Modulational instability criteria for two-component Bose–Einstein condensates

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(Dated: Submitted 13 April 2005; revised 12 May 2005)

The stability of colliding Bose–Einstein condensates is investigated. A set of coupled Gross-Pitaevskii equations is thus considered, and analyzed via a perturbative approach. No assumption is made on the signs (or magnitudes) of the relevant parameters like the scattering lengths and the coupling coefficients. The formalism is therefore valid for asymmetric as well as symmetric coupled condensate wave states. A new set of explicit criteria is derived and analyzed. An extended instability region, in addition to an enhanced instability growth rate is predicted for unstable two component bosons, as compared to the individual (uncoupled) state.

PACS numbers: 03.75.Lm, 05.45.-a, 67.40.Vs, 67.57.De
Keywords: Bose-Einstein Condensation, Modulational Instability, Gross-Pitaevskii Equations.

I. INTRODUCTION

Bose-Einstein condensation of dilute gases in traps has attracted a great deal of interest recently, as witnessed in recent reviews and monographs 1,2. Mean-field theory provides a consistent framework for the modeling of the principal characteristics of condensation and elucidates the role of the interactions between the particles. A generic theoretical model widely employed involves the Gross-Pitaevskii equation, which bears the form of a non-linear Schrödinger-type equation, taking into account boson interactions (related to a scattering length $a$), in addition to the confinement potential imposed on the Bose-Einstein condensates (BECs) in a potential trap. The scattering length $a$, although initially taken to be positive (accounting for repulsive interactions and preserving condensate stability), has later been sign-inverted to negative (attractive interaction) via Feshbach resonance, in appropriately designed experiments. This allowed for the prediction of BEC state instability, eventually leading to wave collapse, which is only possible in the attractive case ($a < 0$) 1. As expected from previous know-how on problems modelled by generic nonlinear Schrödinger-type equations (in one or more dimensions), the analysis of BEC dynamics revealed the possibility for the existence of collective excitations including bright- (for $a < 0$) and dark- (holes, for $a > 0$) type envelope excitations, as well as vortices, which were quite recently observed in laboratories 3,4,5,6,7. The evolution of coupled (“colliding”) BEC wavepackets was recently considered in theoretical and experimental investigations 3,4,5,7,8. Pairs of nonlinearly coupled BECs are thus modeled via coupled Gross-Pitaevskii equations, involving extra coupling terms whose sign and/or magnitude are a priori not prescribed. Although theoretical modeling, quite naturally, first involved symmetric pairs of (identical) BECs, for simplicity, evidence from experiments suggests that asymmetric boson pairs deserve attention 2.

In this paper, we investigate the stability of a nonlinearly coupled BEC pair, from first principles. Both BECs are assumed to lie in the ground state, for simplicity, although no other assumption is made on the sign and/or magnitude of relevant physical parameters. We shall derive a set of general criteria for the stability of BEC pairs (allowing for asymmetry in the wave functions).

II. THE FORMALISM

The wave-functions $\psi_1$ and $\psi_2$ of two nonlinearly interacting BECs evolve according to the coupled Gross-Pitaevskii equations (CGPEs)

\begin{align}
\frac{i\hbar}{\partial t} \psi_1 &= \frac{\hbar^2}{2m_1} \nabla^2 \psi_1 - V_{11} |\psi_1|^2 \psi_1 - V_{12} |\psi_2|^2 \psi_1 + \mu_1 \psi_1 = 0, \\
\frac{i\hbar}{\partial t} \psi_2 &= \frac{\hbar^2}{2m_2} \nabla^2 \psi_2 - V_{22} |\psi_2|^2 \psi_2 - V_{21} |\psi_1|^2 \psi_2 + \mu_2 \psi_2 = 0,
\end{align}

where $\nabla^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$ is the Laplace operator (a three-dimensional Cartesian geometry is considered, for clarity). Here $m_j$ represents the mass of the $j$th condensate. According to standard theory, the nonlinearity coefficients $V_{jj}$ are proportional to the scattering lengths $a_j$, via $V_{jj} = 4\pi\hbar a_j/m_j$, while the coupling coefficients $V_{jl}$ are related to the mutual interaction scattering lengths $a_{jl}$ via $V_{jl} = 2\pi\hbar a_{jl}/m_{jl}$, where $m_{jl} = m_j m_l/(m_j + m_l)$ is the reduced mass. The (linear) last terms in each equation involve the chemical potential $\mu_j$, which corresponds to a ground state of the condensate, in a simplified model. These terms may readily be
eliminated via a simple phase-shift transformation, viz. \( \psi_j = \psi'_j \exp(i\epsilon_j t) \) \((j = 1, 2)\); this is however deliberately not done at this stage, for generality. Nevertheless, one therefore intuitively expects no major influence of the chemical potentials on the coupled BEC dynamics (at least for the physical problem studied here).

### III. LINEAR STABILITY ANALYSIS

We shall seek an equilibrium state in the form \( \psi_j = \psi_{j0} \exp[i\varphi_j(t)] \), where \( \psi_{j0} \) is a (constant real) amplitude and \( \varphi_j(t) \) is a (real) phase, into the CGP Eqs. We then find a monochromatic (fixed-frequency) Stokes’ wave solution in the form: \( \varphi_j(t) = \Omega_{j0} t \), where

\[
\Omega_{j0} = -\frac{V_{jj} \psi_{j0}^2}{\hbar} - \frac{V_{jl} \psi_{l0}^2}{\hbar} + \mu_j,
\]

for \( j \neq l = 1, 2 \).

Let us consider a small perturbation around the stationary state defined above by taking \( \psi_j = (\psi_{j0} + \epsilon \psi_j(t)) \exp[i\varphi_j(t)] \), where \( \psi_j(r, t) \) is a complex number denoting the small \( (\epsilon \ll 1) \) perturbation of the slowly varying modulated bosonic wave-functions (it includes both amplitude and phase corrections), and \( \varphi_j(t) \) is the phasor defined above. Substituting into Eqs. and separating into real and imaginary parts by writing \( \psi_j = a_j + ib_j \), the first order terms in \( \epsilon \) yield

\[
-\hbar \frac{\partial b_j}{\partial t} + \frac{\hbar^2}{2m_j} \nabla^2 a_j - 2V_{j2} \psi_{j0} a_j - 2V_{jl} \psi_{j0} a_l = 0,
\]

where \( j \) and \( l \neq j = 1, 2 \) (this will be henceforth understood unless otherwise stated). Eliminating \( b_j \), these equations yield

\[
\left[ \frac{\hbar^2}{2m_j} \frac{\partial^2}{\partial t^2} + \frac{\hbar^2}{2m_j} \left( \frac{\hbar^2}{2m_1} \nabla^2 - 2V_{11} \psi_{10}^2 \right) \nabla^2 \right] a_l
\]

\[
- \frac{\hbar^2}{m_1} V_{12} |\psi_{10}| |\psi_{20}| \nabla^2 a_2 = 0,
\]

(together with a symmetric part, obtained by permuting \( j \leftrightarrow l \)). We now let \( a_j = a_{j0} \exp[i(\mathbf{k} \cdot \mathbf{r} - \Omega_k t)] + a_{j0}^* \exp[-i(\mathbf{k} \cdot \mathbf{r} - \Omega_k t)] \) complex conjugate, where \( \mathbf{k} \) and \( \Omega_k \) are the wavevector and the frequency of the modulation, respectively, viz. \( \partial / \partial t \rightarrow -i \Omega_k \) and \( \partial / \partial x_n \rightarrow ik_n \) \((x_n \equiv \{x, y, z\} \) for \( n = 1, 2, 3 \)) i.e. \( \partial^2 / \partial t^2 \rightarrow -\Omega_k^2 \) and \( \nabla^2 \rightarrow -k^2 \). After some algebra, we obtain the eigenvalue problem: 

\[
\mathbf{Ma} = (\hbar \omega)^2 \mathbf{a},
\]

where \( \mathbf{a} = (a_1, a_2)^T \), and the matrix elements are given by \( M_{jj} = e_j (V_{jj} \psi_{j0} |\psi_{j0}|) = \hbar^2 \Omega_j^2 \) and \( M_{jl} = -2e_j V_{jl} |\psi_{j0}| |\psi_{l0}| = \hbar^2 \Omega_j^2 \); where we have defined \( e_j = \hbar^2 k^2 / 2m_j \). The frequency \( \omega \) and the wave number \( k \) are therefore related by the dispersion relation

\[
(\Omega_k^2 - \Omega_1^2)(\Omega_k^2 - \Omega_2^2) = \Omega_4^2,
\]

where the coupling is expressed via \( \Omega_4^2 = \Omega_{12}^2 \Omega_{21}^2 \equiv M_{12} M_{21} / \hbar^4 \) in the right-hand side of Eq. (4). We stress that this dispersion relation (which is independent of the chemical potentials \( \mu_j \)) relies on absolutely no assumption on the sign or the magnitude of \( m_j, V_{jj} \) and \( V_{jl} \).

### IV. MODULATIONAL INSTABILITY OF INDIVIDUAL BECS

In the vanishing coupling limit, i.e. for \( V_{jl} \to 0 \), the dispersion relation gives \( \Omega_{k, \pm} = \pm \Omega_j \) \((j = 1, 2)\). Absolute stability is ensured if \( V_{jj} > 0 \). On the other hand, if \( V_{jj} < 0 \), a purely growing unstable mode occurs (viz. \( \Omega_k^2 < 0 \) for wavenumbers below a critical value \( k_{j,c} = 2(m_j |V_{jj}|)^{1/2} |\psi_{j0}| / \hbar \). The growth rate \( \sigma = \sqrt{-\Omega_k^2} \) attains a maximum value \( \sigma_{\text{max}} = |V_{jj}| |\psi_{j0}|^2 / \hbar \) at \( k = k_{j,c} / \sqrt{2} \).

Recalling the definitions of \( V_{jj} \), we see that a repulsive/attractive scattering length (i.e. positive/negative \( V_{jj} \)) prescribes a stable/unstable (single) BEC behavior. In the following, we shall see how this simple criterion for stability (\( V_{jj} > 0 \)) is modified by the presence of interaction between two he condensates.

### V. MODULATIONAL INSTABILITY OF COUPLED BECS

The dispersion relation takes the form of a bi-quadratic polynomial equation

\[
\Omega_k^4 - T \Omega_k^2 + D = 0,
\]

where \( T = \text{Tr} \mathbf{M} / \hbar^2 = \Omega_1^2 + \Omega_2^2 \) and \( D = \text{Det} \mathbf{M} / \hbar^4 = \Omega_{12}^2 \Omega_{21}^2 - \Omega_1^2 \Omega_2^2 \) are related to the trace and the determinant, respectively, of the matrix \( \mathbf{M} \). Eq. has the solution

\[
\Omega_k^2 = \frac{1}{2} \left[ T \pm (T^2 - 4D)^{1/2} \right],
\]

or

\[
\Omega_{k, \pm}^2 = \frac{1}{2} (\Omega_1^2 + \Omega_2^2) \pm \frac{1}{2} \left[ (\Omega_1^2 - \Omega_2^2)^2 + 4 \Omega_4^4 \right]^{1/2}.
\]

We note that the right-hand side is real/complex if the discriminant quantity \( \Delta = T^2 - 4D \) is positive/negative, respectively.

Stability is ensured (for any wavenumber \( k \)) if (and only if) both solutions \( \Omega_{k, \pm}^2 \) are positive. This is tantamount to the following requirements being satisfied simultaneously: \( T > 0, D > 0 \) and \( \Delta > 0 \). Since the three quantities \( T, D \) and \( \Delta \) are all even order polynomials of \( k \), one has to investigate three distinct polynomial inequalities. The topstones of the analysis will be outlined in the following, though trying to avoid burdening the presentation with unnecessary details.

First, the sign of \( T = k^2 (\hbar^2 k^2 / 4) \sum_j (1/m_j^2) + \sum_j V_{jj} |\psi_{j0}|^2 / m_j \) (see definitions above) depends on (the
sign of) the quantity $\sum_{j} V_{jj} |\psi_{j0}|^2/m_j$ which has to be positive for all $k$, in order for stability to be ensured (for any $\psi_{j0}$ and $k$). This requires that

$$V_{11} > 0 \quad \text{and} \quad V_{22} > 0. \quad (8)$$

Otherwise, $T$ becomes negative (viz. $\Omega^2_{k,-} < 0$, at least) for $k$ below a critical value $k_{cr,1} = \sqrt{K_1}$, where $K_1 = 4(-\sum_j V_{jj} |\psi_{j0}|^2/m_j)/[h^2 \sum_j (1/m_j^2)] > 0$ (cf. the single BEC criterion above); this is always possible for a sufficiently large perturbation amplitude $|\psi_{j0}|$ if, say, $V_{11} < 0$ (even if $V_{22} > 0$). Therefore, only a pair of two repulsive type BECs can be stable; the presence of one attractive BEC may destabilize its counterpart (even if the latter would be individually stable).

Second, $D = \Omega^2_{11} - \Omega^2_{22} = 0$, an 8th-order polynomial in $k$, which can be factorized as $D = k^4(k^4 + bk^2 + c)$, where $b = 4 \sum_j (m_j V_{jj})/h^2$ and $c = 16m_1 m_2 (V_{11} V_{22} - V_{12} V_{21}) |\psi_{j0}|^2/|\psi_{20}|^2/h^4$ (note that $b^2 - 4c > 0$). The stability requirements $b > 0$ and $c > 0$ (in order for $D$ to be positive for any value of $k > 0$) amount to $m_1 V_{11} + m_2 V_{22} > 0$ and

$$V_{11} V_{22} - V_{12} V_{21} > 0, \quad (9)$$

respectively. Only the latter condition for stability has to be retained, since the former one is automatically covered by (8) above. To be specific, solving $D = 0$ for $k^2 = K_{2,\pm}$, viz. $K_{2,\pm} = [-b \pm (b^2 - 4c)^{1/2}]/2$, we see that:

(i) if $b < 0 < c$, then $0 < K_{2,-} < K_{2,+}$, and $D < 0$ for $\sqrt{K_{2,-}} < k < \sqrt{K_{2,+}}$ (instability for short wavelengths);

(ii) if $c > 0$ (regardless of $b$), then $K_{2,-} < 0 < K_{2,+}$, and $D < 0$ for $0 < k < \sqrt{K_{2,+}}$;

(iii) if $b > 0$ and $c > 0$, then $K_{2,-} < K_{2,+} < 0$, so that $D > 0$.

We see that this kind of instability, i.e. if the criterion (9) is not met, is due to the mutual interaction potential $V_{ij}$ among the bosons.

Finally, the positivity of $V = T^2 - 4D = (\Omega^2_{11} - \Omega^2_{22})^2 + 4 \Omega^2_{12} \Omega^2_{21}$ is only ensured (for every value of $k$ and $|\psi_{j0}|$) if $\Omega^2_{12} \Omega^2_{21} \sim M_{12} M_{21} > 0$, i.e. if

$$V_{12} V_{21} > 0. \quad (10)$$

If this condition is not met, the solution (8) above has a finite imaginary part, which accounts for amplitude instability due to the external perturbation. For rigour, we note that $\Delta$ bears the form $\Delta = k^4(c_4 k^4 - c_2 k^2 + c_0)$ (where $c_4 > 0$; the complex expressions for $c_0$ are omitted). If $\Delta \equiv c_4 k^4 - 4c_0 c_4 \sim -V_{12} V_{21} < 0$, i.e. if (10) is met, then $\Delta > 0$ for any value of $k$. If $\Delta > 0$, on the other hand, denoting $K_{3,\pm} = [c_2 \pm (c_2^2 - 4c_0 c_4)^{1/2}]/(2c_4)$, we find that:

(i) stability is only ensured (since $K_{3,-} < K_{3,+} < 0 < k^2$) if $c_2 < 0 < c_0$ (nevertheless, this condition depends on the perturbation amplitudes $|\psi_{j0}|$ and may always be violated).

(ii) again, a finite unstable wavenumber interval $k \in (\sqrt{K_{3,-}}, \sqrt{K_{3,+}})$ is obtained for $c_2 > 0$ and $c_0 > 0$.

(iii) finally, instability will be observed for $k \in (0, \sqrt{K_{3,+}})$ if $c_0 < 0$ (regardless of $c_2$).

VI. CONCLUSIONS

Summarizing, we have derived a set of explicit criteria, (8) to (10) above, which should all be satisfied in order for a boson pair to be stable. Therefore, an interacting BEC pair is stable only if the interaction potentials satisfy $V_{11} > 0$ and $V_{22} > 0$ and $V_{11} V_{22} > V_{12} V_{21} > 0$. If one criterion is not met, then the perturbation frequency develops a finite imaginary part and the solution blows up in time. A few comments and qualitative conclusions should however be mentioned.

First, for a symmetric stable boson pair, viz. $V_{11} = V_{22} > 0$ and $V_{12} = V_{21}$, stability is ensured if $V_{12}^2 < V_{11}^2$. Second, if one BEC satisfies $V_{jj} < 0$, the pair will be unstable: only pairs consisting of stable bosons can be stable. Interestingly, in the case of individually unstable BECs (viz. $V_{jj} < 0$, for $j = 1$ or $2$), the instability characteristics are strongly modified. For instance, in the case of a symmetric unstable boson pair (viz. $V_{11} = V_{22} < 0$ and $m_1 = m_2$), an extended unstable wavenumber region and an enhanced growth rate can be obtained, as can be checked via a tedious calculation; cf. Fig. II. Furthermore, we have pointed out the appearance of secondary instability “windows”, i.e. unstable wave number intervals beyond $(k_{cr}, k'_{cr})$, where $k_{cr} \neq 0$.

These results above follow from a set of explicit stability criteria. Both BECs were assumed to lie in the ground state, for simplicity, although no other assumption was made on the sign and/or magnitude of the relevant physical parameters. Naturally, a future extension of this work should consider the external confinement potential, imposed on the trapped condensates. Our results can be tested, and can hopefully be confirmed, by designed experiments.

Acknowledgments

I.K. is grateful to the Max-Planck-Institut für extraterrestrische Physik (Garching, Germany) for the award of a fellowship (project: Complex Plasmas). Partial support from the Deutsche Forschungsgemeinschaft through the Sonderforschungsbereich (SFB) 591 – Universelles Verhalten Gleichgewichtsferner Plasmen: Heizung, Transport und Strukturbildung is also gratefully acknowledged.
FIG. 1: The growth rate $\gamma$ versus the wavenumber $k$ (in units of $|V_{jj}|\psi_{j,0}/\hbar$ and $\sqrt{2m_j|V_{jj}|}\psi_{j,0}/\hbar$, respectively) for a symmetric pair of coupled unstable ($V_{jl} < 0$ for $j,l = 1,2$) BECs (upper curve) as compared to the single BEC case (lower curve).

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