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Formation of Bose-Einstein condensate structures in laser fields: semiclassical approach and electrodynamic effects

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The formation of Bose-Einstein condensate (BEC) structures via electromagnetically induced interactions is analyzed within a semiclassical approach where an improved interaction potential is obtained. This analysis shows how the laser-induced forces can lead to self-confinement of the ground state even with a homogeneous field. It furthermore indicates that the vector character of the field can be crucially important, since it can change the type of nonlinearity, thus strongly modifying the BEC structures.

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Background. Recently, the nonlinear behaviour of Bose-Einstein condensates (BEC) in laser fields has become a subject of growing attention (see, e.g., [1 – 3]and references therein), inspired both by new perspectives in the study of BEC in optical lattices and by new possibilities of having a BEC self-localized in space via laser-induced interactions when the atoms are released from a trap. Since most of the experiments on Bose-Einstein condensation have been accurately described by the mean-field method based on the Gross-Pitaevskii equation (GPE) [4], extensions of this equation are also used for describing BEC in optical fields. However, so far the potential energy of the interaction has been modelled as the single-particle ponderomotive potential in problems of optical lattices or as a sum of the laser-induced dipole-dipole interatomic potentials, see for example [3] or [5].

The purpose of the present work is to provide a general approach for describing the laser-induced interaction of Bose-Einstein condensates where the difference between the local field (the microscopic field acting on an atom) and the macroscopic field (the field averaged over a volume containing many atoms) is taken into account. Of particular interest is to investigate the formation of BEC structures created via such interactions where the nature and stability of a Bose-condensed state are influenced by the self-induced dipole-dipole interaction forces. This analysis provides us with qualitatively new regimes for the formation of condensate structures. To this purpose, we consider an extension of the GPE by using a semiclassical approach for describing the self-induced forces (striction forces) in the laser-condensate interaction. For a large number of atoms, this description can be significantly simplified by using the macroscopic electrodynamics approach. This analysis also shows that the vector character of the field can be crucially important. For instance, for BEC structures well-localized within a laser wavelength along the field, variations of the dielectric permittivity strongly influence the microscopic field, thus qualitatively changing the type of nonlinearity.

Semiclassical approach. The dipole-dipole interactions of a BEC in laser fields as well as in static fields have recently been investigated within the framework of quantum theory [5 – 8]. For models of different effective interaction potentials, simple cases of density modulations and atomic beam guiding have been investigated. The full quantum description is based on the exact Hamiltonian, but for the conditions of interest in laser-condensate interactions and for large laser detunings from the atomic resonance, a semi-classical model can be derived where the atoms are described by a Schrödinger equation with the interaction term given by the self-induced force calculated in the framework of macroscopic electrodynamics. For a high frequency field, the averaged induced force per volume, **f**, in transparent media can be obtained as shown in [9] by time averaging of the corresponding electrostriction force in a static electric field [10]. For a zero-temperature, dilute BEC in a far-off resonant laser field $\mathrm{Re}[\mathbf{E}\exp(-i\omega t)]$, we have (see Ref. [9])

$$\mathbf{f} = \frac{n}{16\pi}\nabla\left[|\mathbf{E}|^2\frac{\partial\varepsilon}{\partial n}\right], \qquad (1)$$

where n is the condensate atom density, and ε is the dielectric permittivity of the condensate gas. To describe the striction forces, we have to find a suitable model for ε. Since we assume a large number of condensate particles in a volume λ^3 (λ is the laser wavelength), the dielectric constant can be modelled in the local-field approach where, for atomic gases, the difference between the local field acting on an atom and the macroscopic field formed by the induced dipoles of the surrounding particles is taken into account, see, for example, [11]. This gives

$$\varepsilon = 1 + \frac{4\pi\alpha n}{1-(4\pi/3)\alpha n}, \qquad (2)$$

where $\alpha = -d^2/\hbar\Delta$ is the atomic polarizability at the laser frequency, with $\Delta = \omega - \omega_a$ being the detuning from the nearest atomic resonance frequency ω_a, and d is the dipole matrix element of the resonant transition. By substituting Eq.(2) into Eq. (1) we obtain the total force acting on a single atom $\mathbf{F} = \mathbf{f}/n = -\nabla V_d$ where the corresponding potential energy is given by

$$V_d = -\frac{\alpha}{4}\frac{|\mathbf{E}|^2}{(1-(4\pi/3)\alpha n)^2}. \qquad (3)$$

For a single particle (n=0), Eq.(3) describes the ponderomotive force in an inhomogeneous laser beam. However, even in a homogeneous laser field, the force does not vanish since it may also be generated by the presence of density gradients. As is easily seen, in the low density limit (or in the weak dipole interaction limit, $4\pi\alpha n/3 \ll 1$), the striction force originating from the induced microscopic dipole-dipole interatomic forces is attractive force, independent of the sign of the frequency detuning, i.e., $V_d \propto -\alpha^2 n$. Although at a first glance the low density approximation seems to describe most of the experiments, the structural dynamics and the subsequent density modulations will, in fact, depend on the character of the nonlinearity, i.e., on the sign of the detuning.

Self-confined BEC. We consider a condensate with repulsive interaction (the s-wave scattering length $a >$ > 0). The above result implies that the dynamics of the BEC atoms in a laser field can be described by a generalized GPE for the condensate wave function $\Psi(\mathbf{r},t)$ [4]:

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_0\Psi + \left[U_0|\Psi|^2 - \frac{\alpha}{4}\frac{|\mathbf{E}|^2}{(1-(4\pi/3)\alpha|\Psi|^2)^2}\right]\Psi, \qquad (4)$$

where $\hat{H}_0$ is the linear single-particle Schrödinger Hamiltonian, the wave function Ψ is normalized as $N =$ $= \int|\Psi|^2 d\mathbf{r}$ with N denoting the total number of atoms, so that the gas density is $n = |\Psi|^2$, $U_0 = 4\pi\hbar^2 a/m$ and m is the atom mass. In Eq.(4), the laser-induced nonlinearity originates from the difference between the macroscopic and local fields in a condensate gas and bears a local character since, for fixed orientation and separation of the dipoles, the interaction energy for a large number of atoms in a physical volume averaged over the relative positions of the dipoles vanishes, see, e.g., [11]. This is consistent with the approach used in [6], where a phenomenological dipole-dipole interaction is assumed to be in the form of a contact potential, rather than with the model used in [3, 5], where the main contribution is due to the long range interaction. As a first approximation in the low density limit, the self-confining dynamics does not depend on the sign of α and when the interparticle interaction is dominated by the dipole-dipole forces, i.e., for laser intensities such that

$$|\mathbf{E}|^2 > \mathrm{E}_{th}^2 = \frac{3U_0}{2\pi\alpha^2} = \frac{6\hbar^4 a\Delta^2}{md^4}, \qquad (5)$$

the dynamics may result in a density modulation of the condensate ground state and even a tendency towards a subsequent collapse-like evolution that usually takes place only in the presence of attractive s-wave interactions [12, 13]. However, the question of what kind of structures the condensate will actually realize, must be answered by using the exact Eq.(4) and, in fact, the evolution will essentially depend on the sign of the laser frequency detuning. In order to clarify this question, we consider the case of a constant (homogeneous) laser field $\mathbf{E}$ = const, and restrict the analysis to the steady-state regime where we can assume $\Psi(\mathbf{r},t) = \psi(\mathbf{r})\exp(-iEt/\hbar)$. Without external potential Eq.(4) reduces to

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + U_0\psi^2 - \frac{\alpha}{4}\frac{|\mathbf{E}|^2}{\left(1-\frac{4\pi}{3}\alpha\psi^2\right)^2}\right]\psi = E\psi, \qquad (6)$$

where ∇^2 is the Laplace operator and E is the ground state energy of the Bose condensate which depends also on the total number of condensate atoms. It is obvious that, due to the focusing nature of the induced dipole-dipole interaction nonlinearity, there are continuous families of symmetrical localized solutions of Eq.(6) for any space dimensionality. However, since the validity of a model with a constant field, as we will see below, depends on the orientation of the density gradients, we will here pay particular attention to 3D axisymmetrical and 1D cases.

In 1D, Eq.(6) is similar to that which describes particle motion in the effective potential $V_e(\psi) = -U_0\psi^4 +$ $+(\alpha/2)|\mathbf{E}|^2\psi^2/(1-(4\pi/3)\alpha\psi^2)+2E\psi^2$. From this analogy, all possible condensate distributions can be inferred from the phase portraits of the system. This is shown in Fig.1 for the different parameters for which localized solutions exist. The main bifurcation inequality when a

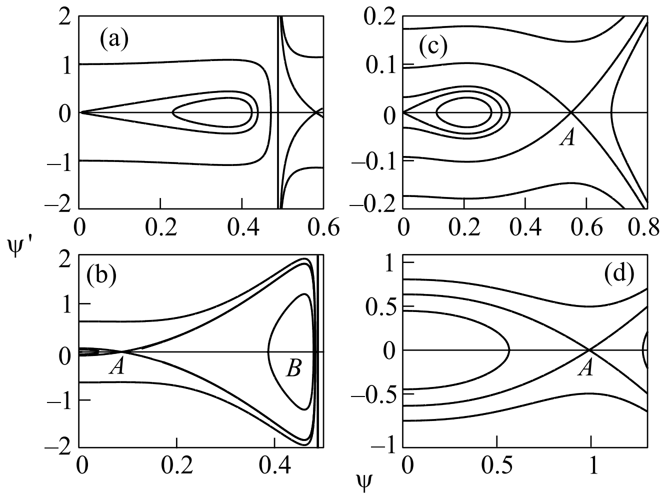

Fig.1. Phase portrait for Eq.(6) for different regimes when the self-confinement of the ground state can occur (symmetrical with respect to the axis ψ'): (a) $\alpha > 0$, $E < -E_c$, for any number of condensate atoms if $|\mathbf{E}|^2 > E_{th}^2$ and otherwise for $N > N_*$, (b) $\alpha > 0$, $E > -E_c$ and $|\mathbf{E}|^2 < E_{th}^2$, (c) $\alpha < 0$, $|\mathbf{E}|^2 > E_{th}^2$; and (d) $\alpha < 0$, $|\mathbf{E}|^2 < E_{th}^2$. Dash line indicates the singularity point in the potential energy $V_e(\psi^2)$

localized BEC can occur is given by Eq.(5). If the laser intensity exceeds this threshold, self-confined states can occur for any number of atoms as seen in Fig.1a,c where the separatrix curve passing through zero corresponds to localized solutions. For weak nonlinearity, the bound state has the shape of the Schrodinger soliton, $\psi(x) \simeq \simeq \sqrt{2\tilde{E}/\tilde{\delta}U_0}\text{sech}(\sqrt{2m\tilde{E}}x/\hbar)$ (where $\tilde{E} = -E - E_c > 0$, $E_c = \alpha|\mathbf{E}|^2/4$, $\tilde{\delta} = (|\mathbf{E}|^2/\mathrm{E}_{th}^2) - 1 > 0$) with the total number of atoms $N = \sqrt{2\tilde{E}/m}(2\hbar/\tilde{\delta}U_0)$ decreasing with decreasing $\tilde{E}$. In fact, the qualitative behaviour of the localized solutions does not depend on the sign of α. However, as we will see below, the sign of α is important for the problem of stability which originates from the singularity in the interaction potential for red frequency detuning ($\alpha > 0$) where the condensate distributions become more narrow for increasing number of atoms in contrast to the case of blue detuning ($\alpha < 0$) where the condensate distributions become more flat due to the saturation behaviour of the nonlinearity.

If the inequality given by Eq.(5) is not fulfilled, self-bound states of the BEC do not exist for $\alpha < 0$. However, for red detuning ($\alpha > 0$) topologically the same phase portrait takes place if the number of condensate atoms exceeds some critical value (see Fig.1a). This critical number of atoms corresponds to the case when the ground energy of the condensate is equal to $E = -E_c$, which can be found by direct integration of Eq.(6). In a case that may be verified experimentally, when laser intensities are near the threshold level, i.e., $0 < \delta = 1 - (|\mathbf{E}|^2/\mathrm{E}_{th}^2) << 1$, the ground state distribution is self-organized to the form

$$\psi_*(x) \simeq \sqrt{\frac{3\delta}{4\pi\alpha}}\frac{1}{1+\gamma^2x^2}, \tag{7}$$

where $\gamma = (\delta/\hbar)\sqrt{3mU_0/4\pi\alpha}$. This solution contains a critical number of atoms, N_*, which does not depend on δ:

$$N_* = \int_{-\infty}^{\infty} \psi_*^2(x)dx \simeq \sqrt{\frac{3\pi\hbar^2}{4mU_0\alpha}}. \tag{8}$$

In a 3D geometry, N_* plays the role of the atom density surface density.

It is interesting to note that Eq.(6) not only has purely localized solutions ($\psi \to 0$ at $x \to \pm\infty$) but also describes localized solutions on a homogeneous condensate background, as a dark soliton corresponding to the separatrix curve from the equilibrium point A to $-A$ (Fig.1b,c,d) and as a hump (compressed) field in the condensate (closed separatrix around the equilibrium point B in Fig.1b). If the dark soliton in Fig.1d can be considered as a generalized version of the well-known solution observed also experimentally (see, for instance, in [14]), the others represent new solutions indicating that new types of collective excitations can be produced in laser-condensate interactions.

The important role of the sign of α is clearly seen for axisymmetric BEC structures that occur if the total number of atoms exceed a critical number, which can easily be calculated by expanding the potential function in the low density limit where the ground state solution is the so called Townes mode [12, 15]. Eq.(6) admits localized solutions for any sign of the detuning. However, it is obvious that for positive α, such solutions are unstable against collapse. This is in accordance with the stability criterion of Kolokolov and Vakhitov [16]. The ground state is unstable when the total number of atoms is an increasing function of the energy $\delta N/\delta E > 0$ as seen in Fig.2a. Otherwise, it is stable (Fig.2b) due to the saturation-type nonlinearity. Thus, for $\alpha > 0$, condensates tend to collapse and can produce even a condensed matter state. It should be noted that one-dimensional states may also be unstable against collapse due to the singularity in the potential energy (see, for example, [17]) and therefore quasi-1D condensed matter structures can also be formed.

Thus, for experimental realization of the predicted self-confined effects it is sufficient that the laser intensity exceeds the threshold given by Eq.(5). For ^{87}Rb

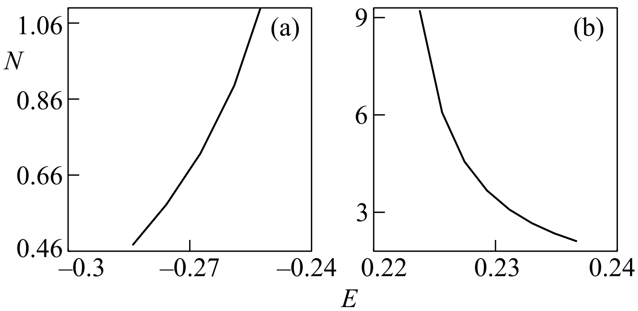

Fig.2. Dependence of the total number of atoms in the self-confined BEC structure on the ground state energy at $|\mathbf{E}|^2 > E_{th}^2$ for positive (a) and negative (b) α. All quantities are dimensionless

and ^{23}Na atoms, and linearly polarized light with a frequency detuning of 0.95 GHz from the $^2S_{1/2} -^2 P_{3/2}$ atomic resonance (irrespective of the sign of the detuning), the threshold intensity is equal to 130 $\mathrm{mW/cm}^2$ and 900 $\mathrm{mW/cm}^2$, respectively. However, it should be noted that below this threshold the density modulation can also occur for red detuning ($\alpha > 0$) only if the total number of atoms exceeds the critical value $N = N_* S$, where S is the transverse cross section (see Eq.(8)). For the same parameters, N_* is equal to $4.7 \cdot 10^{11}\,\mathrm{cm}^{-2}$ and $7 \cdot 10^{11}\,\mathrm{cm}^{-2}$. For example, for $S = 10 \times 10\mu$m $N = 4.7 \cdot 10^5$ and $7 \cdot 10^5$ for Rb and Na condensates, respectively.

Notice that, in the model we have presented, all absorption processes were neglected, a legitimate assumption provided that the laser detuning Δ is so large compared with the spontaneous emission rate γ_o (e.g., for Na $\gamma_o/2\pi \simeq 10\,\mathrm{MHz}$), that the imaginary part of the dielectric permittivity can be considered negligibly small. In this case the effect of resonance absorption on the BEC density modulations is small but will define the life time of these structures. However, even if the laser detuning was chosen to be large enough, $\Delta \gg \gamma_o$, resonance absorption could come into play due to photoassociation which can be an effective mechanism of excitation of the high-lying vibrational levels of an excited molecule created from two atoms during a collisional process [18]. However, as was recently experimentally shown in almost pure condensates, a photoassociation spectrum is quite narrow [19, 20]. At the laser intensities presented in the above estimates, the photoassociation linewidth would be approximately twice the atomic linewidth corresponding to the low intensity limit where it is independent of intensity. For higher intensities the linewidth is broadened (and also shifted) linearly with the intensity up to a maximum of 60 MHz at 1 $\mathrm{kW/cm}^2$ for Na. We note that this intensity value is three orders of magnitude higher than that in our estimates. Thus, our estimates show that by choosing appropriate laser detunings we are able to avoid the photoassociation absorption or even to use it for effectively creating highly vibrationally-excited molecules by employing the considered BEC density modulations.

Electrodynamic effects and 3D limits of small-scaled structures. So far, we have considered the problem of BEC structures in a given laser field. However, in general, Eq.(4) must be considered self-consistently together with Maxwell's equations, which determine the dynamics of the electromagnetic radiation. The condensate density modulations may affect the electromagnetic field propagation and, as a consequence, the self consistent interaction may exhibit features, which differs from what was predicted in the first part of this work. Thus, we will concentrate now on the possible back-effects of BEC density modulations on the electromagnetic field. In particular, we will show that, if the density gradient is along the electric field, the corresponding variations in the dielectric permittivity can strongly influence the microscopic field and may even change the character of the nonlinear effects.

To gain insight into this effect, we consider the structural dynamics of a condensate that is well localized within a laser wavelength. In this case we can use as a governing equation for the field [11]:

$$\nabla \cdot (\varepsilon \mathbf{E}) = 0. \tag{9}$$

The evolution of condensates in electromagnetic fields within the framework of Eqs.(2), (4) and (9) may be referred to as quasielectrostatic BEC dynamics. First of all, the characteristic scales of the density modulations can be obtained from the problem of structural stability of the background state against small perturbations. We assume the background state to be homogeneous: $\Psi = \Psi_0 \exp(-iE_0 t/\hbar)$, $\mathbf{E} = \mathcal{E}_0 \mathbf{e}_y$ and the relation between Ψ_0, E_0, $\mathcal{E}_0$ is given by the algebraic equation $E_0 = U_0\Psi_0^2 - \alpha\mathcal{E}_0^2/4(1 - 4\pi\alpha\Psi_0^2/3)^2$. The latter also defines the equilibrium points in Fig.1. We introduce the electrostatic potential, $\mathbf{E} = -\nabla\varphi$, which implies that Eq.(9) becomes $\varepsilon\nabla^2\varphi + (\nabla\varepsilon \cdot \nabla\varphi) = 0$. By linearizing the basic set of equations for small perturbations, i.e. writing $\Psi = [\Psi_0 + u_1(\mathbf{r}, t) + iv_1(\mathbf{r}, t)] \exp(-iE_0 t/\hbar)$, $\varphi = -\mathcal{E}_0 \mathbf{y} + \varphi_1(\mathbf{r}, t)$ where u_1, v_1, φ_1 are assumed to be real functions, we arrive at a set of linear equations. For solutions of the form $u_1, v_1, \varphi_1 \propto e^{\Gamma t - i\kappa\mathbf{r}}$, the growth rate is given by

$$\Gamma = \frac{\kappa}{\sqrt{2m}} \times$$
$$\left\{ \left[\frac{4\pi\alpha^2\mathcal{E}_0^2(1 - 3\kappa_y^2/\kappa^2\tilde{\varepsilon}_0)}{3(1 - (4\pi/3)\alpha\Psi_0^2)^3} - 2U_0 \right] \Psi_0^2 - \frac{\hbar^2\kappa^2}{2m} \right\}^{1/2}, \tag{10}$$

where $\kappa^2 = \kappa_x^2 + \kappa_y^2 + \kappa_z^2$ and $\tilde{\varepsilon}_0 = 1 + (8\pi/3)\alpha\Psi_0^2$. The growth rate reaches its maximum at $\kappa_y = 0$, i.e., for condensate density modulations extended along the electric field and well localized in the perpendicular direction.

The most striking new feature of the self consistent interaction between the condensate modulation and the electromagnetic radiation is that modulations along the field are strongly suppressed whereas in the first part of this work, fully localized structures were found when only the condensate dynamics was included. The nature of such a behaviour can be understood by considering a simplified model which assumes 1D density variations in a specific geometry. More specifically, we assume the laser field to be homogeneous (on the scale of the wavelength) and the density gradients to be along the direction of the field. Thus the model equation for the BEC dynamics is rewritten by coupling it to the governing equation for the electromagnetic radiation. This model is built to describe exactly the conditions under which we have found from Eq.(10) that no localized BEC structure along the field direction should be formed. While the result of Eq.(10) comes from the general model of Eqs.(4) and (9), we will now focus on a simpler model describing only the 1D case of density modulations parallel to the field. The aim is to understand how the nonlinear interaction is modified in this case and why localized structures are suppressed.

For linearly polarized light, Eq.(9) implies that the macroscopic field generated inside the condensate is given by

$$\mathbf{E}(x,t) = \frac{\mathbf{E}_L}{\varepsilon(x,t)}, \tag{11}$$

where $\mathbf{E}_L = \mathrm{E}_L \mathbf{e}_x$ is the laser field. Substituting Eq.(11), with the dielectric permittivity given by Eq.(2), into Eq.(3), we arrive at the following governing equation

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}_0\Psi + \left[U_0|\Psi|^2 - \frac{\alpha}{4}\frac{\mathrm{E}_L^2}{\left(1+(8\pi/3)\alpha|\Psi|^2\right)^2}\right]\Psi \tag{12}$$

which models the simplified case of density modulations parallel to the laser electric field, so that it differs from the general model equation (4) for the simplifying assumptions between Eq.(11). Eq.(12) is thus intended to shed light on the more general result obtained from the full model and contained in Eq.(10) on the effects of density gradients parallel to the vector electric field. As is easily seen in the low density limit, the interaction energy is $V_d^{nl} \simeq 8\pi\alpha^2\mathrm{E}_L^2|\Psi|^2/3 > 0$ which leads to a defocusing nonlinearity as for repulsive interaction between particles, independently of the sign of α.

Thus, Eq.(12) shows the effects of density modulations along the direction of the field. These density modulations induce variations of the dielectric constant which then affect the electromagnetic field.

It turns out that this effect is of the same order of magnitude as that due to the induced dipole-dipole interaction. In fact, it is strong enough to give rise to a different type of nonlinearity. Apart from a family of localized dark soliton-like solutions which can be excited as collective excitations, an analysis of the steady-state solutions of Eq.(12) shows that there are no localized hump-like solutions for the case of density modulations along the electric field. This means that, in the general 3D case, along the direction of the laser field, self-localized states can be generated only over a length scale comparable to or larger than the laser wavelength. However, as follows from Eq.(4) and (10), in any other direction the focusing nature of the nonlinearity can lead to the formation of more narrow density distributions. Consequently the evolution of a BEC, which is affected by laser-induced interactions in a linearly polarized field, may result in a self-organized cigar-shaped bound state extended along the field.

In conclusion, we have presented an analysis of the density modulations of a BEC produced via laser-induced forces and we have shown that by modifying well-controllable parameters, such as the laser intensity, frequency detuning and field polarization, different self-confined condensate structures can be accomplished. Furthermore we have investigated the self-consistent back-reaction of atom density modulations on the electromagnetic field finding that, when the vector nature of the field is taken into account, spatial localization over a wavelength scale along the electric field is inhibited while still being possible in the transverse direction.

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