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Stability of standing matter waves in a trap

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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 Gross-Pitaevskii equation is reduced to

\[ -\frac{1}{2} \frac{d^2 \Psi_0}{dz^2} + \Psi_0^3 \Psi_0 = 0 \]  

(1)

and has a simple solution describing the kink in the dependence of \( \Psi_0 \) on the \( z \) coordinate (see, e.g., [7]):
Elementary excitations of the kinkwise condensate are characterized by the quantum number $z$, where a particle at distances of order $l$ is a condensate part of the field operator of atoms can be represented as $\hat{b}_k^\dagger \hat{b}_k$ of the excitations, the above-condensate part of the field operator of atoms can be represented as $\Sigma_k \exp(ik \cdot r )[\hat{u}_{k\nu}(z)\hat{b}_{k\nu}^\dagger - \nu_{k\nu}(z)\hat{b}_{k\nu}]$, and we obtain the following Bogolyubov–de Gennes equations for the excitation energies $\epsilon_{k\nu}$ and wave functions $\tilde{f}_\nu(z)$:

$$\epsilon_{k\nu} f^\dagger_{\nu}(z) = [h_+ + (k^2/2)] f^\dagger_{\nu}(z),$$

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

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

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

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 $h_+ f^\dagger_{\nu} = 0$. Those which do not exponentially grow at large $z$ are $f_{\nu} = \tanh z$, $f_{\nu}^\dagger = 0$, $f_{\nu}^\dagger = \cosh^{-2};$ and $f_{\nu}^\dagger = z \tanh z^{-1}$, $f_{\nu}^\dagger = 0$. The mode $f_{\nu}^\dagger$, 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 mode $f_{\nu}^\dagger$. For transverse momenta $k \ll 1$ the excitation wave functions in distances $z \ll k^{-1}$ can be found as a series in powers of $k$. Since the leading term in the expansion for the function $f^\dagger$ is proportional to $\cosh^{-2}$, from Eq. (4) one can find that the leading terms in the expansion for the function $f^\dagger$ should be $f^\dagger = \text{const}$ and $f^\dagger = f_{\nu}^\dagger$. Hence, this expansion takes the form

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

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

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

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

$$\epsilon_{k} = i k/\sqrt{3}.$$

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 $\text{Im} \epsilon_{k}$ 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 $\text{Im} \epsilon_{k}$, which becomes zero at $k = 1$. At this critical point we have one more zero-energy solution of Eqs. (4):

$$\epsilon_{k} = 0, \quad f^\dagger = 1/\cosh z, \quad f^- = 0.$$

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 $\epsilon_{k}$.
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, $n_{0a,U}$, 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 $\gamma=\n_{0a,U}/\hbar\omega_r$, at which the kinkwise Bose-condensed state is still dynamically stable, i.e., all excitation modes have real frequencies. If $\gamma>\gamma_c$, there are excitations with imaginary frequencies, and the kinkwise Bose-condensed state is dynamically unstable.

We have solved the Gross-Pitaevskii equation
\[
\left[ \frac{\hbar^2}{2m} \Delta + \frac{m}{2} (\omega_z^2 z^2 + \omega_r^2 \rho^2) + U_n |\Psi_0|^2 - \mu \right] \Psi_0 = 0, \tag{11}
\]

together with the Bogolyubov–de Gennes equations for the excitations, which we write in the form
\[
\begin{align*}
&\epsilon_n f^+ = \frac{\hbar^2}{2m} \left[ -\Delta + \frac{\Delta |\Psi_0|^2}{\Psi_0} \right] f^+ + (1+\Omega) U_n |\Psi_0|^2 f^+, \tag{12}
\end{align*}
\]

Equation (12) gives real $\epsilon_n^2$, which depends continuously on $\gamma$ and the aspect ratio. In the range of $\gamma$ and $\omega_r/\omega_z$, where a given mode $n$ is dynamically unstable, $\epsilon_n^2<0$ and the energy $\epsilon_n$ is purely imaginary. In the region of dynamical stability $\epsilon_n$ is purely real ($\epsilon_n^2>0$) and, hence, at the border between the two regions we have $\epsilon_n=0$.

At the critical point $\gamma=\gamma_c$ all excitation energies $\epsilon_n$ 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):
\[
(-\Delta + \Delta |\Psi_0|^2 / |\Psi_0|) f^+ = 0. \tag{13}
\]

Equation (13) is the Schrödinger equation for the motion of a particle (with zero energy) in a cylindrically symmetric potential $V=\hbar^2 \Delta |\Psi_0|^2/2m$. The potential $V$ depends on $\gamma$ and the aspect ratio. Thus, for a given ratio $\omega_r/\omega_z$, one finds the critical value $\gamma_c$ by selecting the parameter $\gamma$ such that there is an even (nonzero) solution of Eq. (13), remaining finite at the origin and tending to zero at infinity. This was checked numerically on the basis of Eqs. (11)–(12) for a wide range of $\gamma$ and the aspect ratio.

As it follows from our calculations, $\gamma_c$ is minimal for excitations with the projection of the orbital angular momentum on the symmetry axis, $M=1$. The dependence of $\gamma_c$ on the aspect ratio is presented in Fig. 3. For $\omega_r<\omega_z$, even an arbitrary small interparticle interaction leads to instability, since the axial “kink-related” energy per particle in the condensate ($\hbar\omega_z$) can be always transferred to the radial mode with $M=1$ which, by itself, has energy $\hbar\omega_r$. For $\omega_r>\omega_z$, the critical value $\gamma_c$ increases with the ratio $\omega_r/\omega_z$ and reaches $\gamma_c \approx 2.4$ for $\omega_r / \omega_z$. We also found that the decay of dynamically unstable kink states is accompanied by the undulation of the nodal plane and the formation of vortex-antivortex pairs, similar to the decay of dark optical solitons [16].

The criterion of dynamical stability of a kinkwise condensate, $\gamma<\gamma_c$, can be satisfied in the conditions of current BEC experiments. For a rubidium condensate in a cylindrical trap with $\omega_r \approx 200$ Hz $\gg \omega_z$, it requires the maximum density $n_{0a} \approx 10^{14}$ cm$^{-3}$.

Although for $\gamma<\gamma_c$ the kinkwise condensate is dynamically stable, there is a thermodynamic instability related to the presence of an excitation with negative energy. For a very strong radial confinement of the axially Thomas-Fermi kinkwise condensate ($\hbar\omega_r \approx n_{0a,U} \gg \hbar\omega_z$; $\gamma \ll \gamma_c$), we calculate a negative excitation energy close to $\epsilon_n = -\hbar\omega_z / \sqrt{2}$ characteristic for the 1D Thomas-Fermi kinkwise condensate in a harmonic trap.

In the 1D case we calculate the negative excitation energy analytically by solving the Bogolyubov–de Gennes equations at distances $z$ from the origin, much smaller than the Thomas-Fermi size of the condensate $R = (2\mu / m\omega_z^2)^{1/2}$. We represent $\Psi_0$ and the excitation wave functions as a series of expansion in powers of small parameter $\xi = \hbar\omega_z / \mu$. Then, in the same dimensionless units as in the absence of trapping field, the Gross-Pitaevskii equation is given by Eq. (1) with an extra term $\xi^2 \hat{z}^2 |\Psi_0|^2 / 2$ on the left-hand side. Confining ourselves to the expansion up to $\xi^2$, we obtain

**FIG. 2.** Imaginary part of the excitation energy (in units of $\mu$) vs the transverse momentum $k$ (in units of $l^{-1}$) for a kinkwise condensate in the absence of a trapping field.

**FIG. 3.** Critical parameter $\gamma_c$ vs the aspect ratio for a kinkwise condensate in a cylindrical trap.
\[ \Psi_0 = \tanh z + \zeta^2 \eta(z), \quad (14) \]

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

\[ h_\eta \eta(z) + (\zeta^2/2) \tanh z = 0, \quad (15) \]

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 \(|z| \ll R/1\). The Bogolyubov-de Gennes equations take the form

\[ e_{nf}^\infty = h = f^\infty + \zeta^2 [\zeta^2/2 + (4/2) \eta(z) \tanh z] f^\infty. \quad (16) \]

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 \( \zeta \) and proportional to \( \zeta^2 \) in the expansion for the function \( f^+ \). Then, similarly to Eq. (7), we obtain \( f^\infty \propto \{1 + \zeta^2 G(z)\} \). The equation for \( G(z) \) follows from Eqs. (16), and by using Eqs. (6) and (15) it is transformed to

\[ \left( \frac{\varepsilon_n^2}{\zeta^2} - \frac{1}{2} \right) = h_\eta [h_\eta G(z) + z^2] - 2 \cosh^2 z \]

\[ \times \frac{d}{dz} \left[ \tanh z \frac{d}{d|\zeta|} \left[ \frac{\cosh^2 z \eta(z)}{\zeta^2} \right] \right]. \quad (17) \]

Integration of Eq. (17) gives at large \(|z|\) the relation \( d^2 G/dz^2 = (\varepsilon_n^2/\zeta^2 - 1/2) \cosh^2 z - 1 \) and, since \( G \) should not contain exponentially growing terms, we obtain \( \varepsilon_n^2 = \zeta^2/2 \). The normalization condition \( \int dz f^+ f^- = 1 \) allows one then to conclude that the excitation energy is negative and, hence, equal to \(-h_\eta \omega_f/\sqrt{2}\). The frequency \( \omega_f \sqrt{2} \) 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 \( \varepsilon_f > 0 \) 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 \( \varepsilon_f = h \omega_f \sqrt{\nu(n+1)/2} \), 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 \( \varepsilon_f > 0 \), this conservation of energy cannot be satisfied while creating a moderate number of excitations with the above found negative energy \(-h_\eta \omega_f/\sqrt{2}\).

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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