Matter-Wave Gap Solitons in Atomic Band-Gap Structures

Elena A. Ostrovskaya[1,2] and Yuri S. Kivshar[1]

[1]*ARC Centre for Quantum-Atom Optics, Nonlinear Physics Group, Research School of Physical Sciences and Engineering, The Australian National University, Canberra ACT 0200, Australia*

[2]*Department of Physics and Theoretical Physics, The Australian National University, Canberra ACT 0200, Australia*

(Received 8 November 2002; published 24 April 2003)

We demonstrate that a Bose-Einstein condensate in an optical lattice forms a reconfigurable matter-wave structure with a band-gap spectrum, which resembles *a nonlinear photonic crystal* for light waves. We study in detail the case of a two-dimensional square optical lattice and show that this *atomic band-gap structure* allows nonlinear localization of atomic Bloch waves in the form of two-dimensional matter-wave gap solitons.

DOI: 10.1103/PhysRevLett.90.160407 PACS numbers: 03.75.Lm

Recent experiments [1–4] have demonstrated that a Bose-Einstein condensate (BEC) loaded into an optical lattice is a perfect test ground for a range of fascinating physical effects. In particular, this is because the effective potential of an optical lattice can be easily manipulated by changing the geometry, polarization, phase, or intensity of the laser beams. Because of inherent nonlinearity of the coherent matter waves introduced by interatomic interactions, BEC in a lattice potential can form a periodic nonlinear system, which is expected to display rich and complex dynamics.

On the other hand, propagation of light in dielectric structures with a periodic variation of the refractive index is receiving growing attention. Photonic band-gap (PBG) materials [5]—artificial periodic structures with a high index contrast—can be used to effectively control the flow of light. The study of photonic crystals made of a Kerr nonlinear material, the so-called *nonlinear photonic crystals*, has revealed that such structures exhibit a wealth of nonlinear optical phenomena and, in particular, they can support self-trapped nonlinear localized modes of the electromagnetic field in the form of optical gap solitons [6,7]. Dynamically reconfigurable PBG structures—optically induced refractive index gratings in nonlinear materials—are now offering new ways to control light propagation and localization [8].

As demonstrated in this Letter, BEC in an optical lattice can be regarded as a *fully reconfigurable* analog of a nonlinear photonic crystal for matter waves—an "atomic band-gap" (ABG) structure. A deep analogy between coherent light and matter waves suggests that the concepts employed in the study of nonlinear PBG structures can be borrowed for analyzing BEC in optical lattices. Many properties of ABG structures can potentially be exploited for high-precision control and manipulation of coherent matter waves in a similar way to how PBG structures are used to manipulate light. The effect of nonlinear localization in band gaps is one of these properties.

Localized nonlinear excitations of coherent matter waves—*bright atomic solitons*—could be very useful for applications such as atomic interferometry due to their robust nature. However, their generation has so far been experimentally achieved only in BECs with attractive atomic interactions (analogous to self-focusing optical media) which are unstable against collapse above a small ($\sim 10^3$) critical number of particles.

In theory, a shallow 1D optical lattice can support bright matter-wave solitons even in repulsive BEC [9] with large atom numbers. These solitons, described in a framework a coupled-mode theory [9], are localized on a large number of lattice wells, and are predicted to exist only in atomic band gaps. In the opposite case of a deep lattice, the condensate can be described by the superposition of ground state modes in the individual wells. The mean-field treatment of the condensate in this regime leads to a discrete equation which admits solutions in the form of stationary modes localized on a few lattice sites—*discrete solitons* [10,11], in complete parallel with spatial solitons in periodic optical structures [12] and localized modes of atomic lattices [13].

The theory of the nonlinear localized matter waves in optical lattices is mostly limited to 1D case [14]. However, as can be deducted from the analogous studies of 2D PBG structures [6], the nonlinear localization of in BEC in higher-dimensional lattices is qualitatively different because both the symmetry and dimensionality of the lattice start to play an important role in the formation and properties of the band-gap structure and corresponding nonlinear modes. In this Letter, we analyze the as yet unexplored problem of the existence and stability of 2D matter-wave gap solitons of BEC with repulsive interatomic interactions loaded into optical lattices, which are analogous to localized states of light waves in nonlinear photonic crystals. We show that their accurate description is possible only within a full mean-field model of BEC in a periodic lattice potential, beyond the tight-binding approximation or coupled-mode theory often employed for the study of BEC in 1D optical lattices.

The dynamics of a three-dimensional BEC cloud loaded into a two-dimensional optical lattice can be described by the Gross-Pitaevskii (GP) equation for the macroscopic wave function, $\Psi(\boldsymbol{r}, t)$ of the condensate,

$$i\frac{\partial\Psi}{\partial t} = \left[-\frac{1}{2}\nabla^2 + V(t) + \gamma_{3D}|\Psi|^2\right]\Psi. \qquad (1)$$

This equation has been made dimensionless by using the natural length, time, and energy scales of the optical lattice. The characteristic length scale in this model, $a_L = k_L^{-1} = d/\pi$, defines the size of a single well of the lattice potential through the lattice constant that depends on the laser wavelength as $d = \lambda/2$. The depth of the lattice potential, measured in the lattice recoil energy $E_L = \hbar^2/(2ma_L^2)$, is proportional to the laser intensity and can be varied from 0 to $\sim 20E_L$ in experiment. The characteristic frequency scale is $\omega_L = E_L/\hbar$. The interatomic interactions are characterized by the coefficient $\gamma_{3D} = 8\pi(a_s/a_L)$, where a_s is the s-wave scattering length, positive for repulsive interactions.

In the simplest case of a square optical lattice, the combined potential of the lattice and magnetic trap, $V(\boldsymbol{r}) = V_L(\boldsymbol{r}) + V_T(\boldsymbol{r})$, can be written as $V(\boldsymbol{r}) = V_0(\sin^2 x + \sin^2 y) + \omega_i^2\boldsymbol{r}^2/2$, where V_0 is the amplitude of the optical lattice, and ω_i are the (normalized) trapping frequencies in the corresponding directions. The current experiments with 2D optical lattices are performed with a strongly anisotropic BEC cloud, with the ratio of the trapping strengths $\Omega = \omega_x/\omega_{y,z} \sim 10^{-1}$ [2]. To simplify our analysis, we assume that the relatively weak magnetic confinement characterized by trap frequencies ω_i has a small effect on the stationary states of the condensate in the lattice. Under this assumption, the trap component of the confining potential in the lattice plane can be neglected, and the model can be reduced to a two-dimensional GP equation by assuming separable solutions of the form, $\psi(\boldsymbol{r}; t) = \Phi(z)\psi(x, y; t)$ where the function $\Phi(z)$, describing the condensate in the direction of the tight confinement, perpendicular to the lattice, is a solution of the 1D quantum harmonic oscillator problem, with the normalization condition $\int \Phi^2(z)dz = 1$. Then the standard dimensionality reduction procedure [15], leads to the following equation for the 2D condensate wave function in the 2D lattice potential:

$$i\frac{\partial\psi}{\partial t} = \left[-\frac{1}{2}\nabla_\perp^2 + V_{\rm L}(\boldsymbol{r}) + |\psi|^2\right]\psi, \qquad (2)$$

where $\nabla_\perp^2 = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $V_{\rm L}(\boldsymbol{r}) \equiv V_{\rm L}(x, y)$ is the periodic potential of the optical lattice, and the wave function is rescaled as $\psi \to \psi\sqrt{\gamma_{2D}}$, with $\gamma_{2D} = \gamma_{3D}/\sqrt{2}$.

Spectrum of atomic Bloch waves in the optical lattice can be found by exploiting the analogies with the theory of single-electron states in crystalline solids. Stationary states of the condensate in an infinite periodic potential of a 2D optical lattice are described by solutions of Eq. (2) of the form: $\psi(\boldsymbol{r}, t) = \phi(\boldsymbol{r})\exp(-i\mu t)$, where μ is the chemical potential, corresponding to the energy level of the stationary state in the lattice potential. The case of noninteracting condensate formally corresponds to Eq. (2) being linear in ψ. According to the Bloch theorem, the stationary wave function can then be sought in the form $\phi(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r})\exp(i\boldsymbol{k}\boldsymbol{r})$, where the wave vector $\boldsymbol{k}$ belongs to a Brillouin zone of the square lattice, and $u_{\boldsymbol{k}}(\boldsymbol{r}) = u_{\boldsymbol{k}}(\boldsymbol{r} + \boldsymbol{d})$ is a periodic (Bloch) function with the periodicity of the lattice. For the values of $\boldsymbol{k}$ within an nth Brillouin zone, the dispersion relation for the 2D Bloch waves, $\mu_n(\boldsymbol{k})$, is found by solving the following linear eigenvalue problem

$$\left[\frac{1}{2}(-i\boldsymbol{\nabla}_\perp + \boldsymbol{k})^2 + V_L(\boldsymbol{r})\right]u_{n,\boldsymbol{k}} = \mu_n(\boldsymbol{k})u_{n,\boldsymbol{k}}. \qquad (3)$$

The eigenvalue problem (3) is simpler than a general 2D problem due to the separability of the lattice potential. The typical dispersion relation for the energy of the Bloch states in the lowest Brillouin zones is shown in Fig. 1 for a moderate value of the lattice depth $V_0 = 5$. The dispersion diagram is presented in the reciprocal lattice space, and the dispersion relations are calculated along the characteristic high-symmetry directions of the irreducible Brillouin zone (see Fig. 1, bottom right). It can be seen that the absolute bands and gaps are determined by the spectra of the Bloch waves in the middle (point Γ) and on the edge (point M) of the Brillouin zone.

To understand how the variation in the lattice parameters affects the band structure, we note that, owing to the scaling properties of the model, any increase in the well spacing, a_L, translates into decreasing the well depth V_0. Thus the global behavior of the band structure can be understood by examining the Bloch wave spectrum as

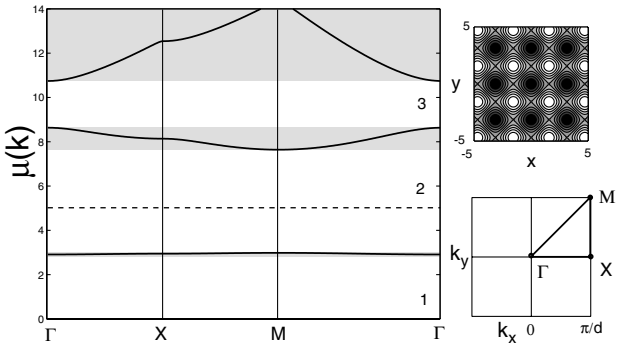

FIG. 1. Dispersion diagram for atomic Bloch waves in a 2D lattice in the reduced zone representation: shaded, first three energy bands; numbered, band gaps ($V_0 = 5.0$). Dashed, the line $\mu = V_0$. Right top: contour plot of the lattice potential in Cartesian space, black shading corresponds to potential minima. Right bottom: the first Brillouin zone of the 2D lattice in the reciprocal lattice space; marked are the high-symmetry points of the irreducible zone.

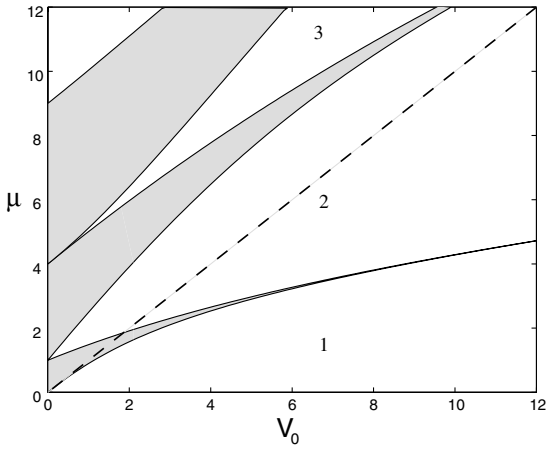

FIG. 2. Band-gap structure of the atomic Bloch-wave spectrum as a function of the lattice amplitude V_0. Shaded: Bloch-wave bands; numbered, gaps. Dashed, the line $\mu = V_0$.

a function of the lattice depth. Figure 2 presents the chemical potentials corresponding to the atomic Bloch waves at the edges of the absolute bands plotted as functions of V_0. The dashed line $\mu = V_0$ (dashed line in Fig. 1) separates the quasiunbound ($\mu > V_0$) and strongly bound ($\mu < V_0$) condensate states in the lattice (see also Ref. [16]). By varying the interwell separation or the amplitude of the lattice, different regimes of the atomic band-gap structure can be accessed. The tight-binding regime of the condensate dynamics corresponds to the domain $V_0 \gg V_0^* = \mu$, where the bands "collapse" to discrete levels of bound states in a single isolated well (see Fig. 2). The narrow-gap regime of a shallow lattice, where the coupled-mode theory applies, is found for the opposite case, $V_0 \ll V_0^*$.

The study of the 1D atomic band-gap structures [15,17] indicates that the correct structure and dynamical properties of the nonlinear localized modes can be revealed only through the analysis of the full continuous mean-field GP model that bridges the gap between the coupled-mode theory and discrete tight-binding approach. One promising development in approximate analysis would be generalization of the Wannier function formalism [18] to the 2D case. However, the complexity involved in the generation of optimally localized higher-dimensional Wannier functions [19] may not provide significant advantage compared with the direct solution of the model Eq. (2).

Here, we find spatially localized stationary solutions of Eq. (2) numerically. Our numerical procedure involves minimization of the functional $\mathbb{N} = \int f^\dagger f d\boldsymbol{r}$, where $f(\phi) = [\nabla_\perp^2 + \mu - V_L(\boldsymbol{r}) - |\phi|^2]\phi$, by following a descent technique with Sobolev preconditioning [20]. The minimization procedure yields a stationary state when $\mathbb{N}(\phi) = 0$. Previous applications of this method to the analysis of optical solitons has shown that it is suitable for tackling both the fundamental and higher-order nonlinear localized modes. Our numerical method is independent of the lattice symmetry; it offers a versatile technique for finding and analyzing nonlinear localized modes in a range of different band-gap structures, and for making accurate predictions about their density, degree of localization, and spatial structure in different areas of the parameter space.

We have identified different families of matter-wave gap solitons of the repulsive BEC in the 2D atomic band-gap structure. These solitons can exist in all gaps, excluding the semi-infinite gap of the spectrum (marked by 1 in Figs. 1 and 2) below the first band. We note in passing that only conventional self-focusing of BEC with attractive interactions is possible in the semi-infinite gap. The change in the peak amplitude of the lowest-order "fundamental" gap solitons across the first gap, along with their spatial localization properties, are demonstrated in

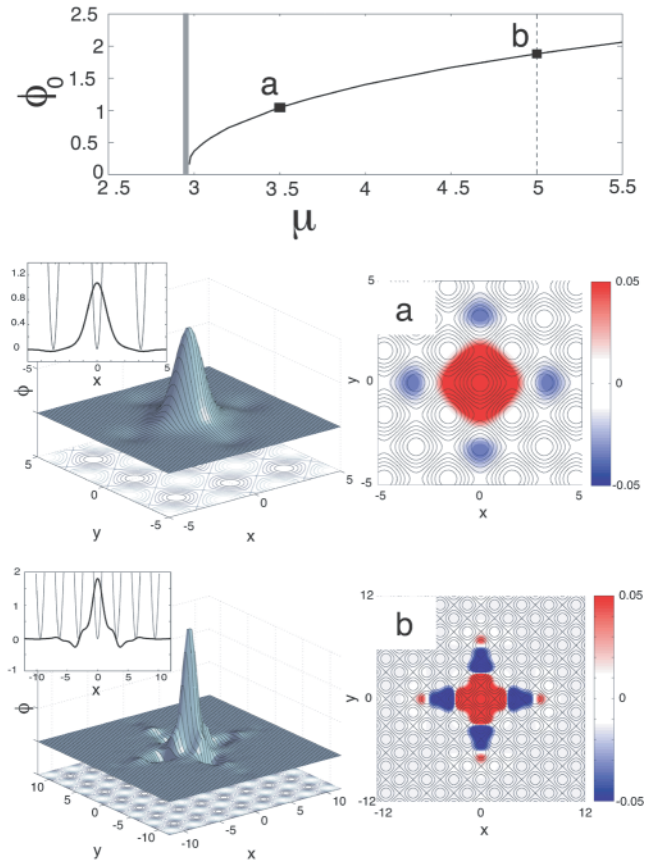

FIG. 3 (color online). Peak amplitude, $\phi_0 \equiv \phi(0,0)$, of the fundamental gap soliton in the first gap ($V_0 = 5.0$); shaded, the first band; dashed, the line $\mu = V_0$. Below: Spatial structure of the gap solitons (a) near the high-energy edge of the first band, $\mu = 3.5$, and (b) at the top of the lattice potential, $\mu = 5.0$. Contour plots on the 3D plots (left) show the structure of the lattice potential, darker contours correspond to potential minima. Potential contours on the right are guides to the eye. Insets: the cross sections of the localized modes and the potential along the line $(x, 0)$.

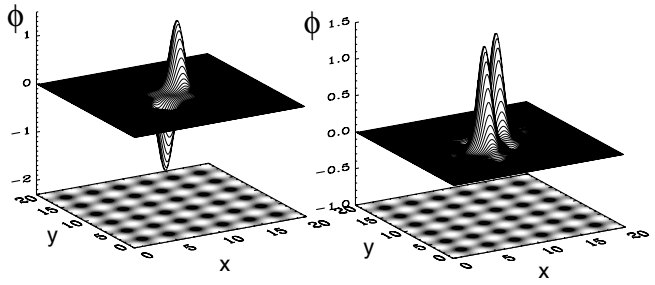

FIG. 4. Spatial structure of the higher-order gap solitons formed by two (left) out-of-phase and (right) in-phase fundamental modes ($V_0 = 5.0$, $\mu = 4.0$). Filled contours show the lattice potential; dark shading corresponds to potential minima.

Fig. 3, for $V_0 = 5$. Gap solitons of repulsive BEC branch off the lower-energy (i.e., smaller values of μ) gap edge (see Figs. 3, top). Near this edge, i.e., at low particle numbers and amplitudes, they are weakly localized. Further within the gap, the localized mode of the BEC contains larger numbers of atoms, and has a strongly localized central peak [see Figs. 3(a) and 3(b)]. Near the linear tunnelling threshold, $\mu \sim V_0$, the nonlinear localized states develop extended tails in the orthogonal directions (x, y), along which the tunneling is assisted by the lower interwell barrier heights (compared to $2V_0$ in diagonal directions). Although the stability analysis of the states localized on the extended background (for $\mu > V_0$) is difficult due to the large computational domain, we have confirmed that strongly localized 2D modes are dynamically stable. In the lattice geometry under consideration, the line $\mu = V_0$ lies within the first gap (marked 2 in Figs. 1 and 2), and only localized modes within this gap have been analyzed.

The higher-amplitude gap solitons have a nontrivial structure of the tails [see Fig. 3(b)], i.e., the zeros of the matter-wave are centered within individual lattice wells (see Figs. 3, insets), rather than on the potential maxima. This structure is determined by the spatial structure of the Bloch wave at the lower-energy edge of the second band (point M in Fig. 1), and cannot be described within the framework of the discrete model.

We have also found families of higher-order gap modes that can be identified as bound states of the fundamental gap solitons. These states can be centered on the lattice potential minima or maxima, similarly to higher-order "odd" and "even" states in 1D lattices [15], and can exhibit symmetry-breaking instabilities. Two examples of the lowest-order in- and out-of-phase odd modes, centered on a lattice maximum, are shown in Fig. 4.

The crucial issue of the potential observation of 2D gap solitons is the stability of the 2D localized state in a 3D BEC cloud, i.e., dynamical stability of the 3D state $\Psi(x, y, z; t)$ with the initial condition given by $\Phi(z)\phi(x, y)$, where $\phi(x, y)$ is the two-dimensional stationary gap soliton. The analysis of stability of 2D solitons in a 3D BEC cloud, which will provide clues for possible experimental observation of multidimensional gap solitons, is the subject of our separate study.

In conclusion, we have demonstrated that the interaction of BEC with the lattice potential is analogous to the light scattering by a nonlinear photonic band-gap structure. We have studied the properties of two-dimensional atomic band-gap structures and demonstrated the existence of gap solitons, the spatially localized states of BEC existing in the gaps of the matter-wave spectrum. We believe the analogy between the physics of BEC in optical lattices and photonic crystals can be useful for revealing many novel features of the matter-wave dynamics in reconfigurable atomic band-gap structures.

The authors thank C. M. Savage and J. J. García-Ripoll for invaluable advice. This work is supported by the Australian Partnership for Advanced Computing and Australian Research Council.

[1] M. Christiani *et al.*, Phys. Rev. A **65**, 063612 (2002).
[2] M. Greiner *et al.*, Phys. Rev. Lett. **87**, 160405 (2001).
[3] M. Greiner *et al.*, Nature (London) **415**, 39 (2002).
[4] J. H. Denschlag *et al.*, J. Phys. B **35**, 3095 (2002).
[5] J. D. Joannopoulos, R. D. Meade, and J. N. Winn, *Photonic Crystals: Molding the Flow of Light* (Princeton University Press, Princeton, 1995).
[6] S. Mingaleev and Y. Kivshar, Phys. Rev. Lett. **86**, 5474 (2001).
[7] *Nonlinear Photonic Crystals*, edited by R. Slusher and B. Eggleton (Springer-Verlag, Berlin, 2003).
[8] J.W. Fleischer *et al.*, Nature (London) **422**, 147 (2003); D. Neshev *et al.*, Opt. Lett. **28**, 710 (2003).
[9] O. Zobay *et al.*, Phys. Rev. A **59**, 643 (1999).
[10] A. Trombettoni and A. Smerzi, Phys. Rev. Lett. **86**, 2353 (2001).
[11] F. K. Abdullaev *et al.*, Phys. Rev. A **64**, 043606 (2001).
[12] Y. Kivshar and G. Agrawal, *Optical Solitons: From Fibers to Photonic Crystals* (Academic Press, San Diego, 2003).
[13] S. Flach and C. Willis, Phys. Rep. **295**, 181 (1998).
[14] After submission of this manuscript, the generation of 2D arrays of localized states via modulational instability of Bloch waves was theoretically demonstrated in B. B. Baizakov, V.V. Konotop, and M. Salerno, J. Phys. B **35**, 5105 (2002).
[15] P. J. Y. Louis *et al.*, Phys. Rev. A **67**, 013602 (2003).
[16] K. Drese and M. Holthaus, Chem. Phys. **217**, 201 (1997).
[17] G. L. Alfimov, V.V. Konotop, and M. Salerno, Europhys. Lett. **58**, 7 (2002).
[18] G. L. Alfimov *et al.*, Phys. Rev. E **66**, 046608 (2002).
[19] N. Marzari and D. Vanderbilt, Phys. Rev. B **56**, 12 847 (1997).
[20] J. J. García-Ripoll and V. M. Pérez-García, SIAM J. Sci. Comput. **23**, 1316 (2001).