma = -\frac{\lambda}{\beta \hbar} \frac{[1+c_n(P+Q+R)][1+c_s(P+R)] - c_n c_s (P-R)^2}{c_n(\hat{p}+\hat{q}+\hat{r}) + c_n c_s [\hat{q}(P+R) + Q(\hat{p}+\hat{r}) + 4(P\hat{r}+\hat{p}R)] + c_s(\hat{p}+\hat{r})}
$$
\n(26)

where

$$
\hat{p} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_+},\tag{27a}
$$

$$
\hat{q} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_0},\tag{27b}
$$

$$
\hat{r} = \frac{\beta}{16\pi\lambda^3} \frac{1}{\sigma_{-}},\tag{27c}
$$

and P, Q, R are given by equations (14). One can see the numerator of Γ is equal to the denominator of the susceptibility (13d), so $\omega(k)$ becomes soft near the critical point like in conventional theory.

7 Summary and discussion

We have studied the magnetic properties of the homogeneous, ferromagnetic, spin-1 Bose gas above the temperature of BEC in the absence and in the presence of a magnetic field. The phase diagram of the system was given in the space of intensive thermodynamical parameters for temperature values higher than that of the BEC

[Fig. 2]. The tricritical point of the magnetic transition $(\mu = \mu^{(1)}, B = 0, T = T^{(1)})$ was numerically estimated for $c_n/|c_s| \approx 151.5$. Varying the temperature for $\mu > \mu^{(1)}$ fixed (or the chemical potential for $T > T^{(1)}$ fixed) there is a magnetic transition only at $B = 0$ showing a continuous character, while for $\mu < \mu^{(1)}$ (or for $T < T^{(1)}$) the transition is of first order and survives even in the presence of a magnetic field up to $B_c(\mu)$ (or $B_c(T)$) which can be understood as a critical point. We have showed that the first order magnetic transition is always accompanied by a phase separation, i.e. the particle densities of the coexisting magnetic phases are also different. The difference between the two densities vanishes in the limit $c_n/|c_s|\to\infty$ (rigid limit).

At the critical point $B_c(\mu)$ (or $B_c(T)$) the static and long wavelength limit of the longitudinal spin correlation function $D_{zz}(\mathbf{k} \to 0,0)$ diverges, as is expected on general grounds. Since in a magnetized phase D_{nn} and D_{zz} hybridize [12] D_{nn} also diverges in this critical point, resulting in a vertical tangent in the $n-\mu$ diagram of a given isotherm at temperature T and $B = B_c(T)$ [see Fig. 1a]. The critical magnetic field is higher than that obtained in the rigid limit [19], indicating that phase separation in the density drives the system towards phase transition. It is also interesting to note that in the rigid limit density fluctuations are suppressed and $D_{nn}(\mathbf{k} \to 0,0)$ is zero. As a signal of this property one can find an $n - \mu$ diagram of the nonrigid system for a magnetic field value smaller than $B_c(T)$, where the curve has a point with a horizontal tangent (corresponding to $D_{nn}(\mathbf{k} \to 0,0) = 0$). Further decreasing the magnetic field the tangent reaches positive values inside the unstable region of the isotherm [see Fig. 1a]. However as the stability analysis shows this part of the isotherm still remains unstable as ζ_2 remains negative [see Fig. 3].

The investigations performed here become even more interesting when applied to situations with constant particle number and magnetic moment. To obtain an isotherm with prescribed particle number one has to read the value of the chemical potential from the $n-\mu$ diagram of the system. When the system is in a state of coexisting phases the Maxwell construction yields the chemical potential and the weight of the two phases. The chemical potential thus determined, the magnetization can be read from the $m-\mu$ isotherm or already yielded by Maxwell construction for the state of coexisting phases. With such a procedure one obtains an $m-B$ diagram of the system [Fig. 4]. With the total magnetization also prescribed one obtains the magnitude of the magnetic field, which, we recall now, is the addition of the external magnetic field and the Lagrange multiplier η . The first order transition can be observed through phase separation in this case.

Furthermore the magnetic phase transition can be observed also through the dynamical properties of the system. As shown, the excitation spectrum of the longitudinal spin fluctuations is a Lorentzian, centered around zero frequency. The full width of half maximum, i.e. equation (26), vanishes at the critical point showing the character of a soft mode.

Finally we note that the extension of the Hartree approximation to the Bose-Einstein condensed phase provides a consistent description of the dynamics in the whole temperature region (see [12] for $B = 0$ and [21] for $B \neq 0$, and for the analogous problem in case of the scalar condensates [22] and references therein). In particular it reproduces the well known results at $T = 0$ [8,9], while it leads to Landau-type dampings for the collective modes (including density wave and various spin waves) [12]. The key point is that a series of diagrams common in the random phase approximation are generated in the self energies from the self-consistent Hartree loop due to the presence of the condensate.

The present work has been supported by the Hungarian National Research Foundation under Grant No. OTKA T046129.

References

- 1. M.H. Anderson, J.R. Ensher, M.R. Matthews, C.E. Wieman, E.A. Cornell, Science **269**, 198 (1995)
- 2. K.B. Davis, M.-O. Mewes, M.R. Andrews, N.J. van Druten, D.S. Durfee, D.M. Kurn, W. Ketterle, Phys. Rev. Lett. **75**, 3969 (1995)
- 3. D.M. Stamper-Kurn, M.R. Andrews, A.P. Chikkatur, S. Inouye, H.-J. Miesner, J. Stenger, W. Ketterle, Phys. Rev. Lett. **80**, 2027 (1998)
- 4. J. Stenger, D.M. Stamper-Kurn, M.R. Andrews, A.P. Chikkatur, S. Inouye, H.-J. Miesner, W. Ketterle, J. Low Temp. Phys. **113**, 167 (1998)
- 5. J. Stenger, S. Inouye, D.M. Stamper-Kurn, H.-J. Miesner, A.P. Chikkatur, W. Ketterle, Nature **396**, 345 (1999)
- 6. H.-J. Miesner, D.M. Stamper-Kurn, J. Stenger, S. Inouye, A.P. Chikkatur, W. Ketterle, Phys. Rev. Lett. **82**, 2228 (1999)
- 7. D. Stamper-Kurn, W. Ketterle, in *Les Houches, Session LXXII, Coherent atomic matter waves*, edited by R. Kaiser, C. Westbrook, F. David (EDP Sciences, Les Ulis; Springer-Verlag, Berlin, 2001), p. 137
- 8. T.-L. Ho, Phys. Rev. Lett. **81**, 742 (1998)
- 9. T. Ohmi, K. Machida, J. Phys. Soc. Jpn **67**, 1822 (1998)
- 10. T. Isoshima, T. Ohmi, K. Machida, J. Phys. Soc. Jpn **69**, 3864 (2000)
- 11. W. Zhang, S. Yi, L. You, Phys. Rev. A **70**, 043611 (2004)
- 12. P. Sz´epfalusy, G. Szirmai, Phys. Rev. A **65**, 043602 (2002)
- 13. G. Szirmai, P. Sz´epfalusy, K. Kis-Szab´o, Phys. Rev. A **68**, 023612 (2003)
- 14. S. Ohtsuka, S. Kurihara, Phys. Rev. A **68**, 013601 (2003)
- 15. Q. Gu, R.A. Klemm, Phys. Rev. A **68**, 031604(R) (2003)
- 16. M. Simkin, E. Cohen, Phys. Rev. A **59**, 1528 (1999)
- 17. A. S¨ut˝o, J. Phys. A **26**, 4689 (1993)
- 18. Q. Gu, K. Bongs, K. Sengstock, Phys. Rev. A **70**, 063609 (2004)
- 19. K. Kis-Szabó, P. Szépfalusy, G. Szirmai, Phys. Rev. A (2005, accepted); e-print arXiv:cond-mat/0410501
- 20. J.E. Robinson, Phys. Rev. **83**, 678 (1951)
- 21. K. Kis-Szabó, P. Szépfalusy, G. Szirmai, to be published
- 22. A. Griffin, in *Excitations in a Bose-condensed liquid* (Cambridge University Press, Cambridge, 1993)