Physics Letters A 379 (2015) 2619–2622

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Lower bound for the variation of the hyperfine populations in the ground state of spin-1 condensates against a magnetic field

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ARTICLE INFO

Article history:
Received 11 April 2015
Received in revised form 6 June 2015
Accepted 8 June 2015
Available online 10 June 2015
Communicated by V.A. Markel

Keywords:
Spin-1 condensates
Hyperfine populations
Ground state
Effect of magnetic field

ABSTRACT

A simple and analytical expression for the variation of the lower bound and upper bound of the population density ρ_0 of hyperfine component $\mu = 0$ particles in the ground state of spin-1 condensates against a magnetic field B has been derived. The lower bound has a distinguished feature, namely, it will tend to the actual ρ_0 when B tends to zero and infinite. This feature assures that, in the whole range of B, the lower bound can provide an effective constraint. Numerical examples are given to demonstrate the applicability of the bound.

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The spinor condensates, as tunable systems with active spin-degrees of freedom, are rich in physics and promising in application. Since the pioneering experiment on spin-1 condensates [1] the study of spin-f systems becomes a hot topic. In this study an important observable is the population of the particles lying in a given hyperfine-component $\mu = -f$ to f. This quantity is popularly measured in various experiments and is a key to relate experiments to theories [1–5].

Let the population density of $\mu = 0$ particles in the ground state (g.s.) of spin-1 condensates be denoted as ρ_0. Recently, an inequality for the lower bound of ρ_0 under a magnetic field B has been derived [6]. However, when the related parameters are given in a broad domain frequently accessed in experiments, this lower bound appears as a negative value (refer to Appendix A). Since a negative lower bound for a positive value is not useful, a substantial improvement is necessary.

The aim of this paper is to derive an applicable lower bound for ρ_0 so that it could be qualitatively known before any precise theoretical calculations and/or experimental measurements are performed. In Ref. [6] the term $\langle \Phi_{gs}|\hat{V}|\Phi_{gs}\rangle$ (where Φ_{gs} is the g.s. wave function and $\hat{V}$ is the total interaction) is assumed to be non-negative, and its minimum (which is zero) is used to derive the inequality. Alternatively, we think that $\langle \Phi_{gs}|\hat{V}|\Phi_{gs}\rangle$ is an important term, therefore it has been fully taken into account in our derivation. In addition, a reasonable approximation for Φ_{gs} has been introduced. In this way, a much higher lower bound together with an upper bound for ρ_0 can be obtained. Besides, the bound given in [6] is only for the case with the total magnetization $M = 0$. However, under a magnetic field B, M is a good quantum number depending on how the condensate is experimentally prepared. Thus, different choices of M are allowed. Furthermore, it has been found as early as in 1998 that the g.s. of the ^{87}Rb and ^{23}Na condensates have the ferromagnetic and polar phases, respectively. Since their spin-textiles differ from each other greatly [7,8], a more precise lower bound should depend strongly on the species. Therefore, in the following derivation, both the M-dependence and the species-dependence have been considered.

Note that, for spin-1 atoms, the dipole–dipole interaction is very weak, thus the coupling between the spatial modes and spin-modes is weak (incidentally, the light-induced quasi-spin–orbit coupling is not in the scope of this paper). Furthermore, the spin-dependent force is nearly two orders weaker than the central (spin-independent) force[1] thus the spin-modes are much easier to get excited. Accordingly, a group of states free from any spatial

[1] Let c_0 and c_2 be the strengths of the spin-independent (central) and spin-dependent interaction, respectively. For ^{87}Rb, $|c_0/c_2| = 215$; while for ^{23}Na, $|c_0/c_2| = 31.9$. Thus, the spin-independent force is much stronger. Note that eq. (1) can be called the single mode approximation (SMA). However, it is not the same as the SMA usually adopted under the framework of the mean-field theory. In Eq. (1)

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http://dx.doi.org/10.1016/j.physleta.2015.06.019
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excitations would be the lowest and would contain various spin-modes. With this in mind, it is reasonable to assume that the g.s. would have all the particles falling into the same spatial state which is most advantageous for binding. Thus the g.s. appears as

$$\Phi_{\text{gs}} = \Pi_i \phi(\mathbf{r}_i)\Theta_{\text{gs}} \tag{1}$$

where Θ_{gs} denotes the total spin-state of the g.s. (see footnote 1). If some particles were not in $\phi(\mathbf{r}_i)$ but in a higher state, spatial excitation would be involved and therefore should be avoided. Eq. (1) is the basic assumption of this paper. The following derivation is based on this assumption.

The Hamiltonian is

$$\hat{H} = \hat{H}_0 + \hat{V}_0 + \hat{V}_2 - p\sum_i \hat{f}_{iz} + q\sum_i \hat{f}_{iz}^2 \tag{2}$$

where $\hat{H}_0 = \sum_i(-\frac{\hbar^2}{2m}\nabla_i^2 + U(\mathbf{r}_i))$ includes the kinetic and trap energies, $\hat{V}_0 = c_0\sum_{i<j}\delta(\mathbf{r}_i - \mathbf{r}_j)$ and $\hat{V}_2 = c_2\sum_{i<j}\delta(\mathbf{r}_i - \mathbf{r}_j)\ \hat{\mathbf{f}}_i \cdot \hat{\mathbf{f}}_j$, where $\hat{\mathbf{f}}_i$ is the spin-operator of the i-th particle (c_0 and c_2 are related to the scattering lengths of the spin-channels, refer to [7]). The last two terms are for the linear and quadratic Zeeman energies, where $p \propto B$ and $q \propto B^2$. An important feature of $\hat{H}$ is the conservation of M as mentioned. For convenience, $M \ge 0$ and $N - M$ being even are assumed (the generalization to other choices of M is straightforward).

For any normalized state $\Psi \neq \Phi_{\text{gs}}$, obviously we have

$$\langle\Phi_{\text{gs}}|\hat{H}|\Phi_{\text{gs}}\rangle \le \langle\Psi|\hat{H}|\Psi\rangle \tag{3}$$

Let us introduce the Fock-spin-state $|N_1, N_0, N_{-1}\rangle$, where N_μ particles are in the μ-component, $\mu = 0, \pm 1$. When M is conserved, we have $N_{\pm 1} = (N - N_0 \pm M)/2$, therefore the Fock-spin-state can be simply denoted as $|N_0\rangle$. Let us make the first choice $\Psi \equiv \Pi_i\phi(\mathbf{r}_i)|N - M\rangle$ where Ψ and Φ_{gs} have the same spatial wave function and the same magnetization M. Due to this specific choice, it is straightforward to prove

$$\langle\Phi_{\text{gs}}|\hat{H}_0 + \hat{V}_0 - p\sum_i \hat{f}_{iz}|\Phi_{\text{gs}}\rangle = \langle\Psi|\hat{H}_0 + \hat{V}_0 - p\sum_i \hat{f}_{iz}|\Psi\rangle \tag{4}$$

Furthermore, we have the identity

$$\sum_{i<j}^{N} \hat{f}_i \cdot \hat{f}_j = \frac{1}{2}\hat{S}^2 - N \tag{5}$$

where $\hat{S}$ is the operator of the total spin. In addition, for any all-symmetric total spin-state Θ, we have the equality

$$\langle\Theta|\sum_i \hat{f}_{iz}^2|\Theta\rangle = \langle\Theta|N - \hat{N}_0|\Theta\rangle \tag{6}$$

where $\hat{N}_0$ is the operator for the number of $\mu = 0$ particles.

Making use of Eqs. (4), (5) and (6), the inequality Eq. (3) can be rewritten as

$$\frac{Xc_2}{2}\langle\Theta_{\text{gs}}|\hat{S}^2|\Theta_{\text{gs}}\rangle - q\langle\Theta_{\text{gs}}|\hat{N}_0|\Theta_{\text{gs}}\rangle \le \frac{Xc_2}{2}\langle N - M|\hat{S}^2|N - M\rangle - q(N - M) \tag{7}$$

where $X \equiv \int|\phi|^4 d\mathbf{r}$. The second term at the left is just $qN\rho_0$. The first term at the right can be obtained by using the more general formula given in Eq. (A5) of Ref. [9], and we have

$$\langle N - M|\hat{S}^2|N - M\rangle = (M + 1)(2N - M) \tag{8}$$

Let the totally symmetric eigenstates of $\hat{S}^2$ and $\hat{S}_z$ be denoted as ϑ_{SM}, where $N - S$ must be even and $S \ge M$ is required. It has been proved that, for a given pair of S and M, ϑ_{SM} is unique and the set $\{\vartheta_{SM}\}$ is complete [10]. Therefore, Θ_{gs} can be expanded by this set. From the expansion, it is obvious that $M(M + 1) \le \langle\Theta_{\text{gs}}|\hat{S}^2|\Theta_{\text{gs}}\rangle \le N(N + 1)$ disregarding how Θ_{gs} is.

For $c_2 < 0$, $\langle\Theta_{\text{gs}}|\hat{S}^2|\Theta_{\text{gs}}\rangle$ could be replaced by $N(N + 1)$ because the left side of Eq. (7) would become smaller thereby so that the inequality remains hold. With this replacement, Eq. (7) can be rewritten as

$$\rho_0 \ge \frac{N - M}{N}[1 - |c_2|\frac{N - M - 1}{2q}X] \equiv B_{\text{Rb},1} \quad \text{(for Rb)} \tag{9}$$

Whereas for $c_2 > 0$, $\langle\Theta_{\text{gs}}|\hat{S}^2|\Theta_{\text{gs}}\rangle$ could be replaced by $M(M + 1)$, and we have

$$\rho_0 \ge \frac{N - M}{N}[1 - |c_2|\frac{(M + 1)}{q}X] \equiv B_{\text{Na},1} \quad \text{(for Na)} \tag{10}$$

Obviously, the right sides of Eqs. (9) and (10) are the lower bounds of ρ_0 denoted as $B_{\text{Rb},1}$ and $B_{\text{Na},1}$. Note that, when M is conserved, N_1 must be $\ge M$, and therefore N_0 must be $\le N - M$. Thus the first term of $B_{\text{Rb},1}$ and $B_{\text{Na},1}$, i.e., $(N - M)/N$, is just the upper bound of ρ_0, and the second term denotes the difference of these two bounds. Note that the second terms of Eqs. (9) and (10) are negative and $\propto 1/q$. Thus, these two inequalities demonstrate that the lower bound is uprising and tends to the upper bound when $q \to \infty$. Consequently, ρ_0 is restricted in a narrow domain between the two bounds when q is large. Therefore, the value of ρ_0 can be roughly evaluated. The evaluation would become more and more accurate when q is larger. Note that, when $q \to \infty$, N_0 should be maximized so that the quadratic Zeeman energy can be minimized. Due to this physical reason, the upper bound (in which N_0 is maximized) should be the actual value of ρ_0 when $q \to \infty$. Therefore, both $B_{\text{Rb},1}$ and $B_{\text{Na},1}$ tend to the actual ρ_0 when $q \to \infty$. This is a notable feature and is confirmed via numerical results shown below.

Let us make the second choice $\Psi \equiv \Pi_i\phi(\mathbf{r}_i)\vartheta_{NM}$ (for Rb) or $\Pi_i\phi(\mathbf{r}_i)\vartheta_{MM}$ (for Na).[2] It is reminded that, in the first choice, Ψ is close to the g.s. under a strong q. In this choice Ψ is close to the g.s. under a weak q. Accordingly, while the left side of the inequality Eq. (7) remains unchanged, the right side becomes $\frac{Xc_2}{2}N(N + 1) - q\langle\vartheta_{NM}|\hat{N}_0|\vartheta_{NM}\rangle$ (if Rb), or $\frac{Xc_2}{2}M(M + 1) - q\langle\vartheta_{MM}|\hat{N}_0|\vartheta_{MM}\rangle$ (if Na). From Eqs. (18) and (21) of Ref. [11], we have

$$\langle\vartheta_{NM}|\hat{N}_0|\vartheta_{NM}\rangle = \frac{(N - M)(N + M)}{N(2N - 1)} \tag{11}$$

and

$$\langle\vartheta_{MM}|\hat{N}_0|\vartheta_{MM}\rangle = \frac{N - M}{N(2M + 3)} \tag{12}$$

These two formulae are exact. With these formulae and with the same logic in deriving Eqs. (9) and (10), the inequality becomes

$$\rho_0 \ge \frac{N^2 - M^2}{N(2N - 1)} \equiv B_{\text{Rb},2} \quad \text{(for Rb)} \tag{13}$$

and

$$\rho_0 \ge \frac{N - M}{N(2M + 3)} \equiv B_{\text{Na},2} \quad \text{(for Na)} \tag{14}$$

Note that, $B_{\text{Rb},2}$ and $B_{\text{Na},2}$ do not depend on q and they both are $\le$ the upper bound $(N - M)/N$. Note that, when $q \to 0$, the g.s. Φ_{gs}

only the spatial wave function is bound by the SMA, while the spin-degrees of freedom are completely free.

[2] This choice is for $N - M$ being even. If $N - M$ is odd, ϑ_{MM} should be replaced by $\vartheta_{M+1,M}$ because $N - S$ must be even [10].

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