Matter-wave gap solitons in atomic bandgap structures

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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 bandgap structure allows nonlinear localization of atomic Bloch waves in the form of two-dimensional matter-wave gap solitons.

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Recent experiments\textsuperscript{1, 2, 3, 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. Due to inherent nonlinearity of the coherent matter waves introduced by inter-atomic 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 bandgap (PBG) materials\textsuperscript{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\textsuperscript{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\textsuperscript{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 bandgaps 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 (\textasciitilde 10\textsuperscript{3}) critical number of particles.

In theory, a shallow 1D optical lattice can support bright matter-wave solitons even in repulsive BEC\textsuperscript{9} with large atom numbers. These solitons, described in a framework a coupled-mode theory\textsuperscript{10}, are localized on a large number of lattice wells, and are predicted to exist only in atomic bandgaps. 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\textsuperscript{11, 12}, in complete parallel with spatial solitons in periodic optical structures\textsuperscript{12} and localized modes of atomic lattices\textsuperscript{12}.

The theory of the nonlinear localized matter waves in optical lattices is mostly limited to 1D case\textsuperscript{20}. However, as can be deduced from the analogous studies of 2D PBG structures\textsuperscript{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 bandgap 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 only possible 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 wavefunction, $\Psi(r,t)$ of the condensate,

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

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{figure1.png}
\caption{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.}
\end{figure}

In the simplest case of a square optical lattice, the combined potential of the lattice and magnetic trap, $V(r) = V_L(r) + V_T(r)$, can be written as $V(r) = V_0 \left( \sin^2 x + \sin^2 y \right) + \omega_i^2 r^2/2$, where $V_0$ is the amplitude of the optical lattice, and $\omega_i$ 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 $\omega_i$ has 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, $\psi(r,t) = \Phi(z)\psi(x,y,t)$ where the function $\Phi(z)$, describing the condensate in the direction 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 [14], leads to the following equation for the 2D condensate wavefunction in the 2D lattice potential:

$$\frac{\partial \psi}{\partial t} = \left[ -\frac{1}{2} \nabla^2 + V_L(r) + |\psi|^2 \right] \psi, \hspace{1cm} (2)$$

where $\nabla = \partial^2/\partial x^2 + \partial^2/\partial y^2$, $V_L(r) \equiv V_L(x,y)$ is the periodic potential of the optical lattice, and the wavefunction is rescaled as $\psi \rightarrow \psi/\sqrt{\gamma_{2D}}$, 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: $\psi(r,t) = \phi(r) \exp(-i\mu t)$, where $\mu$ 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 $\psi$. According to the Bloch theorem, the stationary wavefunction can then be sought in the form $\phi(r) = u_k(r) \exp(ikr)$, where the wavevector $k$ belongs to a Brillouin zone of the square 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 the following linear eigenvalue problem

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

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 $\Gamma$) 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 parameters affects the band structure, we note that, owing to the spectra of the Bloch waves in the middle (point $\Gamma$) and on the edge (point M) of the Brillouin zone. The typical dispersion relation for the energy of the 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 quasi-unbound ($\mu > V_0$) and strongly bound ($\mu < V_0$) condensate states in the lattice (see also Ref. [12]). By varying the interwell separation or the amplitude of the lattice, different regimes of the atomic bandgap structure can be accessed. The tight-binding regime of the condensate dynamics corresponds to the domain $V_0 > V_0^* = \mu$, 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 bandgap structures [14, 16] indicates that the correct structure and dynamical properties of the nonlinear localized modes can only be revealed 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 [17] to the 2D case. However, the complexity involved in the generation of optimally localized higher-dimensional Wannier functions [18] may not provide significant advantage compared with the direct solution of the model equation [2].

Here, we find spatially localized stationary solutions of Eq. (2) numerically. Our numerical procedure involves minimization of the functional $N = \int f^*fdr$, where $f(\phi) = |\nabla_\perp + \mu - V_{L}(r) - |\phi|^2\phi|$, by following a descent technique with Sobolev preconditioning [19]. The minimization procedure yields a stationary state when $N(\phi) = 0$. 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 bandgap 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 bandgap structure. These solitons can exist in all gaps, excluding the semi-infinite gap of the spectrum (marked by 1 in Figs 1 2 below the first band. We note in passing that only conventional nonlinear localization 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 for $V_0 = 5$. Gap solitons of repulsive BEC branch off the lower-energy (i.e. smaller values of $\mu$) gap edge (see Figs. 3 top). Near this edge, i.e. at low particle numbers and amplitudes, their central peak is localized around a single well [Figs. 3 (a)]. Further within the gap, the localized mode of the BEC

![Image](https://via.placeholder.com/150)
contains larger numbers of atoms, and has a strongly localized central peak. 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 tunnelling is assisted by the lower inter-well 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. 1,2), and only localized modes within this gap have been analyzed.

The higher-amplitude gap solitons have a nontrivial structure of the tails [see Fig. 2(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 [1], 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. 1.

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 $\Psi(z)\phi(x,y)$, 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 multi-dimensional 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 bandgap structure. We have studied the properties of two-dimensional atomic bandgap 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 bandgap structures.

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![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.](Image)

Experimental observation of multi-dimensional gap solitons, is the subject of our separate study.

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