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We discuss excited Bose-condensed states and find the criterion of dynamical stability of a kinkwise state, i.e., a standing matter wave with one nodal plane perpendicular to the axis of a cylindrical trap. The dynamical stability requires a strong radial confinement corresponding to the radial frequency larger than the mean-field interparticle interaction. We address the question of thermodynamic instability related to the presence of excitations with negative energy. [S1050-2947(99)51210-9]

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The discovery of Bose-Einstein condensation (BEC) in trapped clouds of alkali-metal atoms [1] and extensive studies of Bose-condensed gases in recent years have led to the observation of new macroscopic quantum phenomena, such as interference between two independently created condensates [2] and the reduction of the rates of inelastic processes (three-body recombination) in the presence of a condensate [3]. The success in these studies stimulates an interest in macroscopically excited Bose-condensed states, i.e., excited-state solutions of the Gross-Pitaevskii equation, where one can expect to observe novel signatures of BEC. A widely discussed example is the vortex state, well known in superfluid liquid helium [4].

Another option concerns excited Bose-condensed states which have a macroscopic wave function with nodal planes perpendicular to the symmetry axis of a trap. These states represent standing matter waves for which the trap serves as a cavity, and it will be worth studying in which aspects they are similar to light waves. An interesting idea concerns an atom laser for the generation of coherent matter waves out of a ground-state Bose condensate. The waves with one nodal plane (kinks or dark solitons), being the lowest energy phase slip, are of great interest in connection with the decay of persistent currents. Suggested ways of creating standing matter waves in a trap rely on the adiabatic Raman transfer of particles from the ground to the excited Bose-condensed state [5] or on selective population of trap levels by bosonically enhanced spontaneous emission of optically excited atoms of an incoming beam [6].

A principal question concerns the stability of excited Bose-condensed states with respect to the interparticle interaction. In this paper we consider standing matter waves with one nodal plane perpendicular to the axis of a cylindrical trap. For the axially Thomas-Fermi regime (axial frequency $\omega_z$ is much smaller than the mean-field interaction), this state can be called “kinkwise” (see [7] and Fig. 1), since the presence of the nodal plane makes a kink in the dependence of the condensate wave function $\Psi_0$ on the axial coordinate. A characteristic size of the kink is of the order of the correlation length, and the corresponding (axial) kinetic energy of the condensate is of the order of the mean-field interaction. Similar to the case of vortices [8,9], the instability of the kink-wise state is related to the motion of the kink (core) with respect to the rest of the condensate. We analyze the spectrum of elementary excitations of this Bose-condensed state and find the criterion of dynamical stability, i.e., the stability of small-amplitude normal modes; in order to prevent the interaction-induced transfer of (axial) kinetic energy of the condensate to the radial degrees of freedom, one should strongly confine the radial motion by making the radial frequency $\omega_r$ larger than the mean-field interparticle interaction. Under this condition the kink-wise state will be perfectly stable in the limit of zero temperature; the thermodynamic instability related to the presence of an excitation mode with negative energy will not lead to decay in the absence of dissipative processes.

Our conclusion of how tightly one should confine the radial motion to achieve (quasi) one-dimensional (1D) dynamics of a condensate and observe dynamically stable kinks (dark solitons) is directly related to the problem of “engineering the dimensionality of space.” Various experiments aiming for quasi-1D gases are currently being set up.

To gain insight in the nature of the instability, we first consider a kink-wise Bose-condensed state in the absence of trapping field, i.e., the state with one nodal plane $x, y$ plane in an otherwise spatially homogeneous condensate of density $n_0$. We will use the chemical potential $\mu = n_0 U$ and the correlation length $l = \hbar / \sqrt{\mu m}$ as units of energy and length, and $n_0$ as a unit of density. For a positive scattering length the Gross-Pitaevskii equation is reduced to

$$-\frac{1}{2} \frac{d^2 \Psi_0}{dz^2} + |\Psi_0|^2 \Psi_0 = 0$$

and has a simple solution describing the kink in the dependence of $\Psi_0$ on the $z$ coordinate (see, e.g., [7]):

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where the operators $h_+ = -d^2/2dz^2 + \Psi_0^2 - 1$ and $h_- = -d^2/2dz^2 + 3\Psi_0^2 - 1$ take the form

$$h_+ = -\frac{\coth z}{2} \left[ \frac{\tanh z}{dz} \frac{d}{dz} \coth z \right].$$

$$h_- = -\frac{\cosh^2 z}{2} \left[ \frac{1}{\cosh^2 z} \frac{d}{dz} \cosh^2 z \right].$$

The kinkwise state has several excitation modes with zero energy. The ones for $k=0$ are the well-known fundamental modes of a 1D kink state, following from decoupled equations $h f^\pm = 0$. Those which do not exponentially grow at large $z$ are $f_{1}^\pm = \tanh z$, $f_{3}^\pm = 0$, $f_{2}^\pm = \cosh^{-2} z$, and $f_{5}^\pm = z \tanh z - 1$, $f_{3}^\pm = 0$. The mode $f_{2}^\pm$, which is even with respect to inversion of the $z$ coordinate, is localized at distances of order $l$ from the nodal plane.

As an example, we demonstrate the instability of transverse normal modes in the absence of translational motion of the nodal plane. We consider modes that in the limit $k \to 0$ correspond to the localized zero-energy modes $f_{2}^\pm$. For transverse momenta $k \ll 1$ the excitation wave functions at distances $z \ll k^{-1}$ can be found as a series of expansion in powers of $k$. Since the leading term in the expansion for the function $f^\pm$ is proportional to $\cosh^{-2} z$, from Eq. (4) one can find that the leading terms in the expansion for the function $f^\pm$ should be $f^+ = \text{const}$ and $f^- = f_{3}^-$. Hence, this expansion takes the form

$$f^+ = C\left[ 1 + B f_{1}^\pm(z) + k^2 g(z) \right],$$

where $C$ and $B$ are constants. The equation for the function $g$ follows directly from Eqs. (4)–(6):

$$2\varepsilon_{k}^2 = k^2 h_- [2 h_+ g(z) + B f_{2}^\pm(z) + 1] - k^2 \cosh^{-2} z.$$  

Using Eq. (6) and performing the integration of Eq. (8), we obtain the relation $(3\varepsilon_{k}^2/k^2 + 1) \cosh^{-2} z + 4 + 3f_{1}^\pm(z) + 6h_+g(z) = 0$. As $g$ should not contain terms exponentially growing with $z$, we find the dispersion relation corresponding to imaginary excitation energies:

$$\varepsilon_{k} = ik/\sqrt{3}.$$  

The instability of transverse normal modes, following from Eq. (9), originates from the transfer of the (longitudinal) kink-related kinetic energy $K$ of the condensate to these modes. As $K \sim \mu$, it can be transferred by the mean-field interaction to modes with small $k$.

The demonstrated instability and Eq. (9) are similar to those in the case of “domain walls” [15]. In Fig. 2 we present numerical results for $\Im \varepsilon_{k}$ as a function of $k$. For small momenta it increases linearly with $k$, in accordance with Eq. (9), and reaches its maximum at $k = 1/\sqrt{2}$. Further increase of $k$ leads to decreasing $\Im \varepsilon_{k}$, which becomes zero at $k = 1$. At this critical point we have one more zero-energy solution of Eqs. (4):

$$\varepsilon_{k} = 0, \quad f^+ \propto 1/\cosh z, \quad f^- = 0.$$  

For $k > 1$ the energy of free transverse motion, $k^2/2$, exceeds the kink-related kinetic energy $K$, and the normal modes are dynamically stable, with positive $\varepsilon_{k}$.
One can now understand the origin of dynamical instability of a kinkwise Bose-condensed state in a cylindrical harmonic trap: the interparticle interaction can transfer the (axial) kink-related kinetic energy of the condensate to the radial degrees of freedom. In order to suppress this instability one has to significantly confine the radial motion. As the (axial) kinetic energy per particle in the axially Thomas-Fermi condensate is of the order of the mean-field interaction at maximum density, \( n_{0\infty} U \), the radial frequency should be the same or larger.

We have performed calculations for various ratios of the radial to axial frequency, \( \omega_r/\omega_z \), and found the maximum value \( \gamma_c \) of the parameter \( \gamma = n_{0\infty} U/\hbar \omega_r \), at which the kinkwise Bose-condensed state is still dynamically stable, i.e., all excitations have real frequencies. If \( \gamma > \gamma_c \), there are excitations with imaginary frequencies, and the kinkwise condensate is dynamically unstable.

We have solved the Gross-Pitaevskii equation

\[
\frac{\hbar^2}{2m} - \frac{\hbar^2}{2m} \Delta + \frac{m}{2} (\omega_r^2 z^2 + \omega_z^2 r^2) + \tilde{U} |\Psi_0|^2 - \mu \Psi_0 = 0, \tag{11}
\]

together with the Bogolyubov–de Gennes equations for the excitations, which we write in the form

\[
\epsilon^+_\nu \mathcal{F}^+ = \frac{\hbar^2}{2m} \left[ \Delta + \frac{\hbar^2}{2m} \frac{\Psi_0}{\Psi_0} \right] f^+ + \left( \frac{\hbar^2}{2m} \frac{\Psi_0}{\Psi_0} \right) f^+ = 0. \tag{12}
\]

Equation (12) gives real \( \epsilon^+_\nu \), which depends continuously on \( \gamma \) and the aspect ratio. In the range of \( \gamma \) and \( \omega_r/\omega_z \), where a given mode \( \nu \) is dynamically unstable, \( \epsilon^+_\nu < 0 \) and the energy \( \epsilon^+_\nu \) is purely imaginary. In the region of dynamical stability \( \epsilon^+_\nu \) is purely real \( (\epsilon^+_\nu > 0) \) and, hence, at the border between the two regions we have \( \epsilon^+_\nu = 0 \).

At the critical point \( \gamma = \gamma_c \) all excitation energies \( \epsilon^+_\nu \) are real, and one of the excitations has zero energy. This is just the mode which for \( \gamma > \gamma_c \) becomes dynamically unstable. Similar to the mode of Eq. (10) in the absence of trapping field, this mode is even with respect to inversion of the \( z \) coordinate. The function \( f^* = 0 \), and \( f^+ \) follows directly from Eq. (12):

\[
(\Delta + \Delta \Psi_0 / \Psi_0) f^+ = 0. \tag{13}
\]
\[ \Psi_0 = \tanh z + \xi^2 \eta(z), \]  
(14)

where the function \( \eta(z) \) is determined by the equation

\[ h \cdot \eta(z) + (z^2/2) \tanh z = 0, \]  
(15)

and is not given because of its complexity. For \( |z| \gg 1 \) we have \( \eta = -\text{sgn} z (1 + 2z^2)/8 \), and Eq. (14) recovers the Thomas-Fermi result at \( z \approx R/1 \). The Bogolyubov-de Gennes equations take the form

\[ \epsilon_k \tilde{f}^\dagger = h \cdot \epsilon_k + \xi^2 [z^2/2 + (4 + 2)(\eta(z)) \tanh z] f^\dagger. \]  
(16)

Just as in the absence of a trapping field, we consider a mode for which the leading term in the expansion for the function \( f^- \) is proportional to \( 1/\cosh^2 z \). In order to find the excitation energy, it is sufficient to keep the terms independent of \( \xi \) and proportional to \( \xi^2 \) in the expansion for the function \( f^+ \). Then, similarly to Eq. (7), we obtain \( f^+ \propto [1 + \xi^2 G(z)] \). The equation for \( G(z) \) follows from Eqs. (16), and by using Eqs. (6) and (15) it is transformed to

\[ \left( \frac{\epsilon_k^2}{\xi^2} - \frac{1}{2} \right) = h \cdot [G(z) + z^2] - 2 \cosh^2 z \times \frac{d}{dz} \left[ \tanh z, \frac{d}{\cosh^2 z} \frac{d}{dz} [\cosh^2 z \eta(z)] \right]. \]  
(17)

Integration of Eq. (17) gives at large \( |z| \) the relation \( d^2 G/\cosh^2 z = (\epsilon_k^2/\xi^2 - 1/2) \cosh^2 z - 1 \) and, since \( G \) should not contain exponentially growing terms, we obtain \( \epsilon_k^2 = \xi^2/2 \). The normalization condition \( \int dz f^+ f^- = 1 \) allows one then to conclude that the excitation energy is negative and, hence, equal to \(-\hbar \omega_1 \sqrt{2} \). The frequency \( \omega_1 \sqrt{2} \) for the oscillations of the kink in a 1D Thomas-Fermi condensate has also been found in recent work [13] from the equation of motion for the kink.

The excitation spectrum for \( \epsilon_\nu > 0 \) follows from the solution of the Bogolyubov-de Gennes equations at large \( |z| \), where the Thomas-Fermi shape of \( |\Psi_0| \) is not influenced by the kink. Then, along the lines of the theory for the 3D case [10-12], we obtain a discrete spectrum \( \epsilon_\nu = \hbar \omega_\nu \sqrt{\nu (\nu + 1)/2} \), where \( \nu \) is a positive integer.

Finally, we analyze the influence of the excitation with negative energy on the stability of the kink-wise condensate. Beyond the Bogolyubov-de Gennes approach, there is a small coupling of this excitation to the excitations with positive energies. But at temperatures \( T \to 0 \) there will be no real decay processes. Those require a simultaneous creation of excitations with positive and negative energies, with the total excitation energy equal to zero. Due to the structure of the discrete spectrum for \( \epsilon_\nu > 0 \), this conservation of energy cannot be satisfied while creating a moderate number of excitations with the above found negative energy \(-\hbar \omega_1 \sqrt{2} \).

Thus, under the condition of dynamical stability the kink-wise Bose-condensed state is perfectly stable at \( T \to 0 \). The decay mechanism in the presence of a thermal cloud is in some sense similar to that of temperature-dependent damping of excitations in trapped Bose-condensed gases (see [14]) and originates from the scattering of thermal particles on the kink. Accordingly, the decay time can be made large by decreasing temperature well below the value of the mean-field interparticle interaction. A detailed analysis of dissipative dynamics of a kink state at finite \( T \) requires a separate investigation.

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