Excitation spectrum of a toroidal spin-1 Bose-Einstein condensate

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We calculate analytically the excitation spectrum of a toroidal spin-1 Bose-Einstein condensate that is subjected to a homogeneous magnetic field and contains vortices with arbitrary winding numbers in the $m_F = \pm 1$ components of the hyperfine spin. The spectrum can be tuned by varying external parameters, such as the strength of the magnetic field. A rotonlike spectrum can be obtained, or an initially stable condensate can be made unstable by adjusting the magnitude of the magnetic field or trapping frequencies. The structure of the instabilities can be analyzed by measuring the particle density of the spin components.

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Bose-Einstein condensates (BECs) confined in toroidal traps have been subject to many experimental studies recently \cite{1,2,3}. This research covers topics such as the observation of persistent current \cite{4,5}, phase slips across a stationary barrier \cite{6}, stochastic \cite{7} and deterministic \cite{8} phase slips between vortex states, the use of toroidal condensates in interferometry \cite{9}, and the stability of superfluid flow in a spinor condensate \cite{10}. These experiments have given rise to theoretical studies discussing, e.g., the excitation spectrum and critical velocity of a superfluid BEC \cite{11,12} and the simulation of the experiment \cite{13} using the Gross-Pitaevskii equation \cite{14,15} and the truncated Wigner approximation \cite{16}. Most of the experimental and theoretical studies concentrate on the properties of persistent currents. The phase of a toroidal superfluid flow in a spinor condensate \cite{17} and the simulation of the experimental results of Refs. \cite{18,19} have been subject to many experimental studies which are straightforward to prepare experimentally and makes it possible to observe the proliferation of instabilities by measuring the density of the $m_F = 0$ component.

The order parameter of a spin-1 Bose-Einstein condensate is $\psi = (\psi_1, \psi_0, \psi_{-1})^T$, where $T$ denotes the transpose, and it fulfills the identity $\psi^\dagger \psi = n_{3D}$, where $n_{3D}$ is the total particle density. The condensate is confined in a toroidal trap given in cylindrical coordinates as $U(r, z, \varphi) = m \left[ \omega_r^2 (R - r)^2 + \omega_z^2 z^2 \right] / 2$, where $R$ is the radius of the torus and $\omega_r, \omega_z$ are the trapping frequencies in the radial and axial directions, respectively. We assume that the condensate is quasi 1D, so that the order parameter factors as $\psi(r, z, \varphi; t) = \psi_{r,z}(r, z) \psi_{\varphi}(\varphi; t)$, where $\psi_{r,z}$ is complex-valued and time independent. If the system is exposed to a homogeneous magnetic field oriented along the z-axis the energy functional becomes

$$E_{1\text{D}}[\psi_{\varphi}] = \int_0^{2\pi} d\varphi \left\{ \psi_{\varphi}^\dagger \left[ -\frac{\partial^2}{\partial \varphi^2} - \mu - p \tilde{F}_z + q \tilde{F}_z^2 \right] \psi_{\varphi} + \frac{1}{2} n \left[ g_0 (\psi_{\varphi}^\dagger \psi_{\varphi})^2 + g_2 (\hat{F}_z \psi_{\varphi})^2 \right] \right\}, \quad (1)$$

where $\epsilon \equiv h^2/2mR^2$, $\mu$ is an effective one-dimensional chemical potential, and $\mathbf{F} = (\tilde{F}_z, \tilde{F}_y, \tilde{F}_z)$ is the (dimensionless) spin operator of a spin-1 particle. The magnetic field introduces the linear and quadratic Zeeman terms, given by $p$ and $q$, respectively. The sign of $q$ can be controlled experimentally by using a linearly polarized microwave field \cite{20}. The strength of the atom-atom interaction is characterized by $g_0 = 4\pi \hbar^2 (a_0 + 2a_2) / 3m$ and $g_2 = 4\pi \hbar^2 (a_2 - a_0) / 3m$, where $a_F$ is the s-wave scattering length for two atoms colliding with total angular momentum $F$. The scattering lengths of $^{87}\text{Rb}$ used here are $a_0 = 101.8a_B$ and $a_2 = 100.4a_B$ \cite{21}, measured in units of the Bohr radius $a_B$. For $^{23}\text{Na}$ the corresponding values are $a_0 = 50.0a_B$ and $a_2 = 55.1a_B$ \cite{22}. The magnetization in the $z$-direction, $f_z \equiv \int d\varphi |\psi_{\varphi}(\varphi)|^2 / N$, is a conserved quantity; the corresponding Lagrange multiplier can be included into $p$. Here $N$ is the condensate particle number. We assume that in the initial state the spin is parallel to the $z$ axis. In \cite{23} it was argued that...
in a homogeneous system the most unstable states are almost always of this form. The initial state reads

\[ \psi_{\|}(\varphi) = \left( e^{ik_1\varphi} \sqrt{\frac{1 + f}{2} - 0}, e^{i\varphi} e^{ik_{-1}\varphi} \sqrt{\frac{1 - f}{2}} \right)^T, \tag{2} \]

where \( \theta \) is the relative phase and the integer \( k_{\pm 1} \) is the winding number of the \( m_F = \pm 1 \) component. The energy and stability are independent of \( \theta \) and therefore we set \( \theta = 0 \). If \( k_1 = 1 \) and \( k_{-1} = 0 \), \( \psi_{\|} \) describes a half-quantum vortex (Alice string), see, e.g., Refs. 16 18. The populations of \( \psi_{\|} \) are time independent and the Hamiltonian reads \( \hat{H}_g = (g_0 n - \mu) \hat{I} + (g_2 n f_2 - p_{\text{eff}}) \hat{F}_z + q_{\text{eff}} \hat{F}_z^2 \), where \( p_{\text{eff}} = p - \epsilon (k_1^2 - k_2^2) / 2 \) and \( q_{\text{eff}} = q + \epsilon (k_1^2 - k_2^2) / 2 \). The time evolution operator of \( \psi_{\perp} \) is \( \hat{U}_g(t) = e^{-it\hat{H}_g/\hbar} \). We calculate the excitation spectrum in a basis where \( \psi_{\|} \) is stationary \[ \text{13 19} \]. In this basis, the energy of an arbitrary state \( \psi \) is given by \( E_{\text{1D}}^{\psi} := E_{\text{1D}}[\hat{U}_g \psi] + \hbar i \dot{\psi} \left( \frac{\partial}{\partial \varphi} \hat{U}_g^{-1} \right) \hat{U}_g \psi \) and the time evolution of \( \psi \) can be obtained from \( \hbar \partial \psi / \partial t = \delta E_{\text{1D}}^{\psi} / \delta \psi \). We write \( \psi(\varphi; t) = \psi_{\|}(\varphi) + \delta \psi(\varphi; t) \) and expand the time evolution equation to first order in \( \delta \psi \). The perturbation is written as

\[ \delta \psi_j(\varphi; t) = e^{ik_j\varphi} \sum_{s=0}^{\infty} u_{j,s}(t) e^{is\varphi} - v_{j,s}^*(t) e^{-is\varphi}, \tag{3} \]

where \( j = 0, \pm 1 \) and \( k_0 \equiv 0 \). Straightforward calculation gives the equation

\[ i\hbar \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{w}_0 & \mathbf{w}_1 \end{pmatrix} = \left( \hat{B}_2 \oplus \hat{B}_4 \right) \begin{pmatrix} \mathbf{w}_0 & \mathbf{w}_1 \end{pmatrix}, \tag{4} \]

where \( \oplus \) indicates the direct sum of matrices and the subscript \( i \) gives the dimension of \( \hat{B}_i \). Only \( \hat{B}_2 \) depends on time. The vectors \( \mathbf{w}_0 \) and \( \mathbf{w}_{1,-1} \) are defined as \( \mathbf{w}_0 = (u_{0;0,1}^{\perp}, v_{0;0,-1})^T \) and \( \mathbf{w}_{1,-1} = (u_{1;1,0}^{\perp}, u_{1,-1}^{\perp}, v_{1;1,0}^{\perp}, v_{1,-1}^{\perp})^T \). The matrix elements of \( \hat{B}_2 \) read

\[ \begin{align*}
(\hat{B}_2)_{11} &= \epsilon (s^2 + 2g_2 n), \\
(\hat{B}_2)_{12} &= -e^{-i[(\epsilon k_1^2 + \epsilon k_2^2) + 2g_2 n]} \sqrt{1 - f_z^2}, \\
(\hat{B}_2)_{22} &= \epsilon (s - k_1 - k_{-1})^2 + 2g_2 n, \tag{5-7}
\end{align*} \]

and \( \hat{B}_{21} = -(\hat{B}_2)^*_{12} \). The operator \( \hat{B}_4 \) can be written as

\[ \hat{B}_4 = \begin{pmatrix} \epsilon s^2 \hat{I}_2 + \hat{X} + \hat{D} & -\hat{X} \\
\hat{X} & -\epsilon s^2 \hat{I}_2 - \hat{X} + \hat{D} \end{pmatrix}, \tag{8} \]

where \( \hat{I}_2 \) is the 2 \( \times \) 2 identity matrix, \( \hat{D} = 2\epsilon s \text{ diag}(k_1, k_{-1}) \), and \( \hat{X} \) is defined as

\[ \hat{X}_{11,22} = 2g_+ (1 \pm f_z), \quad \hat{X}_{12} = 2g_- \sqrt{1 - f_z^2}, \tag{9} \]

and \( \hat{X}_{21} = \hat{X}_{12} \). Here \( g_\pm \equiv (g_0 \pm g_2) n / 4 \) and \( (\pm) \) refers to \( \hat{X}_{11} (\hat{X}_{22}) \). The 6 \( \times \) 6 matrix \( \hat{B}_2 \oplus \hat{B}_4 \) is in a block diagonal form, the blocks being the \( \hat{B}_2 \) and \( \hat{B}_4 \) matrices. It is then possible to calculate the eigenvalues and eigenvectors of \( \hat{B}_2 \) and \( \hat{B}_4 \) independently. \( \hat{B}_2 \) affects only the \( m_F = 0 \) component, that is, the magnetization remains unchanged but the direction of the spin vector is modified. The corresponding modes are therefore called spin modes. For similar reasons, the eigenvalues of \( \hat{B}_4 \) are called magnetization modes.

The eigenvalues of \( \hat{B}_2 \) can be calculated straightforwardly but they are too long to be shown here. The eigenvalues are independent of \( q \) and can be written as \( \hbar \omega_j(s) = 2\epsilon g_+ + \hbar \omega_j(s) \), where \( \omega_j \) depends on \( k_- \equiv (k_1 - k_{-1}) / 2 \) but is independent of \( k_+ \equiv (k_1 + k_{-1}) / 2 \). Consequently, modes with differing \( k_+ \) but equal \( k_- \) have identical stability. We denote the real and imaginary parts of \( \omega_j \) by \( \omega_j^r \) and \( \omega_j^i \), respectively. Magnetization modes are unstable if at least one \( \omega_j \) is positive. If \( f_z = 0 \) the eigenvalues simplify and are given by

\[ h\omega_{1,2,3,4}(s)|_{f_z=0} = 2\epsilon g_+ \pm 2 \sqrt{\epsilon^2 \left( \frac{1}{4} (s^2 + 4k_2^2) + g_+ \right) + \epsilon k_1^2 (s^2 + 4g_+)} + g_2^2 \tag{10} \]

The signs are defined such that \( ++, -+, +-, \), and \( -- \) correspond to \( \omega_1, \omega_2, \omega_3, \), and \( \omega_4 \), respectively. Unstable modes appear when the term inside the square brackets becomes negative. For rubidium and sodium \( g_+ > 0 \), guaranteeing that \( \omega_1 \) and \( \omega_2 \) are real. Only \( \omega_3 \) can have a positive imaginary part, see Fig. \[ \text{11} \]. The amplitude

\[ \begin{array}{c c}
\text{Rb mag.} & \text{Na mag.} \\
(a) & (b) \\
\text{Rb spin} & \text{Na spin} \\
(c) & (d)
\end{array} \]

\[ \begin{array}{c c}
\omega_3 & \omega_3 \\
5 \quad 5 & 5 \quad 5 \\
3 \quad 3 & 3 \quad 3 \\
1 \quad 1 & 1 \quad 1 \\
0 \quad 0 & 0 \quad 0
\end{array} \]

FIG. 1. The amplitudes of the unstable spin and magnetization modes for rubidium and sodium. Here \( \epsilon = 0.75|g_2| n \), \( q = 0 \), and the unit of \( \omega_3 \) is \( |g_2| n / \hbar \). The lines have been drawn by treating \( s \) as a continuous parameter; dots indicate the actual allowed non-vanishing values of \( \omega_3(s) \). In (c) and (d) the curves are reflection symmetric with respect to \( s = k_- = (k_1 + k_{-1}) / 2 \).

of the unstable modes grows as \( |k_-| \) increases. Now the allowed values of \( s \) are integers; the modes corresponding to \( s = 0 \) are always stable, but unstable modes are
present for \( s = 1, 2, \ldots, \lfloor \sqrt{4k^2 - 2g2n/\epsilon} \rfloor \). Here \( \lfloor \cdot \rfloor \) indicates the floor function. It is therefore not possible to choose the parameters in such a way that a single mode \( s > 1 \) is unstable. A lower bound for the value of \( \epsilon \) yielding at least one unstable mode in a sodium BEC is given by the equation \( \epsilon(4k^2 - 1) \geq 2g2n \). Because \( \epsilon > 0 \), the magnetization modes of a sodium condensate \((g_2 > 0)\) with \( k_- = 0 \) and \( |k_+| = 1/2 \) are always stable. This is visualized in Fig. 1(b), where \( \omega_5^i(s) \) corresponding to \((k_1, k_-) = (0, 0)\) and \((k_1, k_-) = (2, 1)\) is seen to vanish for every \( s \). In a rubidium condensate \((g_2 < 0)\) with \( k_- = 0 \) unstable modes exist if \( \epsilon \leq 2g2n/n; \) if \( |k_-| > 0 \), instabilities are present regardless of the value of \( \epsilon \). For both rubidium and sodium the wavenumber of the fastest-growing instability is approximately given by the integer closest to \( \sqrt{2/3(4k^2 - 2g2n/\epsilon)} \). Assume next that there is one dominant unstable mode. This is in particular the case if only the \( s = 1 \) mode is unstable. Using the eigenvector corresponding to \( \omega_5^i(s)_{|f_2=0} \) we find that the position-dependent population difference \( \Delta F_z(\varphi; t) \equiv \rho_1(\varphi; t) - \rho_1(\varphi; t)\), where \( \rho_j = (|\psi_j|)_j + \delta\psi_j^2, \) is given by

\[
\Delta F_z(\varphi; t) = \alpha e^{\omega_5^i t} \cos(\theta) + \beta e^{2\omega_5^i t} \sin(2\theta),
\]

where \( \theta = \text{arg}[u_1;i(0)/2 + s_\varphi + \omega_5^i t] \) and \( \alpha \) and \( \beta \) are constants that depend on \( s, k_-, \) and the interaction coefficients. The presence of unstable magnetization modes can be experimentally confirmed by measuring \( \Delta F_z (\varphi) \). If \( k_- = 0 \) we obtain \( \beta = 0 \), leading to \( \Delta F_z \) having \( s \) peaks as a function of the coordinate \( \varphi \). For nonzero \( k_- \) both \( \alpha \) and \( \beta \) are in general nonvanishing and \( \Delta F_z \) is a sum of two competing terms with periodicity \( s \) and \( 2s \). If \( \omega_5^i(s) > 0 \) we get \( \omega_5^i(s) = 2\pi s k_+ \), so that the nodes of \( \Delta F_z \) rotate around the torus as time evolves if \( k_+ \) is nonzero. We see that although the value of \( k_+ \) does not affect the stability, it can alter the behavior of the density perturbations resulting from the instabilities.

We now turn to the spin modes. The time dependence of \( B_2 \) can be eliminated by a simple change of basis. In the new basis, the eigenvalues giving the spin modes read

\[
\hbar \omega_{5,6}(s) = 2\epsilon k_+ (s - k_+)
\]

\[
\pm \sqrt{\epsilon[(s - k_+)^2 - k_+^2] + g2n - q}^2 - (1 - f_2^2)(g2n)^2,
\]

where \( + (\sim) \) corresponds to \( \omega_5 (\omega_6) \). If \( k_+ = 0 \), the effect of vortices can be taken into account by scaling \( q \rightarrow q_{\text{eff}} = q + \epsilon k_+^2 \), i.e., the spin modes of a system with \((k_1, k_-) = (k,-k)\) and \( q = \tilde{q} \) are equal to the spin modes of a vortex-free condensate with \( q = \tilde{q} + \epsilon k_+^2 \). Spin modes are unstable only if and only if the term inside the square root is negative. Now only \( \omega_5 \) can have a positive imaginary part. The fastest-growing unstable mode is obtained at \( \epsilon[(s - k_+)^2 - k_+^2] + g2n - q = 0 \) and has the amplitude \( \hbar \omega_5^i(s) = |g_2|n\sqrt{1 - f_2^2} \). Unlike in the case of the magnetization modes, the maximal amplitude is bounded from above and is independent of the winding numbers. By adjusting the strength of the magnetic field, the fastest-growing unstable mode can be chosen to be located at a specific value of \( s \), showing that it is easy to adjust the stability properties experimentally. At \( f_2 = 0 \) the width of the region on the \( s \)-axis giving positive \( \omega_5^i \) is \( \sqrt{k_+^2 + q/\epsilon} - \sqrt{k_+^2 + q/\epsilon - 2g2n/\epsilon} \). This region can thus be made narrower by increasing \( \epsilon, k_- \), or \( q \). Since the magnetization modes are insensitive to the magnetic field, the properties of the spin and magnetization modes can be tuned independently. The winding number dependence of unstable spin modes is illustrated in Figs. 1(c)-(d). Interestingly, by tuning \( \epsilon \) and \( q \) a rotonlike spectrum can be realized, see the solid and dotted blue lines in Fig. 2.

Now the phonon part of the spectrum is missing, but the roton-maxon feature is present. For \( f_2 = k_+ = 0 \) the roton spectrum exists if \( q \geq \max(0,2g2n) \). Because only integer values of \( s \) are allowed, it may happen that the imaginary parts \( \omega_5^i \) and \( \omega_6^i \) are nonzero only in some interval of the \( s \) axis that does not contain integers, see Figs. 1(c)-(d) and Fig. 2(a). In this case rotonic excitations are stable. Alternatively, there can be unstable modes close to the roton minimum, see Fig. 2(b) and Ref. 20. As evidenced by the orange dashed lines in Fig. 2 the roton spectrum can be made to vanish simply by decreasing \( q \). It is known that a rotonlike spectrum can exist in various types of BECs, such as in a dipolar condensate (see, e.g., 21,22), in a Rydberg-excited condensate 23, or in a spin-1 sodium condensate prepared in a specific state 20. In the present case the rotonlike spectrum exists both in a sodium and rubidium BEC and the state \([12] \) giving rise to it is easy to prepare experimentally. Note that the roton-maxon feature exists also in a vortex-free condensate and for any \(|f_2| < 1\). These results suggest that the roton-maxon character of the spectrum is rather a rule than an exception in spinor BECs. By changing the value of \( q \) an unstable spin mode
can be introduced or made to vanish. For example, using the parameter values corresponding to the blue solid line in Fig. 2a), we find that by decreasing (increasing) the value of \( q_{\text{eff}} \) from 5.5\( |g_2|n \) to 4\( |g_2|n \) (6\( |g_2|n \)), the \( s = 4 \) (\( s = 5 \)) modes can be made unstable. This opens the way for quench experiments of the type described in [23, 20]. In the present system the number of excited unstable modes and their wavenumbers can be controlled with a high precision. Instead of altering \( q \), instabilities can also be induced by making \( \epsilon \) smaller by changing the trapping frequencies.

The properties of unstable spin modes can be studied experimentally by measuring the density and phase of the density vanishes. This holds true regardless of the value of \( \epsilon \). We see that the sign of \( \delta \psi = \{e\epsilon\} \) is such that only spin modes are unstable. If \( \delta \psi = \{e\epsilon\} \) components were found to give the density of the magnetic field, an initially stable condensate can be made unstable. We have also shown that some unstable modes lead to a dark soliton-like wavefunction of the \( m_F = 0 \) spin component. Finally, by considering two recent experiments on toroidal single-component BECs, we argued that various types of instabilities can be realized in a spin-1 condensate having the same parameter values as these experiments.

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