Abstract: The problem of resonant generation of nonground-state condensates is addressed aiming at resolving the seeming paradox that arises when one resorts to the adiabatic representation. In this picture, the eigenvalues and eigenfunctions of a time-dependent Gross-Pitaevskii Hamiltonian are also functions of time. Since the level energies vary in time, no definite transition frequency can be introduced. Hence no external modulation with a fixed frequency can be made resonant. Thus, the resonant generation of adiabatic coherent modes is impossible. However, this paradox occurs only in the frame of the adiabatic picture. It is shown that no paradox exists in the properly formulated diabatic representation. The resonant generation of diabatic coherent modes is a well defined phenomenon. As an example, the equations are derived, describing the generation of diabatic coherent modes by the combined resonant modulation of the trapping potential and atomic scattering length.

Generation of nonground-state condensates and adiabatic paradox

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1. Origin of adiabatic paradox

Nonequilibrium ultracold Bose-condensed gases are well described by the time-dependent Gross-Pitaevskii equation [1–10], which is a nonlinear Schrodinger equation

\[ i \dot{\psi}(t) = H[\psi(t), t] \psi(t) , \]

Here \( h \equiv 1 \) and, to simplify the notation, the condensate wave function \( \psi(t) \) is assumed to be a vector in spatial variables and the nonlinear Hamiltonian \( H[\psi(t), t] \) is a matrix in these variables. The overdot means the differentiation with respect to time \( t \). The temperature is close to zero, so that all \( N \) atoms are supposed to be in the coherent Bose-condensed state. Generally, the condensate wave function is normalized to the total number of condensed atoms. If this function is denoted as \( \eta(t) \), it is always possible to introduce, by means of the relation

\[ \eta(t) = \sqrt{N} \psi(t) , \]

the function \( \psi(t) \) that is normalized to one,

\[ \| \psi(t) \|^2 \equiv \langle \psi(t) | \psi(t) \rangle = 1 . \]

It is the latter function that is assumed in Eq. (1). The system of trapped atoms is subject to the action of an externally induced modulation field, so that the nonlinear Hamiltonian \( H[\psi(t), t] \) depends on time directly as well as through the function \( \psi(t) \).

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It is possible to consider the adiabatic eigenvalue problem
\[ H[\psi_n, t] \psi_n(t) = E_n(t)\psi_n(t), \]
(3)
treating time as a fixed parameter. Then, of course, the eigenfunctions \( \psi_n(t) \) and the eigenvalues \( E_n(t) \) depend on time. The multi-index \( n \) labels the eigenfunctions and eigenvalues. The energy spectrum, for trapped atoms is discrete. The eigenfunctions can be normalized to one:
\[ \| \psi_n(t) \|^2 \equiv \langle \psi_n(t) | \psi_n(t) \rangle = 1. \]
(4)
These functions correspond to the adiabatic coherent modes.

The nonlinear Eq. (1) can possess different solutions. A wide and important class of solutions can be represented as the expansion over the adiabatic coherent modes:
\[ \psi(t) = \sum_n a_n(t) \exp \{ i\chi_n(t) \} \psi_n(t), \]
(5)
where the phase
\[ \chi_n(t) = \delta_n(t) + \zeta_n(t) \]
(6)
is the sum of the dynamic phase
\[ \delta_n(t) \equiv - \int_0^t E_n(t') dt' \]
(7)
and of the geometric phase
\[ \zeta_n(t) \equiv i \int_0^t \langle \psi_n(t') | \dot{\psi}_n(t') \rangle dt'. \]
(8)
Formula (5) does not exhaust all admissible solutions of the nonlinear Schrödinger equation (1). But here we are interested in the class of solutions that are representable as expansion (5).

The problem of dealing with the nonlinear Hamiltonian \( H[\psi, t] \) is that the form \( H[\psi_n, t] \) is not a Hermitian operator since
\[ \langle \psi_m(t) | H[\psi_n, t] \psi_n(t) \rangle \neq \langle H[\psi_n, t] \psi_m(t) | \psi_n(t) \rangle. \]
(9)
Therefore, the eigenfunctions \( \psi_m(t) \) and \( \psi_n(t) \) for \( m \neq n \), generally, are not orthogonal,
\[ \langle \psi_m(t) | \psi_n(t) \rangle \neq \delta_{mn}. \]
These functions do not necessarily compose a complete basis. However, in the space that is a closed linear envelope \( \text{Span} \{ \psi_n(t) \} \), they form a total normalized basis, so that the functions from this space can be represented in the form of expansion (5). Substituting the latter into Eq. (1) yields
\[ \sum_m \tilde{a}_m(t) \langle \psi_n(t) | \psi_m(t) \rangle + a_m(t) \langle \psi_n(t) | \dot{\psi}_m(t) \rangle \times (1 - \delta_{mn}) + \]
\[ + i a_m(t) \langle \psi_n(t) | H[\psi, t] - E_m(t) | \psi_m(t) \rangle \]
\[ \times \exp \{ i\zeta_m(t) \} = 0. \]
This equation is difficult to simplify because of the nonorthogonality of the basis \( \{ \psi_n(t) \} \).

If the time dependence in the Hamiltonian \( H[\psi, t] \) enters through an external alternating field with a fixed frequency \( \omega \), then the latter cannot be tuned to resonance with any of the time-dependent transition frequencies \( E_m(t) - E_n(t) \). Moreover, the eigenenergies enter expansion (5) not explicitly but through the dynamic phases (7). Thus, no resonance condition can be defined, making the resonant generation of adiabatic coherent modes impossible. It is this argument that one raises against the possibility of generating nonground-state condensates of trapped atoms.

2. Paradox-free diabatic representation

Now we show that no paradox arises in a properly formulated diabatic representation. Let the Hamiltonian be a sum
\[ H[\psi, t] = H_0[\psi] + V[\psi, t], \]
(11)
where the first term describes the system of cold trapped atoms, while the second term contains the direct time dependence from externally induced modulation fields.

The diabatic coherent modes are defined as the solutions to the time-independent eigenproblem
\[ H_0[\varphi_n] \varphi_n = E_n \varphi_n. \]
(12)
The definition of the diabatic coherent modes as time-independent, stationary solutions makes them principally different from the adiabatic modes of Sec. 1. It is this definition of coherent modes that was introduced in [11–13]. Particular examples of such modes are vortices [14], though many other types of modes are admissible [11–13]. The lowest diabatic coherent mode corresponds to the usual ground-state Bose-Einstein condensate. While the excited diabatic coherent modes represent nonground-state condensates.

The nonlinear Hamiltonian \( H_0[\varphi_n] \) is not Hermitian. Hence the eigenmodes \( \varphi_m \) and \( \varphi_n \), with \( m \neq n \), are not orthogonal, although all of them can be normalized to one:
\[ \| \varphi_n \|^2 \equiv \langle \varphi_n | \varphi_n \rangle = 1. \]
(13)
But again, in the space that is a closed linear envelope \( \text{Span} \{ \varphi_n \} \), the family \( \{ \varphi_n \} \) forms a normalized total basis. In this space, the corresponding class of solutions to Eq. (1) can be represented as the expansion
\[ \psi(t) = \sum_n c_n(t) \exp(-iE_n t) \varphi_n \]
(14)
over the stationary coherent modes.
Substituting expansion (14) into Eq. (1) results in the equation
\[
\sum_{m} \tilde{c}_m(t) \langle \varphi_n | \varphi_m \rangle \exp(-i\omega_m t) = \left( \sum_{m} c_m(t) \langle \varphi_n | H[\psi, t] - E_m | \varphi_m \rangle \exp(-i\omega_m t) \right),
\]
in which
\[
\omega_m \equiv E_m - E_n.
\]
The latter expression defines transition frequencies that do not depend on time. Consequently, a given frequency \( \omega \) in which \( \kappa \) is the transition frequencies with one of these transition frequencies.

Introducing the notation \( \kappa_{nm} \equiv \frac{\omega_m}{E_m - E_n} \),

where \( m \) is atomic mass and \( a_s \), scattering length. The nonlinear Hamiltonian takes the form
\[
H[\psi, t] = -\frac{\nabla^2}{2m} + U(r, t) + N\phi(t)|\psi(r, t)|^2,
\]
where the term
\[
U(r, t) = U(r) + V(r, t)
\]
consists of a trapping potential \( U(r) \) and an external driving field \( V(r, t) \). The interaction part
\[
\phi(t) = \phi_0 + \varepsilon(t)
\]
contains the static interaction potential \( \phi_0 \), defined in Eq. (21), and an additional term describing a possible modulation of the scattering length by means of the Feshbach resonance technique [19].

The generation of coherent modes by modulating the trapping potential, as in Eq. (23), its properties, and different applications were considered in [11–13,20–35]. The analytical treatment, using the averaging method, was compared and found to be in good agreement with the direct simulation of the Gross-Pitaevskii equation [36,37]. The possibility of the resonant creation of coherent modes by modulating the atomic scattering length using Feshbach resonance was considered in [38]. This method can be preferred for those atomic species that demonstrate high tunability of their scattering length [39]. In the present paper, we take into account both these ways, simultaneously modulating the trapping potential as well as the scattering length. By combining both these techniques can give additional advantage for generating nonground-state condensates. For instance, the combination of these two techniques can be employed for generating two different excited coherent modes, in addition to the ground-state one, or for enhancing the generation of the chosen mode.

Hamiltonian (22) can be presented in form (11), with
3. Generation of coherent modes

To specify the above equations, let us consider the atoms interacting through the local potential
\[
\phi(r) = \phi_0 \delta(r) \quad \left( \phi_0 \equiv 4\pi a_s^2 \right),
\]
where \( m \) is atomic mass and \( a_s \), scattering length. The nonlinear Hamiltonian takes the form
\[
\phi(t) = \phi_0 + \varepsilon(t)
\]
contains the static interaction potential \( \phi_0 \), defined in Eq. (21), and an additional term describing a possible modulation of the scattering length by means of the Feshbach resonance technique [19].

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Hamiltonian (22) can be presented in form (11), with
\[
H_0[\psi] = -\frac{\nabla^2}{2m} + U(r, t) + N\phi_0|\psi(r, t)|^2
\]
and
\[
V[\psi, t] = V(r, t) + N\varepsilon(t)|\psi(r, t)|^2.
\]
Eigenproblem (12) becomes
\[
H_0[\varphi_n] = E_n\varphi_n(r),
\]
and expansion (14) takes the form
\[
\psi(r, t) = \sum_n c_n(t) \exp(-iE_n t) \varphi_n(r).
\]
Then we should follow the consideration of Sec. 2.

To explicitly accomplish the averaging procedure of Eq. (18), we have to concretize the trap modulation and the type of the interaction alternation. We take the general form of the oscillating trapping modulation

$$V(r, t) = V_1(r) \cos \omega t + V_2(r) \sin \omega t$$

(29)

and the similar type of the interaction alternation

$$\epsilon(t) = \epsilon_1 \cos \omega t + \epsilon_2 \sin \omega t.$$  

(30)

The oscillation frequency is taken the same for both modulations, so that the same nonground-state coherent mode be excited. In principle, two different frequencies could be taken for modulations (29) and (30), if we would wish to excite two different nonground-state modes simultaneously. The frequency $\omega$ is tuned to the resonance with a chosen transition frequency

$$\omega_{21} \equiv E_2 - E_1.$$  

(31)

If the generation procedure starts with an equilibrium Bose-Einstein condensate, then $E_1$ is the lowest energy of atoms in the trap, corresponding to the condensate chemical potential [10]. The resonance condition reads as

$$\left| \frac{\Delta \omega }{\omega_{21}} \right| < 1 \quad (\Delta \omega \equiv \omega - \omega_{21}).$$

(32)

For what follows, it is convenient to introduce the notation for the transition amplitudes

$$\alpha_{mn} \equiv N \Phi_0 \int \left| \varphi_m(r) \right|^2 \left[ 2 \left| \varphi_n(r) \right|^2 - \left| \varphi_m(r) \right|^2 \right] d r,$$

$$\beta_{mn} \equiv \int \varphi_m^*(r) \left[ V_1(r) - i V_2(r) \right] \varphi_n(r) d r,$$

$$\gamma_n \equiv N (\epsilon_1 - i \epsilon_2) \int \varphi_1^*(r) \left| \varphi_n(r) \right|^2 \varphi_2(r) d r.$$  

The first of them is the amplitude due to atomic interactions, the second one is caused by the trap modulation, and the third amplitude is due to the interaction oscillation. To satisfy condition (17), these amplitudes to be small, such that

$$\left| \frac{\alpha_{mn}}{\omega_{mn}} \right| \ll 1, \quad \left| \frac{\beta_{mn}}{\omega_{mn}} \right| \ll 1, \quad \left| \frac{\gamma_n}{\omega_{mn}} \right| \ll 1,$$

where $\omega_{mn} \neq 0$.

Substituting expressions (29) and (30) into Eq. (20), under the resonance condition (32), yields the evolution equations for the coefficient functions $c_n = c_n(t)$ defining the fractional mode populations

$$p_n(t) \equiv |c_n(t)|^2.$$  

(34)

Under the resonance condition (32), the system of equations reduces to only two equations for the considered coherent modes:

$$i \frac{d c_1}{d t} = \alpha_{12} |c_2|^2 c_1 +$$

$$+ \frac{1}{2} \left( 2 \gamma_1 |c_1|^2 + \gamma_2 |c_2|^2 + \beta_{12} \right) c_2 \exp(i \Delta \omega t) +$$

$$+ \frac{1}{2} \gamma_1 c_2^* \exp(-i \Delta \omega t),$$

$$i \frac{d c_2}{d t} = \alpha_{21} |c_1|^2 c_2 +$$

$$+ \frac{1}{2} \left( 2 \gamma_2 |c_2|^2 + \gamma_1 |c_1|^2 + \beta_{21} \right) c_1 \exp(-i \Delta \omega t) +$$

$$+ \frac{1}{2} \gamma_2 c_1^* \exp(i \Delta \omega t).$$

Solving these equations gives the dynamics of the fractional mode populations (34).

Here we have considered the case of zero temperature and asymptotically weak atomic interactions, when the whole atomic cloud is in a coherent state described by the Gross-Pitaevskii equation. It is possible to extend the consideration to the case of finite temperatures and interactions, when, in addition to the fraction of condensed atoms, there exists a fraction of uncondensed atoms. This can be done by invoking, for instance, a stochastic variant of the Gross-Pitaevskii equation [40–42] or by employing the fully self-consistent theory [43–45]. The possibility of generating nonground-state condensates, even at finite temperatures and interactions, is due to the resonant nature of the generation procedure; since the energy levels of the coherent modes in a trap are discrete, while the spectrum of uncondensed atoms is continuous [43].

Eqs. (35) describe the dynamics of the guiding centers that correspond to the first approximation of the averaging techniques [15–18]. In this approximation, under the resonance condition (32), the system of equations for the functions $c_n(t)$ reduces to only two Eqs. (35), if at the initial time $t = 0$ other modes were not populated, so that

$$c_n(0) = 0 \quad (n \neq 1, 2).$$

Then $c_n(t) = 0$, if $n \neq 1, 2$, for all $t > 0$. Generally, there also exist nonresonant transitions between the coherent modes. These nonresonant transitions can be taken into account by the higher-order approximations of the scale separation approach [16–18]. In the higher-order approximations, the mode amplitudes $c_n(t)$ for the nonresonant modes, for which $n \neq 1, 2$, become nonzero, even if at the initial time these modes were not populated. However, the amplitudes of these nonresonant modes remain small during the time interval $0 < t < t_{res}$, when they can be neglected. But for longer times $t > t_{res}$, the nonresonant modes cannot be neglected. Thus, the resonant generation of coherent modes is limited by the time $t_{res}$, which was estimated in [25,43]. By the order of magnitude, the resonance time $t_{res}$ can be made comparable to the lifetime of atoms in a trap, provided the absolute values of the transition amplitudes $|\alpha_{12}|$, $|\beta_{12}|$, $|\gamma_1|$, and $|\gamma_2|$ are much smaller than the transition frequency $\omega_{21} \approx \omega$. Thus, Eqs. (35) are valid only for $t < t_{res}$. But the time $t_{res}$, being of the order of the atom lifetime in a trap, is sufficiently
long for realizing the process of the resonant mode generation.

In conclusion, we have demonstrated that the appearance of the adiabatic paradox, precluding the generation of the adiabatic modes, exists solely in the adiabatic picture. The adiabatic representation is unsuitable for the case of resonance. However, the diabatic representation, developed in Sec. 2, contains no paradoxes and is perfectly appropriate for describing the resonant generation of coherent modes characterizing nonground-state condensates. Such a generation can be realized by the resonant modulation of either the trapping potential, or the scattering length, or by the combined modulation of both.

The appearance of the resonantly generated nonground-state condensates can be observed, for instance, by means of collective light scattering [46–49]. Another way of their registration is through the time-of-flight experiments, as is discussed in [50].

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