Photonic crystals for matter waves: Bose-Einstein condensates in optical lattices

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Abstract: We overview our recent theoretical studies on nonlinear atom optics of the Bose-Einstein condensates (BECs) loaded into optical lattices. In particular, we describe the band-gap spectrum and nonlinear localization of BECs in one- and two-dimensional optical lattices. We discuss the structure and stability properties of spatially localized states (matter-wave solitons) in 1D lattices, as well as trivial and vortex-like bound states of 2D gap solitons. To highlight similarities between the behavior of coherent light and matter waves in periodic potentials, we draw useful parallels with the physics of coherent light waves in nonlinear photonic crystals and optically-induced photonic lattices.

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References and links
1. Introduction

Photonic band-gap materials [1] – artificial periodic structures fabricated in a dielectric medium with a high refractive index contrast – offer new possibilities for the control and manipulation of coherent light waves. Diffraction management, localization, and controlled steering of light in periodic band-gap structures, such as fiber Bragg gratings and photonic crystals, has revolutionized modern photonics and laid the foundation for the development of novel types of integrated photonic devices. The study of nonlinear photonic crystals made of a Kerr nonlinear material [2, 3], has revealed that such structures can support self-trapped localized modes of the electromagnetic field in the form of optical gap solitons [4] with the energies inside the photonic gaps of a periodic structure. Recent demonstration of the light scattering in dynamically reconfigurable photonic structures – optically-induced refractive index gratings in nonlinear materials – has opened up novel ways to control light propagation and localization [5, 6, 7].

On the other hand, many recent experimental studies of Bose-Einstein condensates (BECs) in periodic potentials of optical lattices [8, 9, 10] demonstrate an unprecedented level of control and manipulation of coherent matter waves in the reconfigurable crystal-like structures created by light. Due to the inherent nonlinearity of coherent matter waves which is introduced by the interactions between atoms, BEC in a lattice potential forms a periodic nonlinear system which is expected to display rich and complex dynamics.

The modelling of both nonlinear optical and nonlinear matter-wave dynamics is often based on the nonlinear Schrödinger equation, which is used to describe both the electromagnetic field envelope and the BEC macroscopic wavefunction (mean-field). This model reflects similarities between the physics of coherent light and matter waves, which aid in understanding and predicting the nonlinear behavior of BEC in an optical lattice. Similar to periodic photonic
structures for coherent light waves, optical lattices form band-gap structures for coherent matter waves [11] which modify the diffraction properties of atomic wavepackets. Different diffraction regimes were predicted to lead to nonlinear localization of condensates with both attractive and repulsive interactions in the spectral gaps of the atomic band-gap structure [12, 13, 14, 15, 16]. Recent experiments on nonlinear dynamics of BEC in a lattice have demonstrated both diffraction management [17, 18] and nonlinear localization of the atomic wavepackets in the form of the matter-wave gap solitons [19].

In this paper we describe the structure and stability properties of nonlinear localized states of BEC in one- and two-dimensional optical lattices, and make links to parallel studies in nonlinear optics of periodic photonic structures such as nonlinear photonic crystals and optically-induced photonic lattices.

2. Model

The dynamics of a Bose-Einstein condensate loaded into an optical lattice can be described in the mean-field approximation, by the nonlinear Gross-Pitaevskii (GP), or nonlinear Schrödinger, equation for the macroscopic condensate wavefunction $\Psi(r,t)$,

$$i\hbar \frac{\partial \Psi}{\partial t} = \left\{ -\frac{\hbar^2}{2m}\nabla^2 + V(r) + g_{3D}|\Psi|^2 \right\} \Psi$$

where $V(r)$ is the time-independent trapping potential, and $g_{3D} = 4\pi\hbar^2a_s/m$ characterizes the two-body interactions for a condensate with atoms of mass $m$ and s-wave scattering length $a_s$. The scattering length $a_s$ is positive for repulsive interactions and negative for attractive interactions.

We consider a trapping potential $V(r)$ of the form

$$V(r) = \frac{1}{2}m(\omega_x^2 + \omega_y^2 + \omega_z^2) + V_L,$$

where the first term describes an anisotropic parabolic potential due to a magnetic trap. The effective periodic potential, $V_L$, is formed by an optical lattice, which we consider to be either one-dimensional (1D),

$$V_L(x) = V_0 \sin^2(Kx),$$

or two-dimensional (2D):

$$V_L(x,y) = V_0 \left[ \sin^2(Kx) + \sin^2(Ky) \right].$$

The 1D (2D) lattice is created by a pair (two pairs) of counter-propagating laser beams with the wavelength $\lambda = 2\pi/K$, and the lattice depth, $V_0$, is proportional to the intensity of the standing light wave.

Equation (1) can be made dimensionless using the characteristic length $a_L = 1/K$, energy $E_{rec} = \hbar^2/ma_L^2$, and time $\omega_L^{-1} = \hbar/E_{rec}$ scales of the lattice. In dimensionless units, the two-body interaction coefficient is given by $g_{3D} = 4\pi(a_s/a_L)$, and the lattice depth is measured in units of the lattice recoil energy, $E_{rec}$.

3. One-dimensional atomic band-gap structures

We now assume a cigar-shaped condensate weakly trapped in $x$-direction ($\omega_x \ll \omega_y, \omega_z \equiv \omega_\perp$). In the directions of tight confinement, the condensate wavefunction can be described by the ground state of a two-dimensional radially symmetric quantum harmonic oscillator potential, with the normalization $\int_{-\infty}^{\infty} |\Phi|^2 d\mathbf{r} = 1$. The 3D wavefunction then separates as $\Psi(r,t) = \Phi(y,z)\psi(x,t)$.
and the transverse dimensions can be integrated out in the dimensionless Eq. (1), yielding the 1D GP equation:

$$i \frac{\partial \psi}{\partial t} = \left\{ -\frac{1}{2} \frac{\partial^2}{\partial x^2} + V_L(x) + \sigma |\psi(x,t)|^2 \right\} \psi$$

where the wavefunction is rescaled as $\psi \rightarrow \psi \sqrt{g_{1D}}$, $g_{1D} = 4(a_s/a_L)(\omega_\perp/\omega_L)^2$, $\sigma = \text{sign}(g_{1D})$, and the external potential is approximated by the quasi-1D periodic potential of the optical lattice, $V_L(x) = \sin^2(x)$, by neglecting the contribution of a weak magnetic confinement.

The stationary states of a condensate in a quasi-1D infinite periodic potential are described by solutions of Eq. (5) of the form: $\psi(x,t) = \phi(x) \exp(-i\mu t)$, where $\mu$ is the corresponding chemical potential. The case of a noninteracting condensate formally corresponds to $g_{1D} = 0$, and the condensate wave function can be represented as a superposition of Bloch waves,

$$\phi(x) = b_1 \phi_1(x) e^{ikx} + b_2 \phi_2(x) e^{-ikx},$$

where $\phi_{1,2}(x)$ have periodicity of the lattice potential, $b_{1,2}$ are constants, and $k$ is the Floquet exponent. The linear matter-wave spectrum consists of bands of eigenvalues $\mu_{n,k}$ in which $k(\mu)$ is a (real) wavenumber of amplitude-bounded Bloch waves [14]. The bands are separated by spectral gaps in which $\text{Im}(k) \neq 0$. The solutions at the band edges are stationary Bloch states corresponding to the condensate density which is strongly and periodically modulated by the lattice.

For an interacting condensate ($g_{1D} \neq 0$), bright solitons can exist for chemical potentials corresponding to the gaps of the linear matter-wave spectrum. The mechanism for nonlinear localization in the gaps was first described for light waves in nonlinear periodic photonic structures by using the Bloch-wave envelope approximation near the band edge [20]. It has been pointed out that, near the band edges, the characteristic diffraction coefficient for a coherent wave is proportional to the band curvature at that edge, which can be both negative and positive. For a matter wave in an optical lattice, the group velocity, $v_g = \partial \mu / \partial k$, and the effective diffraction coefficient, $D = \partial^2 \mu / \partial k^2$ (analogous to the inverse effective mass of an electron in crystalline solids [21]), are shown in Fig. 1 for the Bloch waves in the first lowest-order bands of a relatively shallow lattice. The balance of the repulsive (attractive) interactions and anomalous, $D < 0$, (normal, $D > 0$) diffraction near the top (bottom) of the bands (see Fig. 1), can lead...
Fig. 2. Band-gap spectrum of matter waves in an optical lattice shown as the Bloch bands (shaded) and gaps (open), combined with the families of bright gap solitons in (left) repulsive and (right) attractive condensates ($V_0 = 5$).

to formation of localized wavepackets - \textit{matter wave solitons} - with zero group velocity. The chemical potentials corresponding to such localized waves lie in the gaps of the Bloch-wave spectrum for the matter waves of the noninteracting condensate (open areas in Fig. 1).

Employing the multi-scale perturbation series expansion for the chemical potential and the gap soliton envelope, it is possible to show that, in general, two types of gap solitons bifurcate from each band edge [22]. These are the bright solitons centered on the maximum (off-site) and minimum (on-site) of the lattice potential, respectively. Several families of the lowest-order gap modes are presented in Fig. 2, for the case of both repulsive (left) and attractive (right) condensates. The families are characterized by the norm of the condensate wavefunction, $P = \int |\phi|^2(x)dx$, which is proportional to the number of atoms in a localized state. Such localized states exist in all band gaps, including the semi-infinite gap of the spectrum below the first band [14], which is analogous to the total internal reflection gap of the photonic structures, and where the existence of the localized states is due to conventional self-focusing. Near the bottom (top) gap edge, gap solitons of the repulsive (attractive) BEC are well approximated by a sech-like envelope of the corresponding Bloch wave, centered either on- or off-site. Near the opposite edge of the gap, i.e. approaching the spectral band, the solitons develop extended "tails" with the spatial structure of the Bloch wave at the corresponding band edge [14]. For a sufficiently wide gap (i.e., in the relatively tight binding regime), the soliton deep inside the gap may be strongly localized around a single well of the lattice potential. The bifurcations of the two types of gap solitons from the band edges of the opposite "polarity" (or sign of the effective diffraction) are a general feature of the coherent waves in periodic systems, such as spatial optical solitons in discrete waveguide arrays [23].

Stability of extended and localized modes in nonlinear systems is an important issue, since only dynamically stable modes are likely to be generated and observed in experiments. To
Fig. 3. Examples of a weakly unstable and stable soliton dynamics. Shown is peak density (a) of the repulsive BEC off-site soliton [shown in Fig. 2 (left, b)] in the first gap ($\mu = 3.7$), and (b) of the attractive BEC on-site soliton [shown in Fig. 2 (right, a)] in the semi-infinite gap ($\mu = 1.0$). In (a) the initial state given by the exact (numerical) stationary solution of Eq. (5) is perturbed by a symmetric excitation at 5% of the soliton peak density. In (b) the antisymmetric internal mode is excited by an initial perturbation at 5% of the initial soliton peak density.

determine the stability properties of the localized modes, we consider small perturbations to a stationary gap soliton of the GP equation, $\phi(x)$, in the form

$$\psi(x, t) = \phi(x)e^{-i\mu t} + \epsilon[(u + iw)e^{\lambda t} + (u^* + iw^*)e^{-\lambda t}]e^{-i\mu t},$$  \hspace{0.5cm} (7)

where $\epsilon \ll 1$, and $u(x), w(x)$ are spatially-dependent perturbation modes. We linearize the GP equation (5) around the localized solution and obtain, to the first order in $\epsilon$, a linear eigenvalue problem for the perturbation modes

$$L_-w = \lambda u, \quad L_+u = -\lambda w,$$  \hspace{0.5cm} (8)

where $L_\pm = -(1/2)(\partial^2/\partial x^2) + V_L(x) + 2\sigma \partial^2 \pm \sigma \partial^2 - \mu$. The modes describing the development of instability have either purely real or complex eigenvalues $\lambda$; in this latter case, the instability is called an oscillatory instability.

We solve the eigenvalue problem for the perturbation modes numerically, as a matrix eigenvalue problem with Fourier interpolants for the differential operators. The results reveal that, in agreement with the generalized Vakhitov-Kolokolov criterion (see, e.g., [4]), nodeless localized states of the attractive BEC (such as the fundamental solitons in a semi-infinite gap [Fig. 2 (a), right]) are linearly stable as long as $-\partial P/\partial \mu > 0$. Note that the criterion is “inverted” for our choice of $\mu$. The fundamental gap solitons of repulsive BEC [Fig. 2 (left, a)] are also linearly stable.

The linear stability analysis shows that gap solitons of both attractive and repulsive BEC are associated with a number of internal modes ($\text{Im}\lambda \neq 0$ and $\text{Re}\lambda = 0$). The excitation of these modes usually leads to a persisting dynamics (e.g., amplitude oscillations) of the localized state that does not lead to its decay. However, higher-order gap solitons of both attractive and repulsive condensates can experience oscillatory instability ($\text{Im}\lambda \neq 0$ and $\text{Re}\lambda \neq 0$) initiated by resonances of internal modes with the bands of the inverted spectrum [22]. This mechanism for weak spectral instability was first identified in studies of spatial optical solitons in one-dimensional nonlinear photonic crystals [24]. In Fig. 3 we compare temporal evolution of the weakly unstable gap soliton of the repulsive condensate in the first gap (a) with that of a linearly stable (attractive) BEC soliton in the semi-infinite spectral gap (b). The evolution of the soliton peak density is shown in Fig. 3 for the cases when initial solitons are perturbed by a 5% of the peak density. These results indicate that the oscillatory instability is weak and, on
realistic experimental time scales, can not provide a strong mechanism for the soliton decay into spatially extended lattice states (which would otherwise prevent observation of localized states in experiments).

4. Two-dimensional band-gap structures

The theory of the nonlinear localized matter waves in optical lattices can be extended to the case of two-dimensional lattices [11]. Nonlinear localization of 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 the corresponding nonlinear localized modes. In particular, the problem of the existence and stability of 2D matter-wave gap solitons of BEC with repulsive interatomic interactions loaded into optical lattices, is analogous to the study of localized states of light waves in nonlinear photonic crystals [2].

To simplify our analysis of the model (1), we assume that the weak magnetic confinement characterized by trap frequencies $\omega_{y,z}$ has little effect on the stationary states of the condensate in the 2D lattice formed in the $(x,y)$ plane of the condensate cloud. 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 the dimensionality reduction procedure described above for the 1D case. The condensate wavefunction in the 2D lattice potential is then described by the following equation:

$$i\frac{\partial \psi}{\partial t} = \left\{ -\frac{1}{2} \nabla^2 + V_L(x,y) + |\psi|^2 \right\} \psi, \quad (9)$$

where $\nabla_\perp = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $V_L(x,y)$ is the periodic potential of the optical lattice, and the wavefunction is rescaled as $\psi \rightarrow \psi/\sqrt{g_{2D}}$, with $g_{2D} = g_{3D}/\sqrt{2}$. The equation (9) is made dimensionless by using the "natural" lattice units of energy, length, and frequency, described above. In the simplest case of the square optical lattice, the potential of the optical lattice can be written as $V_L = V_0 \left[ \sin^2(x) + \sin^2(y) \right]$, where $V_0$ is the amplitude of the optical lattice.

Stationary (time-independent) states of the condensate in an infinite periodic potential of a 2D optical lattice are described by solutions of Eq. (9) of the form: $\psi(r,t) = \phi(r) \exp(-i\mu t)$, where $\mu$ is the chemical potential. The case of a noninteracting condensate formally corresponds to Eq. (9) being linear in $\psi$. According to the Bloch theorem, the stationary wavefunction can then be sought in the form $\phi(r) = u_k(r) \exp(ikr)$, where the wave vector $k$ belongs to a Brillouin zone of the square optical lattice, and $u_k(r) = u_k(r + d)$ is a periodic (Bloch) function with the periodicity of the lattice. For the values of $k$ within an $n$-th Brillouin zone, the dispersion relation for the 2D Bloch waves, $\mu_{n,k}$, is found by solving a linear eigenvalue problem:

$$\left[ \frac{1}{2} (-i\nabla_\perp + k)^2 + V_L(r) \right] u_{n,k} = \mu_{n,k} u_{n,k}. \quad (10)$$

The band-gap structure of the spectrum $\mu(k)$ of the atomic Bloch waves in the 2D optical lattice is shown in Fig. 4, in the reduced zone representation usually assumed in the theory of crystalline solids and photonic crystals. Due to separability of the lattice potential, the Bloch waves $u(x,y)$ in the first band, at the high symmetry points $(\Gamma \rightarrow X \rightarrow M)$ of the first irreducible Brillouine zone (see Fig 4), can be found as $u(x,y; k) = u^{(1d)}(x;k_x)u^{(1d)}(y;k_y)$, where $u^{(1d)}$ are the corresponding 1D Bloch states. Different structure of the Bloch states in the first band, at the values of $k$ corresponding to the three symmetry points, are shown in Fig. 4 (right column). By applying an envelope theory near the band edges, it can be deduced that each of the Bloch states is associated with a (partially) localized state in the $\Gamma, X$, or $M$-gap. Similarly
Fig. 4. Left: Dispersion diagram for a 2D square lattice ($V_0 = 1.5$); dotted - the line $\mu = V_0$; shaded - spectral bands, open - the lowest, semi-infinite, and the first complete gaps. Below: lattice potential in the cartesian and reciprocal spaces. Right: Spatial structure of the 2D Bloch waves at the extreme high-symmetry points of the first irreducible Brillouine zone.

to optical gap solitons in indirect gaps of higher-dimensional photonic crystals [25], matter-wave gap solitons can be spatially localized in all directions only in the complete gap located between the $M$ and $X$-edges of the first and the second band, respectively (see Fig. 4). The localization near the lower $M$-edge is possible due to the negative components of the effective diffraction tensor. We find spatially localized stationary solutions of Eq. (9) numerically. Our numerical procedure involves minimization of the norm $N = \int f^* f \, dr$ of the functional $f(\phi) = [(1/2) \nabla^2 - \mu - V(r) - |\phi|^2] \phi$ by following a descent technique with Sobolev preconditioning [26]. The minimization procedure yields a stationary state when $N(\phi) \to 0$.

The family of fundamental bright matter-wave solitons in the first complete gap is presented in Fig. 5. For the repulsive condensate, such gap solitons exist in all band gaps excluding the semi-infinite gap below the first band. The spatial structure of the lowest-order gap solitons near the lower gap edge [Fig. 5(a)] has a characteristic structure of the symmetric envelope superimposed onto the corresponding Bloch state [see Fig. 4]. The threshold value of the number of atoms (and therefore $P_c$) needed for the soliton localization is determined by the theory of lattice-free self-focusing in the 2D geometry. These weakly localized, low density modes are similar to the near-band-edge modes described above for the case of one-dimensional gap solitons. Deeper inside the gap, the matter-wave soliton becomes strongly localized [Fig. 5(b)], before delocalizing again near the upper gap edge. Near that edge, extended tails [see Fig. 5(c)] are developed in the directions along which the tunneling is assisted by lower inter-well barrier heights and positive (normal) effective diffraction. By direct numerical simulations we have confirmed that the strongly localized two-dimensional fundamental modes are dynamically sta-
The possibility of the formation of periodic trains of such 2D localized structures, triggered by the modulational instability of the nonlinear Bloch states, has been suggested in Ref. [27]. We have also found different families of higher-order localized gap modes that can be identified as in-phase and out-of-phase bound states of the fundamental gap solitons. These states can be centered at the lattice potential minima or maxima, similarly to higher-order states in one-dimensional lattices [14], and they can exhibit symmetry-breaking instabilities. In particular, Figs. 6(a-c) shows three different examples of higher-order gap solitons. The simplest structure of this kind is described by a pair of two fundamental gap solitons which are out-of-phase and form a dipole [see Fig. 6(a)]. The similar structure of four solitons can exist as a quadrupole state where the neighboring solitons are π out-of-phase [see Fig. 6(b)]. However, the most interesting structure, which is shown in Fig. 6(c), possesses a vortex-like phase dislocation, with the phase winding by 2π around the low-density centre [as seen in Fig. 6(d)]. Such a bound state can be identified as a gap vortex [29].

5. Optically-induced photonic lattices

Although many similarities (including the structure of localized modes and their stability properties) exist between nonlinear atom optics in optical lattices and nonlinear optics in fabricated photonic structures, the closest analog of the matter-wave band-gap structures can be found in the new and rapidly developing field of optically-induced photonic lattices [5, 6, 7].

Fig. 5. Top: Family of bright atomic gap solitons of repulsive BEC in a 2D optical lattice (V₀ = 1.5). Bottom: spatial structure of the BEC wavefunctions at the marked points of the existence curve inside the gap.
Fig. 6. Spatial structures of the BEC wavefunctions corresponding to higher-order gap solitons ($V_0 = 1.5$): (a) dipole ($\mu = 2.0, P = 9.02$), (b) quadrupole ($\mu = 2.0, P = 9.8$), (c) charge-one gap vortex ($\mu = 2.0, P = 16.2$). (d) Phase structure of the gap vortex shown in (c) (color-bar refers to the phase plot only).

In the existing experimental realizations of optically-induced photonic lattices, a periodic modulation of the refractive index is induced by a plane wave interference pattern illuminating a photorefractive crystal with a strong electro-optic anisotropy [28]. The spatially periodic interference pattern modulates the space-charge field in the crystal, which relates to the refractive index via electro-optic coefficients. The latter are substantially different for different polarizations. As a result, the material nonlinearity experienced by waves polarized in the main direction of the crystal is up to two orders of magnitude larger than that experienced by the orthogonally polarized ones. When the lattice-forming waves are polarized orthogonally to the main axis, their nonlinear self-action as well as any cross-action from the co-propagating probe beam (polarized along the main axis) can be neglected. Thus, the periodic interference pattern propagates in the diffraction-free linear regime and creates a stationary refractive-index grating [5, 6]. The effective induced grating exhibited by the probe light is almost identical to the effective periodic potential experienced by matter waves in an optical lattice. Optically induced lattices open up an exciting possibility for creating dynamically reconfigurable photonic structures in bulk nonlinear media, with a degree of control over the parameters of the periodic structure approaching that of BECs in optical lattices. Nonlinear localization of coherent light waves has been observed in both 1D and 2D optically-induced photonic lattices [5, 6, 7], in the self-focusing regime (which is analogous to the attractive matter-wave localization regime).
6. Conclusions

We have studied the spectrum of matter waves and localization of Bose-Einstein condensates in one- and two-dimensional optical lattices and demonstrated that the interaction of the condensate with a periodic lattice potential can be compared to the propagation of coherent light waves in a nonlinear periodic photonic structure. Using the analogy with the physics of photonic band-gap structures, we have described some basic properties of matter-wave band-gap structures and demonstrated numerically the existence of one- and two-dimensional matter-wave gap solitons, spatially localized states of the condensate existing in the gaps of the matter-wave linear spectrum. We believe that the analogy between the physics of BEC in optical lattices and light waves in nonlinear photonic crystals, as well as other types of periodic photonic structures, is useful to reveal many novel features of the matter-wave dynamics in reconfigurable optically-induced structures.

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