Coupled-mode theory for Bose-Einstein condensates

Elena A. Ostrovskaya, Yuri S. Kivshar, Mietek Lisak, Bjorn Hall, Federica Cattani, and Dan Anderson
1 Optical Sciences Centre, Australian National University, Canberra ACT 0200, Australia
2 Department of Electromagnetics, Chalmers University of Technology, S-41296 Göteborg, Sweden

We apply the concepts of nonlinear guided-wave optics to a Bose-Einstein condensate (BEC) trapped in an external potential. As an example, we consider a parabolic double-well potential and derive coupled-mode equations for the complex amplitudes of the BEC macroscopic collective modes. Our equations describe different regimes of the condensate dynamics, including the nonlinear Josephson effect for any separation between the wells. We demonstrate macroscopic self-trapping for both repulsive and attractive interactions, and confirm our results by numerical simulations.

A system of interacting bosons confined within an external potential at zero temperature can be described by a macroscopic theory having the meaning of an order parameter and satisfying the Gross-Pitaevskii (GP) equation \[ \dot{\psi} = -\frac{i}{\hbar} \left( \frac{\nabla^2}{2m} + U_{\text{ext}} + \frac{\lambda}{2} |\psi|^2 + \frac{\sigma}{a} |\psi|^4 \right) \psi. \] The GP equation is a nonlinear equation that takes into account the effects of the particle interactions through an effective mean field, and it describes the condensate dynamics in a confined geometry. Similar models of the confined dynamics of macroscopic systems appear in other fields, e.g., in the case of an electron gas confined in a quantum well, or optical modes of a photonic microcavity. In all such systems, confined single-particle states are restricted to discrete energies that form a set of eigenmodes.

The physical picture of eigenmodes remains valid in the nonlinear case \[ \sigma > 0 \], and nonlinear collective modes correspond to the ground and higher-order (excited) states of the Bose-Einstein condensate (BEC). Moreover, it is possible to observe at least the first excited (antisymmetric) collective mode experimentally, through the collapses and revivals in the dynamics of strongly coupled two-component BECs. The interest in the non-ground-state collective modes of BECs has dramatically grown with the study of vortex states, very recently successfully created in the experiment [6].

The modal structure of the condensate macroscopic (ground and excited) states allows us to draw a deep analogy between BEC in a trap and guided-wave optics, where the concept of nonlinear guided modes is widely used [7]. The physical description of confined condensate dynamics is in time akin to that of stationary beam propagation along a nonlinear optical waveguide, with the BEC chemical potential playing the role of the beam propagation constant. As is well known from nonlinear optics, the guided waves become coupled in the presence of nonlinearity, and the mode coupling can lead to the nonlinear phase shifting between the modes, power exchange, and self-trapping.

In this paper, we apply the concepts of nonlinear guided-wave optics to the analysis of mode coupling and intermodal population exchange in trapped BECs. As the most impressive (and also physically relevant) example of the applications of our theory, we consider the BEC dynamics in a harmonic double-well potential, recently discussed in the literature [8]. We study the coupling between the BEC ground-state mode and the first excited (antisymmetric) mode in such a potential, and derive the dynamical equations for the the complex mode amplitudes, valid for any value of the well separation. Our model comprises, in the limiting case of large separation, the theory of Josephson tunneling developed for weakly interacting condensates in two separate harmonic traps [9]. In the limit of close separation, our theory describes a nonlinear population exchange between the interacting modes, similar to the effective Rabi oscillations in two-component BECs, studied both theoretically [10] and experimentally [11].

We consider the macroscopic dynamics of BEC in a strongly anisotropic external potential, \( U = \frac{1}{2} m \omega_z^2 (Y^2 + Z^2 + \lambda X^2) \), created by a magnetic trap with a characteristic frequency \( \omega \). In the case of the cigar-shaped trap, \( \lambda \ll 1 \), the collective BEC dynamics can be described by a one-dimensional GP equation. Details of the derivation and normalization can be found, e.g., in Refs. [12]. The GP equation for the longitudinal profile of the normalized condensate wave function takes the form:

\[
i \frac{\partial \psi}{\partial t} + \frac{\partial^2 \psi}{\partial x^2} - U(x) \psi + \sigma |\psi|^2 \psi = 0.
\]

According to normalization, the number of condensate particles \( N \) is defined as \( N = (\hbar \omega / 2 U_0) / \sqrt{\lambda} \), where \( U_0 = 4 \pi \hbar^2 (a/m) \) characterizes two-particle interaction proportional to the s-wave scattering length \( a \), and the functional \( N = \int_{-\infty}^{\infty} |\psi|^2 dx \) is the integral of motion for the normalized nonstationary GP equation [8]. The value of \( \sigma = \text{sgn}(a) = \pm 1 \) in front of the nonlinear term is defined by the sign of the scattering length of the two-body interaction, repulsive for \( a > 0 \), and attractive for \( a < 0 \). The potential \( U(x) = k (|x| - x_0)^2 \) (below we take \( k = 1 \)) describes the double-well structure of the trap in the longitudinal direction.

In the linear limit (i.e., for an ideal non-interacting gas), we should consider \( \sigma = 0 \), and the exact stationary solutions of Eq. (1) in the form \( \psi(x,t) = \Phi_j(x) e^{i \lambda_j t} \) are found in terms of the parabolic algebraic elliptic functions [13] that define a set of confined stationary states existing...
at certain discrete values of $\beta_j$ (linear eigenmodes). For $\sigma \neq 0$, we can introduce, in a similar way, a set of nonlinear eigenmodes described by real functions $\Phi_j(x)$ that satisfy the following nonlinear equation,

$$\frac{d^2\Phi_j}{dx^2} + \beta_j \Phi_j - U(x)\Phi_j + \sigma \Phi_j^3 = 0. \quad (2)$$

While in the case $\sigma = 0$ the eigenvalue for each mode $\beta_j$ is unique for any given trap separation $x_0$, in the nonlinear case there exist families of localized solutions $\Phi_j$ characterized by the dependence of the norm $N_j = \int dx \Phi_j^2(x)$ on $\beta_j$, and the eigenvalue now becomes a parameter of a continuous family. Figure 1 shows two examples of the ground-state mode $\Phi_0(x)$ and first-order excited mode $\Phi_1(x)$ of the BEC with $N_0 = N_1$ but $\beta_0 \neq \beta_1$, for different values of $x_0$. The dependencies $\beta_0$ and $\beta_1$ on the trap separation $x_0$ are quite different for two signs of $\sigma$, as is seen in Fig. 2.

![Figure 1](image1.png)

**FIG. 1.** Confining potential (bold) with the ground (solid) and first excited (dashed) collective modes for (a) $x_0 = 0.6$, and (b) $x_0 = 2.5$ ($\sigma = -1$, $N_0 = N_1 = 5.0$). Dotted lines - corresponding values of the chemical potential: (a) $\beta_0 = 1.974$, $\beta_1 = 3.162$, and (b) $\beta_0 = 1.889$, $\beta_1 = 1.925$.

![Figure 2](image2.png)

**FIG. 2.** Dependencies $\beta_0(x_0)$ (lower curve) and $\beta_1(x_0)$ (upper curve) for $\sigma = 0$ (dotted) and $\sigma = \pm 1$ (solid, $N_0 = N_1 = 5.0$). Dashed - results of the variational approach.

To develop a coupled-mode theory for BECs, we consider the mode interaction in a double-well potential and assume that the condensate wave function is described by a superposition of two modes of different symmetry, i.e. symmetric and antisymmetric,

$$\psi(x, t) = b_0(t)\Phi_0(x)e^{-i\beta_0 t} + b_1(t)\Phi_1(x)e^{-i\beta_1 t}, \quad (3)$$

where $b_j$ ($j = 0, 1$) are the complex amplitudes, and $\Phi_j(x)$ may, in general, be any two solutions of Eq. (2). Then, the BEC dynamics can be deduced from the rate equations for the modal amplitudes $b_j$. A similar approach has previously been employed in Refs. to describe coherent tunneling between two largely separated harmonic traps, with the basis $\Phi_j$ consisting of the ground-state modes of individual potential wells. In contrary, our basis eigenfunctions are the local nonlinear modes of the entire double-well trap which can be found exactly for any given trap separation. Our approach is therefore similar to the analysis of the power transfer between the cores of a nonlinear optical coupler usually carried out in the terms of the supermodes, i.e. the local modes of a composite core.

To derive the equations for the complex mode amplitudes $b_j(t)$, we use the standard procedure, substituting the ansatz (3) into the nonstationary GP equation (1), and averaging over the spatial dimension after multiplying the GP equation by either $\Phi_0(x)$ or $\Phi_1(x)$. This yields a system of two coupled equations,

$$i\frac{dB_0}{dt} = \sigma C_0|B_0|^2B_0 + \sigma C_{01}(2|B_1|^2B_0 + B_0^*B_1^2e^{-i\Omega t}),$$

$$i\frac{dB_1}{dt} = \sigma C_1|B_1|^2B_1 + \sigma C_{01}(2|B_0|^2B_1 + B_0^*B_1^2e^{i\Omega t}).$$

Here $\Omega = 2(\beta_1 - \beta_0) - 2\sigma(C_0 N_0 - C_1 N_1)$, and the coupling coefficients are defined as $C_j = \gamma_{ij}/N_j^2$, $C_{01} = \gamma_{01}/(N_0 N_1)$, where $\gamma_{ij} = \int dx \Phi_j^2(x)\Phi_i^2(x)$, and $B_j$ are the normalized mode amplitudes, $B_j(t) = \sqrt{N_j}b_j(t)\exp(-i\sigma C_j N_j t)$. These equations conserve the total norm $|B_0|^2 + |B_1|^2 = n_0(t) + n_1(t) \equiv n$, where $n_0$ and $n_1$ have the meaning of the time-dependent population numbers for the two macroscopic states, and $n = N = N_0|b_0|^2 + N_1|b_1|^2$. It is important to note, that the form of the rate equations does not depend on the normalization conditions for the basis functions. For example, the condition $\int_{-\infty}^{\infty} |\Phi_j|^2 dx = \int_{-\infty}^{\infty} |\psi|^2 dx = 1$ simply imposes the constraint $|B_j| = |b_j|$, so that $n = N = |b_0|^2 + |b_1|^2$.

Separating the amplitudes and phases as $B_j(t) = \sqrt{n_j(t)}e^{-i\phi_j(t)}$, we obtain a system of coupled equations for the population difference of the two states $\Delta = n_1 - n_0$, and the relative phase shift, $\Theta = 2(\phi_0 - \phi_1) - \Omega$,

$$\frac{d\Delta}{dt} = \sigma(n^2 - \Delta^2) \sin \Theta,$$

$$\frac{d\Theta}{dt} = -\delta + \sigma(C_0 + C_1)\Delta - 2\sigma C_{01}(2 + \cos \Theta)\Delta, \quad (4)$$

where $\delta = 2(\beta_1 - \beta_0) + \sigma[(n - 2N_0)C_0 - (n - 2N_1)C_1]$. System (4) can be rewritten in a canonical form, $d\Delta/dt = -\partial H/\partial \Theta$, $d\Theta/dt = \partial H/\partial \Delta$, with the Hamiltonian: $H = \sigma(n^2 - \Delta^2)C_0\cos \Theta + \sigma(C_0 + C_1)/2 - 2C_{01}\Delta^2 - \Delta$. A mechanical analog of this system may describe the motion of a non-rigid pendulum with angular momentum $\Delta$ and a generalized angular coordinate $\Theta$. On the other
hand, Eqs. (3) closely resemble the dynamic equations for the guided power and phase difference of two nonlinearly interacting orthogonally polarized optical modes in a birefringent fiber [6]. The exact solution of the system (3) can be obtained in terms of elliptic Jacobi functions and will be presented elsewhere.

The dynamics described by Eqs. (3) depends crucially on the values of the coupling coefficients $C_0$, $C_1$, and $C_{01}$, which are determined by integration over the eigenmode profiles, so that the results can be quite different and rational equations with respect to the parameters $\sigma$. Importantly, for $\sigma = +1$, the energy spectrum becomes degenerate. As expected from the linear theory [13] and results (3), the coupling coefficients are sufficiently different, there are only two fixed states of the relative population: $\Delta = \pm n$, which corresponds to either $n_0 = 0$ or $n_1 = 0$. In both these states, the phase is unbounded, i.e. it is a linear function of time. The other phase trajectories in Figs. 4(a,b) represent the dynamical states with the running phase, that is a delocalized phase. The mechanical analogy of this phenomenon is simple [10]: it corresponds to a self-sustained steady closed-loop rotation of a non-rigid pendulum around its support. In terms of the condensate dynamics, these states describe the nonlinear Rabi-type oscillations between the ground and first excited macroscopic states, for small $x_0$, and the Josephson-type tunneling between the two potential wells, for a sufficiently large separation. Remarkably, the population of either well is never completely depleted.

To visualize the population dynamics, in Fig. 4 we plot the phase portraits $\{\Theta, \Delta\}$ of the dynamical system (3) for the case $\sigma = +1$ and $N_0 = N_1$. For convenience, the population difference, $\Delta$, is measured in the units of $n$.

For small separations [Figs. 4(a,b)], while the coupling coefficients are sufficiently different, there are only two fixed states of the relative population: $\Delta = \pm n$, which corresponds to either $n_0 = 0$ or $n_1 = 0$. In both these states, the phase is unbounded, i.e. it is a linear function of time. The other phase trajectories in Figs. 4(a,b) represent the dynamical states with the running phase, that is a delocalized phase. The mechanical analogy of this phenomenon is simple [10]: it corresponds to a self-sustained steady closed-loop rotation of a non-rigid pendulum around its support. In terms of the condensate dynamics, these states describe the nonlinear Rabi-type oscillations between the ground and first excited macroscopic states, for small $x_0$, and the Josephson-type tunneling between the two potential wells, for a sufficiently large separation. Remarkably, the population of either well is never completely depleted.

The routine of calculating the coupling coefficients numerically can be bypassed by employing the variational approach, using the trial functions in the form of a linear superposition of the ground states of isolated traps: $\Phi_{0,1} = A_{0,1} \{ \exp[(x-x_0)^2/2a_{0,1}^2] \pm \exp[(x+x_0)^2/2a_{0,1}^2] \}$, and the Lagrangian of the stationary GP equation,

$$\mathcal{L} = \frac{1}{2} \left( \frac{d\Phi_j}{dx} \right)^2 + \frac{1}{2} [\beta_j - U(x)] \Phi_j^2 - \frac{1}{4} \sigma \Phi_j^4.$$

By inserting the trial functions into the corresponding variational integral, an explicit, although algebraically complicated integrated Lagrangian is obtained. The variational equations with respect to the parameters $A_{0,1}$ and $A_{0,1}$ yield relations which determine the characteristic eigenvalues $\beta_{0,1}(x_0)$ and the coefficients $C_0$, $C_1$, and $C_{01}$. These relations can be further simplified in the limit $x_0 \gg 1$, but must be solved numerically for a general case. Comparisons between the variational predictions and the results obtained by solving Eq. (3) numerically are shown in Fig. 2, for $\beta_{0,1}(x_0)$, and in Fig. 3, for $C_0$, $C_1$, and $C_{01}$. The agreement is seen to be satisfactory.

The phase plane shown in Fig. 4 also reveals the existence of macroscopic quantum self-trapped (MQST) states, predicted and described in [14] for weakly interacting BECs in largely separated traps. The MQST states are characterized by a nonzero average population imbalance. As the separation between the wells grows, a bifurcation of the fixed points on the phase plane $\{\Delta, \Theta\}$ occurs, and the stable centers, corresponding to the MQST states with a trapped phase, appear [see Figs. 4(c,d)]. This occurs at a certain $x_{0,cr}$, for which the condition $\delta = n(6C_{01} - C_0 - C_1)$ is satisfied. For $\sigma = +1$ and $n = 1$, for example, $x_{0,cr} \approx 1.48$ which agrees very well with the corresponding result of the variational approach, $x_{0,cr} \approx 1.41$. For larger separation, when $C_0 \approx C_1 \approx C_{01}$, the positions of the centers are approximately given by: $\Delta \approx (\beta_0 - \beta_1)/(2C_{01}\sigma)$ at $\Theta = \pm (2m)\pi$, where $m$ is integer.
fixed centers move towards the line $\Delta = 0$, and the saddles form between them, so that the MQST states, other than those identical to the ground states of the individual wells, cease to exist [see Fig. 4(d)]. The oscillations of the population imbalance around the stable fixed points with the trapped phase have been identified in [11] as $\pi$-states. Clearly, the effect we observe here is qualitatively similar, except for the average value of the trapped phase which, due to a different choice of the basis eigenfunctions and definition of $\Theta$, is equal to $\pm(2m)\pi$.

To compare the predictions of our coupled-mode theory with the actual dynamics of the BEC in a double-well potential modeled by the GP equation, we solve Eq. (1) numerically. As an initial condition, for both $\sigma = \pm 1$, we take $\psi(x,0) = b_0(0)\Phi_0(x) + b_1(0)\Phi_1(x)$, with $b_0^2(0) + b_1^2(0) = 1/N_0 = 1/N_1$. In Fig. 5(a), the phase trajectories $\Delta(\Theta)$ are compared with those calculated using Eqs. (1), for $\sigma = -1$, and the trap separation corresponding to sufficiently dissimilar values of $\beta_j$ and $C_j$ (see Figs. 2 and 3). It is clear that the approximate equations of the coupled-mode theory correctly describe the dynamics of the condensate in the states with a running phase [see Fig. 5(c)], as well as the position of the MQST states, one of which is shown in Fig. 5(b). Performing a similar comparison for different $\sigma$ and $x_0$, we can conclude that the eigenfunctions $\Phi_j(x)$ represent a good basis for the modal decomposition of the macroscopic condensate wave function $\psi(x,t)$. The adiabatic evolution of the eigenfunctions with time, although leading to slight deviations of the condensate states from the exact MQSTs [see Fig. 5(a)], does not introduce significant damping into the system, and therefore does not lead to a dramatic switching between the states.

In conclusion, we have employed the concepts of the nonlinear guided-wave optics and developed, for the first time to our knowledge, a consistent coupled-mode theory for BECs. We have studied the BEC dynamics in a double-well harmonic trap, and verified the results by numerical simulations of the nonstationary GP equation. The strong advantage of our theory is its ability to describe the condensate dynamics for any well separation, including the Josephson tunneling effect at large separations, mode coupling and Rabi oscillations in a single harmonic well, and the macroscopic self-trapped states in the crossover regime.

![FIG. 5](image)

FIG. 5. (a) Phase trajectories $\Delta(\Theta)$ calculated from Eqs. (1) for $\sigma = -1$, $x_0 = 1.7$ (thin) compared with the numerical solution of the GP equation (thick). (b) $|\psi|^2$ in the MQST state "1" in (a), at the normalized times $t = 0$ (solid) and $t = 100$ (dashed). (c) $|\psi|^2$ corresponding to the point "2" in (a) at $t = 0$ (solid), and corresponding to the point "3" in (a) at $t = 20$ (dashed). Double-well potential is shown in (b,c) by a dotted curve.

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