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Modulational instability in Bose-Einstein condensates in optical lattices

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A self-consistent theory of a cylindrically shaped Bose-Einstein condensate (BEC) periodically modulated by a laser beam is presented. We show, both analytically and numerically, that modulational instability/stability is the mechanism by which wave functions of soliton type can be generated in a cylindrically shaped BEC subject to a one-dimensional optical lattice. The theory explains why bright solitons can exist in a BEC with positive scattering length and why condensates with negative scattering length can be stable and give rise to dark solitary pulses.

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There has been increasing interest in the study of Bose-Einstein condensates (BECs) in the presence of periodic potentials, such as the one induced by detuned standing waves of light (optical lattices) [1]. Switching on an optical lattice in a continuous BEC induces fragmentation of the original wave function into local wave functions centered around the minima of the potential, leading to a crystal-like structure of mutually interacting BECs. In analogy with the usual theory of crystals, one can think to control the dynamics of this new state of matter by properly choosing the parameters of the lattice. This gives, for example, the possibility to observe macroscopic quantum-interference phenomena with emission of coherent pulses of atoms (Bloch oscillations), as recently reported in Ref. [2] for vertical BEC arrays in the gravitational field. Understanding the properties of the BEC in optical lattices is, therefore, of fundamental importance for developing novel applications of quantum mechanics such as atom lasers and atom interferometers. For small overlapping between local wave functions, a tight-binding model can be developed. This was done, for the one-dimensional (1D) case, in Ref. [3], where it was shown that the mean-field equation for the condensate wave function reduces to the so called discrete nonlinear Schrödinger equation [4]. The tight-binding approximation, however, putting restrictions on the shape of the wave function (i.e., on the number of atoms in the condensate), as well as on the potential profile, is applicable only to particular experimental settings. From this point of view it is desirable to develop a theory of BEC in optical lattices that does not rely on this approximation. Studies in this direction were made in terms of a 1D nonlinear Schrödinger equation (NLS) with trigonometric [5] or elliptical potentials [6]. Bright and dark solitons in BEC in optical lattices, analog to the gap-soliton of photonic crystals [7], were also shown to exist [8,9].

The aim of this paper is to investigate, both analytically and numerically, modulational-instability phenomena of extended states at the border of the Brillouin zone. To this end we construct approximate ground-state solutions of the original 3D by means of a multiple-scale expansion, starting from the exact eigenfunctions of the underlying linear Schrödinger equation with potentials that are parabolic in the transverse direction and periodic in the longitudinal one (periodic cylindrical trap). We show that at the lowest orders in the expansion the condensate evolves according to an effective 1D NLS with the dispersive term depending on the effective mass of the Bloch states of the underlying linear problem. Extended states close to the borders of the Brillouin zone, are then shown to be unstable (stable) against small spatial modulations (modulational instability) depending on the sign of the dispersion in the effective 1D NLS. The stability properties of these states is shown to be the basic mechanism by which bright (dark) solitons are created in BEC with positive (negative) scattering lengths. Numerical simulations of the longitudinal BEC dynamics confirm the predictions of our theory. The possibility to observe the modulational instability phenomena in real BEC is discussed at the end of the paper.

As is well known [10], the condensate wave function is described by the Gross-Pitaevskii equation (GPE)

$$i\hbar\frac{\partial\Psi(\mathbf{r},t)}{\partial t}=\left[-\frac{\hbar^2}{2m}\Delta+V(\mathbf{r})+g_0|\Psi(\mathbf{r},t)|^2\right]\Psi(\mathbf{r},t), \tag{1}$$

with $g_0=4\pi\hbar^2 a_s/m$, m is the atomic mass, and a_s is the s-wave scattering length of atoms that can be either positive or negative. We consider a trap potential of the form $V(\mathbf{r})=\frac{1}{2}m\nu^2\mathbf{r}_\perp^2+V_0\cos(\kappa z)$, which model a cylindrically shaped BEC periodically modulated along the z axis (the results, however, will not depend on the form of periodic potential used, and can be easily generalized to arbitrary z-periodic potentials). Here $\mathbf{r}\equiv(\mathbf{r}_\perp,z)$, V_0 is the potential deepness, ν the trap frequency in the transverse direction, and $2\pi/\kappa$ the period of the modulation. We assume periodic boundary conditions $\Psi(\mathbf{r}_\perp,z,t)=\Psi(\mathbf{r}_\perp,z+L,t)$, with L denoting the length of the cylinder. The change of variables $t\mapsto 2t/\nu$, $\mathbf{r}\mapsto a_0\mathbf{r}$, $\Psi\mapsto(N/a_0^3)^{1/2}\psi$, with $a_0=[\hbar/(m\nu)]^{1/2}$, allows us to rewrite Eq. (1) in the dimensionless form

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$$i\frac{\partial\psi(\mathbf{r},t)}{\partial t}=[\mathcal{L}+\chi|\psi(\mathbf{r},t)|^2]\psi(\mathbf{r},t),\qquad(2)$$

where $\chi=8\pi Na_s/a_0$, and $\mathcal{L}\equiv\mathcal{L}_\perp+\mathcal{L}_z$ with

$$\mathcal{L}_\perp=-\Delta_\perp+r_\perp^2,\qquad \mathcal{L}_s=-\partial^2/\partial z^2+2\Lambda\cos(kz)\qquad(3)$$

(here $\Delta_\perp$ denotes the two-dimensional Laplacian, $k=a_0/\kappa$ and $\Lambda=V_0\nu/\hbar$). In these units the wave function results normalized to 1, i.e.,

$$\int d\mathbf{r}_\perp\int_0^{\tilde{L}}dz|\psi|^2=1,\qquad(4)$$

with $\tilde{L}\equiv L/a_0$ denoting the normalized length of the cylinder. In the following we shall restrict to the small amplitude limit ($\chi|\psi|^2\ll1$) and construct a solution of Eq. (2) perturbatively, starting from the solution of the linear problem. These last can be written as products of eigenfunctions of the operators in Eq. (3)

$$\mathcal{L}_z\phi_{\tilde{n}q}(z)=\mathcal{E}_{\tilde{n}q}\phi_{\tilde{n}q}(z),\qquad \mathcal{L}_\perp\xi_{nm}(\mathbf{r}_\perp)=\varepsilon_{nm}\xi_{nm}(\mathbf{r}_\perp).$$

For the considered potential, $\phi_{\tilde{n}_q}(z)$ are solutions of the Mathieu equation, while $\xi_{nm}(\mathbf{r}_\perp)$ are eigenfunctions of the two-dimensional harmonic oscillator (n and m denote the principal and the angular quantum numbers of the harmonic oscillator, while $\tilde{n}$ and q denote the band index and the wave vector inside the first Brillouin zone of the 1D lattice, respectively). We look for solutions of Eq. (2) of the form

$$\psi=\left(\frac{\tilde{L}}{|\chi|}\right)^{1/2}(\sigma\psi_1+\sigma^2\psi_2+\cdots),\qquad(5)$$

with σ a small parameter whose physical meaning will be clarified later (the prefactor is unimportant and introduced just for convenience). Since we are interested in the ground state we take as the leading-order term in Eq. (5) a small modulation of the linear ground-state wave function ($n_0=0,m_0=0,\tilde{n}_0=1$) of the form

$$\psi_1=A(\mathbf{z},\mathbf{t})\phi_{\tilde{n}_0q}(z_0)\xi_{n_0m_0}(\mathbf{r}_\perp)e^{-i\omega_{n_0m_0\tilde{n}_0}(q)t_0},\qquad(6)$$

with $\omega_{n_0,m_0,\tilde{n}_0}(q)=\varepsilon_{n_0,m_0}+\mathcal{E}_{\tilde{n}_0q}\equiv\omega(q)$. The modulating amplitude $A(\mathbf{z},\mathbf{t})$ is considered to be a function of a set of independent spatial and temporal variables of the form $\mathbf{z}\equiv(z_1,z_2,\ldots,z_n,\ldots)$ with $z_n=\sigma^nz$, and $\mathbf{t}\equiv(t_1,t_2,\ldots,t_n,\ldots)$ with $t_n=\sigma^nt$, respectively. To simplify the notation we introduce the shortcut symbols $\varepsilon_0\equiv\varepsilon_{n_0,m_0}$, $\mathcal{E}(q)\equiv\mathcal{E}_{\tilde{n}_0,q}$, $\phi_q(z)\equiv\phi_{\tilde{n}_0,q}(z)$, and in the modulation amplitude A, we show only the dependence on the most "rapid" variables. The time and coordinate derivatives in Eq. (2) are then expanded as $\partial/\partial t=\Sigma_{\alpha=0}\sigma^\alpha\partial/\partial t_\alpha$ and $\partial/\partial z=\Sigma_{\alpha=0}\sigma^\alpha\partial/\partial z_\alpha$. Substituting the above expansions in Eq. (2) and collecting all the terms of the same order in σ, we obtain at the first order: $i\partial\psi_1/\partial t_0-\mathcal{L}\psi_1=0$, which is evidently satisfied by ψ_1 given by Eq. (6). At the second order in σ, the following equation is obtained:

$$i\frac{\partial\psi_2}{\partial t_0}-\mathcal{L}\psi_2=-i\frac{\partial\psi_1}{\partial t_1}-2\frac{\partial^2\psi_1}{\partial z_0\partial z_1},\qquad(7)$$

whose solution can be searched for in the form

$$\psi_2=\sum_{n,m}\sum_{(\tilde{n},q')\neq(\tilde{n}_0,q)}B_{n,m,\tilde{n}}(q')\phi_{\tilde{n}q'}\xi_{nm}e^{-i\omega(q)t_0}.\qquad(8)$$

Substituting Eq. (8) in Eq. (7) and projecting along the eigenfunctions of operators (3) with $\tilde{n}\neq\tilde{n}_0$, we find that

$$\psi_2=\frac{\partial A}{\partial z_1}\sum_{\tilde{n}\neq\tilde{n}_0}\frac{\Gamma_{\tilde{n}\tilde{n}_0}}{\omega_0(q)-\omega_{n_0m_0\tilde{n}}(q)}\phi_{\tilde{n}_q}\xi_{n_0m_0}e^{-i\omega(q)t_0},\qquad(9)$$

with $\Gamma_{\tilde{n}\tilde{n}_0}(q)=-2\int_0^{\tilde{L}}\overline{\phi}_{\tilde{n}_q}(z)(d/dz)\phi_{\tilde{n}_{oq}}(z)dz$. The solvability condition of Eq. (7) reads as $(\partial A/\partial t_1)+v(\partial A/\partial z_1)=0$, from which we see that $A\equiv A(\zeta;z_2,t_2)$, with $\zeta=z_1-vt_1$. Note that the $v\equiv v(q)=i\Gamma_{\tilde{n}_0\tilde{n}_0}(q)$ can be interpreted as the group velocity of the wave packet in the z direction. Finally, at the third order in σ, we get

$$i\frac{\partial\psi_3}{\partial t_0}-\mathcal{L}\psi_3=-i\frac{\partial\psi_1}{\partial t_2}-i\frac{\partial\psi_2}{\partial t_1}-2\frac{\partial^2\psi_2}{\partial z_0\partial z_1}-\left(\frac{\partial^2}{\partial z_1^2}+2\frac{\partial^2}{\partial z_0\partial z_2}\right)\psi_1+\chi|\psi_1|^2\psi_1.\qquad(10)$$

Requiring orthogonality (to avoid secular terms) between the right-hand side of this equation and the kernel of the operator $i\partial/\partial t_0-\mathcal{L}$, and taking into account the expressions of ψ_1 and ψ_2 derived above, we find that Eq. (10) reduces to the following NLS equation

$$-i\left(\frac{\partial A}{\partial t_2}+v\frac{\partial A}{\partial z_2}\right)-D\frac{\partial^2A}{\partial\zeta^2}+\tilde{\chi}|A|^2A=0,\qquad(11)$$

where $D\equiv D(q)=1+\Sigma_{\tilde{n}\neq\tilde{n}_0}|\Gamma_{\tilde{n}\tilde{n}_0}(q)|^2/(\omega(q)-\omega_{n_0m_0\tilde{n}}(q))$ is the effective group velocity dispersion induced by the periodic potential, and

$$\tilde{\chi}=\mathrm{sgn}(\chi)\frac{\tilde{L}}{2\pi}\int_0^{\tilde{L}}|\phi_0(z)|^4dz,\qquad(12)$$

is the effective nonlinearity (here we integrated on radial variables and used the ground-state wave function of the 2D harmonic oscillator). The above expressions of v and D, in terms of eigenfunctions of the linear operator $\mathcal{L}$, can be simplified by expressing them in terms of the energy spectrum of the noninteracting linear system. This can be done in the same manner as in the theory of optical gap solitons [7]. To this end, we take two close Bloch solutions of the 1D linear problem, of the form $\phi_q(z)=\exp(iqz)u_{\tilde{n},q}(z)$, which differ only by a small δq, so that $u_{\tilde{n},q+\delta q}(z)$ can be considered as a perturbation of $u_{\tilde{n},q}(z)$ generated by the operator $-2i\delta q((d/dz)+iq)+(\delta q)^2$. This perturbation produces a shift $\Delta=\mathcal{E}_{\tilde{n},q+\delta q}-\mathcal{E}_{\tilde{n},q}$ in energy, which can be expanded in a Taylor series in δq. On the other hand, Δ can also be computed from perturbation theory. A comparison of the corresponding expressions leads to $v=d\omega(q)/dq$ and $D=\frac{1}{2}d^2\omega(q)/dq^2$, i.e., v and D are, respectively, the slope (velocity) and the curvature (inverse effective mass) of the energy band (Bloch states) of the underlying linear problem.

From the physical point of view the above results have a number of consequences. First, the group velocity induced by the periodicity at the boundaries of zone dominate the dispersion inherent to NLS. For example, if we take $k=2.0$ and $\Lambda=0.5$, we have that the edges of the first gap $[\mathcal{E}^{(1)},\mathcal{E}^{(2)}]$ are at $\mathcal{E}^{(1)}\approx 0.47$, and $\mathcal{E}^{(2)}\approx 1.47$. The effective dispersion at these points is $\omega_1''\approx -6.13$, and $\omega_2''\approx 10.14$, respectively (here $\omega_j''=d^2\omega/dq^2|_{q=q_j}$). Thus even in the case the group velocity dispersion does not change sign it becomes much larger than the NLS dispersion. Second, for fixed nonlinearity and in presence of the periodic potential, the dynamics will crucially depend on the sign of D. This sign can be controlled by changing the wave number of the initial state, as well as, the potential parameters. Instability phenomena of extended (Bloch) states close to the edges of the Brillouin zone can then appear. To understand this, let us assume positive scattering length ($\tilde{\chi}>0$ in Ref. [11]) and consider the Bloch state at $\mathcal{E}^{(1)}$, for which $D^{(1)}<0$. In the presence of a repulsive interatomic interaction ($\chi>0$), the energy of this state will be shifted upward in the gap where it cannot exist. One can expect then the state to become unstable against small spatial modulations (modulational instability) so that new excitations must arise. Equation (11) predicts that out of the instability bright solitons should appear [recall that for $\tilde{\chi}>0$, and $D<0$ ($D>0$), Eq. (11) has stable bright (dark) soliton solutions]. On the contrary, if we take as initial state the Bloch state at the bottom of the second band, $\mathcal{E}^{(2)}$, where $D=D^{(2)}>0$, one expects modulational stability instead (in this case the nonlinearity is pulling the energy of the state further up in the second band where it can still exist). This extended stable state can be then used as background to construct the dark soliton solution expected in this case from Eq. (11) (see below). Obviously, for negative scattering lengths the opposite situation will occur, i.e., modulational instability will appear at the top of the gap (leading to bright solitons) and stability at the bottom (leading to dark solitons). From this it is clear that the stability properties of the Bloch states at the edge of the Brillouin zone, plays a crucial role for the existence of bright and dark solitons in BEC in optical lattices both for positive and negative scattering lengths.

These predictions can be easily checked by direct numerical integration. In this regard we remark that instabilities along the z direction mainly depend on the spectrum of the operator $\mathcal{L}_z$ (the transverse distribution of the condensate affects only the absolute value of the coefficient $\tilde{\chi}$), so that we can perform numerical simulations in the framework of a 1D NLS equation obtained from Eq. (2) with $\mathcal{L}\approx\mathcal{L}_z$. Moreover, we note that the Bloch state (Mathieu function) at the top of the first band (bottom of the gap), is an odd function of z that can be approximated by $\sin(z)$, while the one at the bottom of the second band (top of the gap) is an even function of z very close to $\cos(z)$. In the following we shall use these approximate states as initial conditions for investigating modulational stability since they are, in real experiments, easier to generate.

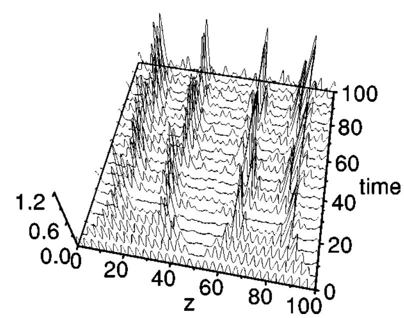

FIG. 1. Modulational instability in Eq. (2) with $\mathcal{L}\approx\mathcal{L}_z$ for parameter values $\tilde{\chi}=1.0$, $k=2.0$, and $\Lambda=0.5$. The initial condition is an approximated eigenfunction, taken as a sine function, of the first band of the linear system at the edge $\mathcal{E}^{(1)}\approx 0.47$ of the Brillouin zone. Quantities plotted are dimensionless.

In Fig. 1 a numerical simulation of the 1D problem with initial condition close to the state at the bottom of the gap, is depicted. We see that, as expected from our analysis, modulational instability develops and, in spite of the fact that we have positive scattering ($\tilde{\chi}=1$), bright solitons are created in agreement with our analysis [the number of solitons coming out from the instability can be estimated as $Lk_{\mathrm{max}}/(2\pi)$, where k_{max} is the wave number of the most unstable linear mode [11]]. We remark that although the theory is valid for small-amplitude excitations, the numerical simulations show that the obtained results extend also above this limit (note that in Fig. 1 $\tilde{\chi}=1$). An intuitive explanation for this is that small-amplitude solitons once formed can only become more and more localized as the nonlinearity is increased. The modulational instability at higher nonlinearity should, therefore, produce solitons that are more localized and of large amplitude. This is precisely what is observed in Fig. 1. In contrast to this, we find that an initial condition corresponding to a Bloch state close to the top of the gap, remains modulationally stable also in the presence of nonlinearity. This is reported in Fig. 2 for an initial profile of cosine type. It is interesting to note that one can use this state to construct the stable dark soliton predicted by Eq. (11). To this end we take

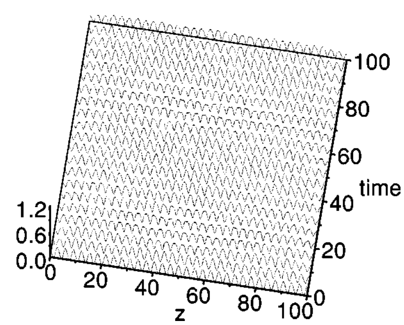

FIG. 2. Same as in Fig. 1 but for the eigenfunction at the top of the gap $\mathcal{E}^{(2)}\approx 1.47$ approximated with a cosine function. Quantities plotted are dimensionless.

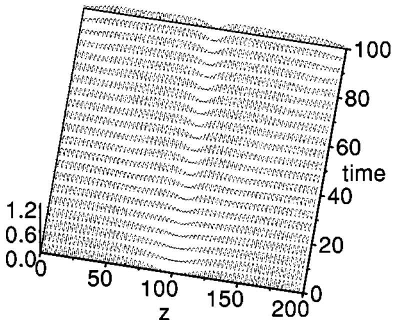

FIG. 3. Same as in Fig. 1 but for a dark-soliton initial condition. Quantities plotted are dimensionless.

as initial condition a modulated Bloch state of the form tanh(λz)cos(z), where the cosine function, taken as background, approximates the Mathieu eigenfunction at the edge $\mathcal{E}^{(2)}$, while the tanh modulation is used to make the profile close to the expected dark state.

In Fig. 3 the corresponding numerical simulation is reported, from which we see that a dark soliton is indeed generated, in perfect agreement with our analysis (the energy of this state is in the gap close to the bottom of the second band). It is interesting to note that for negative scattering lengths this leads to the existence of dark soliton in BEC in optical lattices (in this case one must use the stable Bloch state at the bottom of the gap as background for the dark solution).

In order to check the self-consistency of the theory we shall estimate the size of the parameter σ used for the expansion, and the magnitude of the effective nonlinearity in Eq. (11). To this end we start with the dark soliton or periodic solution and notice that the eigenfunctions $\phi_q(z)$ are normalized to 1, so that $\tilde{L}|\phi_q|^2 \sim 1$ and hence, from Eq. (12) we have that $\tilde{\chi} \sim 1$. Similarly, from the normalization of the wave function (4) and from the expansion (5), we have that $\pi \tilde{L}^2 \sigma^2/|\chi| \sim 1$ from which, after restoring physical units, we get $\sigma^2 = 8 N a_s a_0 / L^2$. If we consider the case of a condensate with $N \approx 10^4$ atoms of ^{87}Rb ($a_s \sim 5.5$ nm) with a radial size $a_0 \sim 17\ \mu$m, and length $L \sim 300\ \mu$m [12], we have that $\sigma^2 \sim 0.08$, this being reasonably small to justify our expansion (smaller values can be achieved by considering longer, thinner, cylinders and smaller values of N). It is worth noting here that the effective reduction of the dimensionality of the problem can lead to a reduction (by a factor much less than unity) of the nonlinear coefficient, as recently reported in Ref. [13].

As to the initial state, we remark that it could be generated from a uniform cylinder by modulating it along the z axis with a sine or cosine wave of light with twice the wavelength of the lattice. Another possibility is to use an initial uniform condensate and accelerate the lattice until the state reaches the edge of the band (it is enough to be close to the edge for the instability to develop). Finally we mention that, although the expansion has been provided for a cylindrically shaped BEC, a number of effects discussed is relevant to a cigar-shaped BEC (i.e., including parabolic confining potential in the direction of periodicity). This is the case when the effect (instability, bright or static dark soliton) observed has a scale much less than the length of the condensate. We hope that the phenomena of modulational instability discussed in this paper will be soon observed in real BEC experiments.

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