On the single mode approximation in spinor-1 atomic condensate

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We investigate the validity conditions of the single mode approximation (SMA) in spinor-1 atomic condensate when effects due to residual magnetic fields are negligible. For atomic interactions of the ferromagnetic type, the SMA is shown to be exact, with a mode function different from what is commonly used. However, the quantitative deviation is small under current experimental conditions (for \textsuperscript{87}Rb atoms). For anti-ferromagnetic interactions, we find that the SMA becomes invalid in general. The differences among the mean field mode functions for the three spin components are shown to depend strongly on the system magnetization. Our results can be important for studies of beyond mean field quantum correlations, such as fragmentation, spin squeezing, and multi-partite entanglement.

Trapped atomic quantum gases have provided a remarkable testing ground for quantum many-body theory \cite{1}. Since the discovery of the first atomic Bose-Einstein condensate \cite{2}, mean field theory has been applied with great success to these systems, arguably because 1) low energy atom-atom interaction can be simply parameterized by a s-wave scattering length \(a_{sc}\) with atoms behave as hard spheres of effective radii \(a_{sc}\); and 2) most current atomic gases are dilute with densities \(n\) satisfying \(na_{sc}^3 \ll 1\) \cite{3}. Increasingly, theoretical and experimental attentions are directed beyond mean field effects. In this regard, spinor-1 atomic condensates have become a prototype system for many recent studies \cite{4,5,6,7,8}. Several interesting results have already been obtained, e.g. multi-particle and continuous variable type entanglement \cite{4}, spin-mixing \cite{5}, spinor four-wave mixing \cite{6}, and super and coherent fragmentation \cite{7}. The single mode approximation (SMA) is often adopted for these studies when a mean-field approach with a vectorial order parameter becomes inappropriate \cite{8,9,10}. Beyond mean field quantum effects are directed both when there is no external fields \cite{4,6,9,10,11} and when there is an external magnetic or optical field \cite{12,13}. To justify the use of the SMA, earlier studies often compared with solutions of the coupled Gross-Pitaevskii (GP) equation for the different spin components and enforced an upper limit on the number of atoms \cite{8,11}. While there is not a generally adopted limit, it is typically estimated that \(N\) should be less than \(10^4\), a rather small number for current experiments.

In this paper, we investigate the validity conditions of the SMA in spinor-1 atom condensate \cite{11,12}. Our initial aim was to provide a reliable thermodynamic phase diagram for a trapped spinor-1 atomic gas \cite{12}. Surprisingly, interesting zero temperature results from the coupled GP equations reveal intricate relationships of the mode functions for the three spin components due to the constraint on the system magnetization.

We consider a spinor-1 atomic condensate in the absence of an external magnetic field. As partitioned by Law et al. \cite{11}, the system Hamiltonian, \(H\), separates into a symmetric part (under spin exchange)

\[
H_S = \int d\vec{r} \left( \Psi^\dagger_\alpha L_{\alpha \beta} \Psi_\beta + \frac{c_0}{2} \Psi^\dagger_\alpha \Psi^\dagger_\beta \Psi_\beta \Psi_\alpha \right),
\]

with \(L_{\alpha \beta} = -\hbar^2 \nabla^2 / 2M + V_{\text{ext}}\), and an asymmetric part

\[
H_A = \frac{c_2}{2} \int d\vec{r} \Psi^\dagger_\alpha (F_\eta)_{\alpha \beta} \Psi_\beta \Psi^\dagger_\mu (F_\eta)_{\mu \nu} \Psi_\nu,
\]

where \(\Psi_\alpha (\alpha = 0, \pm)\) denotes the annihilation field operator for the \(\alpha\)-th component. \(F_\eta = x,y,z\) are the spin 1 matrix representation, and a summation over repeated indices is assumed in Eqs. (1) and (2). The external trapping potential \(V_{\text{ext}}(\vec{r})\) is spin-independent as in an far-off-resonant optical dipole force trap (FORT) which makes atomic spinor degrees of freedom completely accessible. The pair interaction coefficients are \(c_0 = 4\pi \hbar^2 (a_0 + 2a_2) / 3M\) and \(c_2 = 4\pi \hbar^2 (a_2 - a_0) / 3M\), with \(a_0\) (a2) the s-wave scattering length for two spin-1 atoms in the combined symmetric channel of total spin 0 (2). The only state changing collision in Eq. (2) occurs through the coupling \(\Psi^\dagger_0 \Psi^\dagger_\pm \Psi_+ + h.c.\), which conserves the system magnetization \(M = \int d\vec{r} \langle F_\eta \rangle = \int d\vec{r} \Psi^\dagger_0 \Psi_+ - \Psi^\dagger_\pm \Psi_- \rangle\). \(M\)-changing inelastic (“bad”) collisions occur at a much longer time scale as compared with a condensate’s typical lifetime, therefore are excluded here as in all previous studies. Although the real time dynamics governed by \(H_S + H_A\) conserves the total atom number \(N = \int d\vec{r} \Psi^\dagger_0 \Psi_0 + \Psi^\dagger_\pm \Psi_\pm\) and \(M\), the ground state obtained from a global minimization of \(H_S + H_A\) is not automatically guaranteed to have the same \(N\) and \(M\). We therefore introduce separate Lagrange multipliers \(\beta\) to guarantee the conservation of \(M\) and the chemical potential \(\mu\) to conserve \(N\). The ground state is then determined by a minimization of the free energy functional \(F = H_S + H_A - \mu N - BM\). Mathematically, this task turns out to be highly nontrivial. In fact, most previous discussions on spinor-1 condensates did not minimize \(H\) under the constraint of a conserved \(M\). Therefore, their resulting ground states are the global ground states that can only be reached if the system can coherently adjust its initial \(M\) value. Such a situation is inconsistent with current experiments.
shown to lead to effects associated with density waves between spatial and spinor degrees of freedom were then system with the use of a plane wave basis. Correlations 
notable exception is the work by Ueda [20], who went 

It shares similar physics of the often used spin-charge separation in condensate matter systems. Since its introduction, the SMA has been used frequently [4, 5, 6, 7, 19]. The solid line shows 

 The solid line shows $N_0/N = (1 - M^2/N^2)/2$, while the dots are numerical results. The agreement is remarkable.

One of the strongest physics support for the SMA comes from the fact that $a_0 \sim a_2$ for a spinor-1 ($^{87}$Rb) condensate. This gives rise to $|c_2| \ll |c_0| [1, 11]$. Thus $H_A$ is much smaller as compared with $H_S$, and can be considered as a perturbation by assuming the SMA

$$
\Psi_\alpha(\vec{r}) = a_\alpha \phi_{\text{SMA}}(\vec{r}), \quad \alpha = 0, \pm,
$$
i.e., with a common mode function $\phi_{\text{SMA}}(\vec{r})$ (normalized to 1). The Fock state boson operators $a_\alpha$ satisfy $[a_\alpha, a_\beta^\dagger] = \delta_{\alpha\beta}, \ [a_\alpha, a_\beta] = 0$. $\phi_{\text{SMA}}(\vec{r})$ is determined from $H_S$ alone (without $H_A$) according to [3]

$$
\left[ -\frac{\hbar^2 \nabla^2}{2M} + V_{\text{ext}} + c_0 |\phi_{\text{SMA}}|^2 \right] \phi_{\text{SMA}}(\vec{r}) = \mu \phi_{\text{SMA}}(\vec{r}).
$$

It is less critical as the resulting Hamiltonian $H_S$ remains of the same symmetry group in the Schwinger boson representation, although with a different coefficient and the presence of additional linear terms in $J_\mu$. The validity of the SMA in this case has been tested recently using the rigorous positive P-approach [23].

For a spinor-1 condensate, however, complications arise when spin component mode functions are taken to be different. The effective Hamiltonian thus obtained contains no angular momentum symmetry at all in its corresponding Schwinger boson representation. This naturally calls for a critical investigation of the SMA. To check the validity of SMA, we start with the mean field and find separate spin component mode functions ($\Psi_\alpha = \Phi_\alpha$ at zero temperature). The dynamics of $\Phi_\alpha$ for the ground state is governed by $H_S + H_A$, which obeys the following coupled GP equation

$$
i\hbar \dot{\Phi}_+ = [H - B + c_2(n_+ + n_0 - n_-)] \Phi_+ + c_2 \Phi_0^* \Phi_-^*,
$$

FIG. 1: The $M$ dependence of $N_0$ in the ferromagnetic case. The solid line shows $N_0/N = (1 - M^2/N^2)/2$, while the dots are numerical results. The agreement is remarkable.

The same SMA is sometimes also used in a spin 1/2 system by assuming $\phi_0(\vec{r}) = \phi_1(\vec{r})$ [21, 22, 23, 24]. This is not critical as the resulting Hamiltonian $H_S$ remains of the same symmetry group in the Schwinger boson representation, although with a different coefficient and the presence of additional linear terms in $J_\mu$. The validity of the SMA in this case has been tested recently using the rigorous positive P-approach [23, 24].

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$$
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$$

FIG. 2: The original (left column) and the renormalized (right column) wave functions along radial (upper panel) and axial (lower panel) directions for the + (solid line) and the − (dashed line) spin components. Other parameters are $N = 3.16 \times 10^7$, $M/N = 0.5$, and $\lambda = 2$. All lengths are in units of $\sqrt{\hbar/m\omega}$.

$$
i\hbar \dot{\Phi}_0 = [H + c_2(n_+ + n_-)] \Phi_0 + 2c_2 \Phi_0^* \Phi_+ \Phi_-, \quad (5)
$$

with $H = -\hbar^2 \nabla^2 / 2M + V_{\text{ext}} + c_0 n_\alpha$, $n_\alpha = |\Phi_\alpha|^2$, and $n = n_+ + n_0 + n_-$. We have developed a reliable numerical algorithm based on propagating Eq. (3) in imaginary time, which converges to the ground state while maintaining the conservation of both $N$ and $M$. We take the initial wave function to be a complex Gaussian with a constant velocity, i.e., $e^{-(x^2/2\lambda_x^2 + y^2/2\lambda_y^2 + z^2/2\lambda_z^2)} e^{-i\vec{k} \cdot \vec{r}}$, where $\lambda_x$, $\lambda_y$, $\lambda_z$, and $\vec{k}$ are adjustable parameters that shall not affect the final converged solution. In the simplest case for the ground state, we assume $\Phi_\alpha(\vec{r}) = |\Phi_\alpha(\vec{r})| e^{i\theta_\alpha}$ with $\theta_\alpha$ a global phase independent of $\vec{r}$. Then only the relative phase $\Delta = 2\theta_0 - \theta_+ - \theta_-$ shows up in $J_\mu$ with a term $c_2 \Phi_0^* \Phi_+ \Phi_-^* |\Phi_\alpha|^2$. This gives $\Delta = 0$ (for $c_2 < 0$) or $\pi$ (for $c_2 > 0$) when $J_\mu$ is minimized [23], a conclusion also verified by numerical calculations. As first stated by Ho [11], the spinor-1 condensate Hamiltonian $H = H_S + H_A$ is invariant under gauge transformation $e^{i\theta}$ and spin rotations $U(\alpha, \beta, \tau) = e^{-iF_\alpha e^{-iF_\beta e^{-i\tau}}}$ for the ground state that conserves $M$, however, the spin rotation symmetry is reduced to the subgroup SO(2) generated by $e^{-iF_\alpha}$. Thus the signs of the signs of $c_2$, a transformation of the form $e^{-i\theta_0 e^{-i\tau}}$ can always reduce a complex solutions to a real one [23].

When $B = 0$ as for ferromagnetic interactions with any values of magnetization $M \leq N$ or for anti-ferromagnetic interactions with $M = 0$, we find $|\Phi_\alpha| = |\Phi_-| \Phi_\alpha$ from the symmetry of Eq. (2). We then rescale the wave function $\phi_\alpha = \Phi_\alpha / \sqrt{N_\alpha}$ such that $\phi_\alpha$ is normalized to 1 ($\int d^3 \phi_\alpha(\vec{r})^2 = N_\mu$, the number of atoms in $\mu$-th component), the asymmetric interaction energy then becomes

$$
E_A = \frac{c_2}{2} \int d\vec{r} \left[ (N_+|\phi_+|^2 - N_-|\phi_-|^2) \right]^2
$$
For ferromagnetic interactions \( (c_2 < 0 \text{ and } \Delta = 0) \), we thus prove in general that \( E_A \) is minimized when

\[
|\phi_+| = |\phi_0| = |\phi_-| = |\phi|,
\]
and \( N_0/N = (1 - M^2/N^2)/2 \). The latter result (independent of all other parameters) was first obtained in Ref. \([11]\) assuming the SMA, i.e. essentially assuming Eq. \( (5) \). Our numerical solutions closely follow this as shown in Fig. \( 1 \). For anti-ferromagnetic interactions \( (c_2 > 0) \), \( B = 0 \) holds only when \( M = 0 \). In this case, using \( \Delta = \pi \), we prove in general that \( E_A \) is minimized to zero under Eq. \( (7) \), while \( N_0 \) can be any value \( \leq N \).

For anti-ferromagnetic interactions \( (M \neq 0) \), we find that mode functions for the three spin components are different (see Fig. \( 2 \)). Further analysis show that \( E_A \) is minimized if \( N_0 = 0 \).

We now discuss the relationship of Eq. \( (7) \) to the SMA Eq. \( (4) \). We note that the validity of Eq. \( (7) \) (including \( H_A \)) is in fact not equivalent to the validity of the SMA (excluding \( H_A \)). For ferromagnetic interactions, with Eq. \( (5) \) and the relation between \( N_0 \) and \( M \), Eq. \( (8) \) simplifies to

\[
\left[ -\frac{\hbar^2 V^2}{2M} + V_{\text{ext}} + (c_0 + c_2) N |\phi|^2 \right] \phi(\vec{r}) = \mu \phi(\vec{r}).
\]

This shows that \( \phi(\vec{r}) \) is independent of \( M \), and its deviation from \( \phi_{\text{SMA}} \) comes only from the \( c_2 \) term. This result can in fact be easily understood. Since \( c_0 + c_2 = 4\pi \hbar^2 a_2/M \), \( \phi(\vec{r}) \) of Eq. \( (8) \) is simply the ground state of the GP equation for an atomic scattering length of \( a_2 \). In a ferromagnetic state, atomic spins are aligned locally. Two such atoms \( (F_{1.2} = 1) \) only collide in the symmetric total spin \( F = 2 \) channel. For quantitative results, we compared \( |\langle \phi|\phi_{\text{SMA}} \rangle| \) for \( ^{87}\text{Rb} \) atoms with \( a_0 = 101.8 a_B \) and \( a_2 = 100.4 a_B \) (\( a_B \) the Bohr radius). Other assumptions are: typical radial trap frequency \( \omega_r = 2\pi \times 10^3 \) (Hz), axial trap frequency \( \omega_z = \lambda \omega_r \), and \( \lambda = 0.1, 1, \text{ and } 10 \). We also took

\[
\langle \tilde{F}(\vec{r}) \rangle = \langle \phi(\vec{r}) \rangle^2 \left[ \sqrt{\frac{N^2 - M^2}{M}} \cos(\theta_+ - \theta_0) - \sqrt{\frac{N^2 - M^2}{M}} \sin(\theta_+ - \theta_0) \right].
\]
For anti-ferromagnetic interactions, we find
\[
\langle \vec{F}(\vec{r}) \rangle = \begin{pmatrix}
0 \\
N_+|\phi_+(\vec{r})|^2 - N_-|\phi_-(\vec{r})|^2
\end{pmatrix},
\]
(10)
a state with all spins aligned in the ±z direction. It reduces to \(\langle \vec{F}(\vec{r}) \rangle = 0\) for \(M = 0\).

To conclude, we presented both analytic and numerical studies of the validity of the SMA. We find that deviations of the ground state solution from the SMA could consist of \(\Psi(\vec{r})\) and \(|\lambda_N\rangle\), and 10 (dash-dotted line). We find that deviations of the ground state solution from the SMA become the exact ground state wave function; For \(M > 0\), however, one can still use the SMA for \(\phi_+\), but \(\phi_-\) differs significantly if both \(N\) and \(M\) are large. In this case the SMA term contributes the most to the deviation. Our conclusions from this study apply to the ground states of a spinor condensate. For dynamic problems Ref. [3], the SMA may become worse. Our study suggests that instead of making the SMA as in Eq. (3), an improved SMA could consist of \(\Psi(\vec{r}) = a_0\phi_0(\vec{r})\), where the mean-field solution \(\Phi(\vec{r})\) and its associated effective spin mode function \(\phi_0 = \Phi(\vec{r})/\sqrt{N}\) are obtained under the constraints of conserved \(\epsilon\) and \(M\). Such an approach can be important in studying beyond mean field quantum correlations. In a forthcoming article, we will report some results on condensate fragmentation.

In summary, we have presented a detailed investigation of the SMA for a spinor-1 condensate and pointed out interesting structures of its ground state for both ferromagnetic and anti-ferromagnetic interactions.

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[1] See the extensive list of references at: http://amo.phy.gasou.edu/bibliography.html.
[2] M. H. Anderson et al., Science 269, 198 (1995); K. B. Davis et al., Phys. Rev. Lett. 75, 3969 (1995); C. C. Bradley et al., ibid 75, 1687 (1995) and 79, 1170 (1997).
[3] Observation of Feshbach resonance has raised the hope that with a tunable \(a_{sc}\), one can approach the interesting limit of \(na_{sc}^2 \sim 1\), even \(na_{sc}^2 \gg 1\) when exciting new physics may occur. See for example, Eric Braaten and H-W Hammer, Phys. Rev. Lett. 87, 160407 (2001).
[4] L.-M. Duan, J. I. Cirac, and P. Zoller, quant-ph/0107055.
[5] H. Pu et al., Physica B 280, 27, (2000); C. K. Law et al., Phys. Rev. Lett. 81, 5257 (1998).
[6] E. Goldstein and P. Meystre, Phys. Rev. A 59, 3896 (1998).
[7] T.-L. Ho and S. K. Yip, Phys. Rev. Lett. 84, 4031 (2000).
[8] D. M. Stemper-Kurn et al., Phys. Rev. Lett. 80, 2027 (1998).
[9] M. Barrett et al., Phys. Rev. Lett. 87, 010404 (2001).
[10] T. Ohmi and K. Machida, J. Phys. Soc. Jap. 67, 1822 (1998).
[11] T.-L. Ho, Phys. Rev. Lett. 81, 742 (1998).
[12] C. V. Ciobanu et al., Phys. Rev. A 61, 033607 (2000).
[13] H. Pu et al., Phys. Rev. A 60, 1463 (1999).
[14] H. Pu et al., Phys. Rev. A 61, 023602 (2000).
[15] H. Pu et al., Phys. Rev. A 63, 033603 (2001).
[16] S. Raghavan et al., Opt. Commun. 188, 149 (2001).
[17] M. Koashi and M. Ueda, Phys. Rev. Lett. 84, 1066 (2000).
[18] T. Isoshima et al., J. Phys. Soc. Jpn. 69, 3864 (2000).
[19] M. Koashi and M. Ueda, Phys. Rev. Lett. 84, 1066 (2000).
[20] M. Ueda, Phys. Rev. A 63, 013601 (2000).
[21] A. S. Sorensen et al., Nature (London) 409, 63 (2001).
[22] K. Helmerson and L. You, Phys. Rev. Lett. 87, 170402 (2001).
[23] U. V. Poulsen and K. Mølmer, Phys. Rev. A 64, 013616 (2001).
[24] A. S. Sorensen, cond-mat/0110372.
[25] T. Isoshima et al., Phys. Rev. A 60, 4857 (1999); N. P. Robins et al., cond-mat/0105353.
[26] E.G.M. van Kempen et al., cond-mat/0110610.
[27] A. Crubellier et al., Euro. Phys. Jour. D 6 (2), 211 (1999).