Driving Defect Modes of Bose-Einstein Condensates in Optical Lattices

Valeriy A. Brazhnyi,[1] Vladimir V. Konotop,[1] and Víctor M. Pérez-García[2]

[1]*Centro de Física Teórica e Computacional, Universidade de Lisboa, Complexo Interdisciplinar, Avenida Profesor Gama Pinto 2, Lisbon 1649-003, Portugal*

[2]*Departament de Matemáticas, E.T.S.I. Industriales, Universidad de Castilla-La Mancha, 13071 Ciudad Real, Spain*

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We present an approximate analytical theory and direct numerical computation of defect modes of a Bose-Einstein condensate loaded in an optical lattice and subject to an additional localized (defect) potential. Some of the modes are found to be remarkably stable and can be driven along the lattice by means of a defect moving following a steplike function defined by the period of Josephson oscillations and the macroscopic stability of the atoms.

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Loading and manipulating cold bosonic atoms in optical lattices (OLs) is a fascinating and rapidly growing branch of cold atom physics [1–3]. Recent experimental progresses with Bose-Einstein condensates (BECs) in optical lattices [3] and the direct observation of a gap soliton [4] have stimulated studies of the nonlinear dynamics of matter waves in periodic media (see, e.g., Refs. [3,5] and references therein). OLs provide a tool for changing the effective properties of atomic media allowing for the existence of solitary waves in a condensate with positive scattering length. Moreover, OLs also provide ways for manipulating nonlinear matter waves. For instance, smooth modulations of an OL can be used to control the dynamics of gap solitons [5,6], while strongly localized defects generated by narrow laser beams have been used to induce rotational motion of condensed atoms [7] and to study scattering of a soliton on a defect for the sake of understanding BEC expansion in a random potential [8].

In this Letter we consider the combined effect of an OL and of a strongly localized defect on spatial distribution and dynamics of matter waves. We study the existence and stability of defect modes, concentrating on their approximate analytical description and on numerical simulation of their dynamics, establishing the stability properties of the modes. We show that a defect mode can be driven over hundreds of lattice periods, thus representing an effective tool for matter waves management.

In the quasi-one-dimensional (1D) limit a BEC is governed by the dimensionless Gross-Pitaevskii equation [5]

$$i\psi_t = -\psi_{xx} + A\cos(2x)\psi + V_d(x - x_d)\psi + \sigma|\psi|^2\psi, \tag{1}$$

where $\sigma = 1$ (repulsive atom-atom interactions) or $\sigma = -1$ (attractive), A is the amplitude of the lattice, the lattice constant is chosen to be π without restriction of generality and $V_d(x - x_d) = (\eta/\sqrt{2\pi}\ell)\exp[-(x - x_d)^2/2\ell^2]$, is a defect potential of the amplitude characterized by η, width $\ell \lesssim \pi$ (i.e., localized on a distance of the order of 1 lattice period) and center x_d. This situation can be realized experimentally by using narrow Gaussian beams for creating the defect potential and by adjusting the incidence angles of the beams generating the OL.

Since the defect is strongly localized we can expand the solutions over the orthonormal basis of Wannier functions [9]. To do so we first expand $\psi(x, t) = \sum_{\alpha=0}^{\infty} \times \int dk \varphi_{\alpha k}(x) f_\alpha(k, t)$, over the set of Bloch functions $\varphi_{\alpha k}(x)$ solving the eigenvalue problem $[-d^2/dx^2 + A\cos(2x)] \times \varphi_{\alpha k} = E_\alpha(k)\varphi_{\alpha k}$, where $\alpha = 0, 1, \ldots$ stands for a number of the Bloch band, k is the wave vector considered on the first Brillouin zone (BZ), $k \in [-1, 1]$, and hereafter integrals with respect to k are over the first BZ. Inserting this expansion into Eq. (1) we obtain an equation for the envelope $f_\alpha(k)$

$$\begin{aligned} i\dot{f}_\alpha(k) - E_\alpha(k) f_\alpha(k) = \sigma \int dx \bar{\varphi}_{\alpha k}(x)|\psi(x,t)|^2\psi(x,t) \\ + \sum_{\alpha'} \int dk' \int dx \bar{\varphi}_{\alpha k}(x) \\ \times V_d(x - x_d)\varphi_{\alpha' k'}(x) f_{\alpha'}(k'). \end{aligned} \tag{2}$$

Hereafter integration with respect to x is carried out over the real axis and to shorten notations we drop the temporal argument of the envelope f_α.

Next we use the standard definition of Wannier functions: $w_{\alpha n}(x) = (1/\sqrt{2}) \int \varphi_{\alpha k}(x) e^{-i\pi n k} dk$ and introduce the matrix element $V^{nn'}_{\alpha\alpha'} = (1/2) \int dx V_d(x) w_{\alpha n}(x) w_{\alpha' n'}(x)$ describing probability of transitions between the minimum n in the band α and minimum n' in the band α', as well as its Fourier transform $\hat{V}^{kk'}_{\alpha\alpha'} = \sum_{n,n'} V^{nn'}_{\alpha\alpha'} e^{i\pi(k'n' - kn)}$. Then, the last term in Eq. (2) is rewritten in the form $\sum_{\alpha'} \int dk' \hat{V}^{kk'}_{\alpha\alpha'} f_{\alpha'}(k')$.

Let the defect be localized at the origin, $x_d = 0$, which also coincides with a minimum of the lattice potential, for $A < 0$. Matter-wave modes of small amplitude, having width λ exceeding a lattice period, $\lambda \gg \pi$, are well described in the effective mass approximation [5]. In that case, the characteristic scale of $f_\alpha(k)$ in the momentum space is much smaller than the vector of the reciprocal lattice which in our case is equal to 2, i.e., $\Delta k \ll 1$, the latter being the scale of variation of $\hat{V}^{kk'}_{\alpha\alpha'}$. In other words, in

the effective mass approximation the envelope $f_\alpha(k)$ is much more localized than $\hat{V}^{kk'}_{\alpha\alpha'}$.

Let us consider localized modes whose carrier-wave wave vector k_0 borders the BZ: $k_0 = \pm 1$. Then the spatial domain where $f_\alpha(k)$ significantly differs from zero is given by $k \in (k_0 - \Delta k, k_0 + \Delta k)$ allowing us to approximate $\int \hat{V}^{kk'}_{\alpha\alpha'} f_{\alpha'}(k')dk' \approx (\hat{V}_{\alpha\alpha'}/2\pi) \int f_{\alpha'}(k')dk'$, where $\hat{V}_{\alpha\alpha'} = 2\pi \hat{V}^{k_0k_0}_{\alpha\alpha'}$. We also take into account that our approximation is justified when the effective mass, $M_\alpha = [d^2E_\alpha(k)/dk^2]^{-1}$, is of order one and the Wannier functions are localized on a few lattice periods. These conditions are verified for OLs of amplitudes of order of a few recoil energies (in dimensionless units for $|A| \sim 1$) and which are illustrated by examples in Table I.

Now the nonlinear term can be rewritten as $\sum_{\alpha_{1,2,3}} W_{\alpha\alpha_1\alpha_2\alpha_3} Q_{\alpha_1\alpha_2\alpha_3}$ where (see also Ref. [10])

$$W_{\alpha\alpha_1\alpha_2\alpha_3} = \frac{1}{2} \sum_{n_1 n_2 n_3} (-1)^{n_2+n_3-n_1} \times \int dx w_{\alpha 0}(x) w_{\alpha_1 n_1}(x) w_{\alpha_2 n_2}(x) w_{\alpha_3 n_3}(x),$$
$$Q_{\alpha_1\alpha_2\alpha}(k) = \int dk_1 dk_2 \bar{f}_{\alpha_1}(k_1) f_{\alpha_2}(k_2) f_\alpha(k + k_1 - k_2). \quad (3)$$

For our lattice potential the Wannier functions have the symmetry $w_{\alpha n}(x) = (-1)^\alpha w_{\alpha n}(-x)$. Hence, an even defect $V_d(x)$ results in transitions only between bands having the same parity, i.e., $\hat{V}_{\alpha\alpha'} = 0$ if $|\alpha - \alpha'|$ is odd. On the other hand, the nonlinearity by itself, while it couples different modes due to (3), does not affect the averaged densities. Indeed, the total number of particles is given by $N = \int |\psi|^2 dx = \sum_\alpha n_\alpha$, where $n_\alpha = \int |f_\alpha(k)|^2 dk$ is the number of particles in the αth band. Interchange of particles between bands α and α_1 originated by the nonlinearity (3), is determined by the integral $\mathrm{Im} \int dk \bar{f}_\alpha(k) Q_{\alpha_1\alpha_1\alpha}(k)$, which in our case is equal to zero.

Assuming that initially all atoms are loaded in one of the lowest bands we can use the one-band approximation, which neglects the interband transitions and results in decoupling of the equations for $f_\alpha(k)$, reducing Eq. (2) to (hereafter $\hat{V}_\alpha = \hat{V}_{\alpha\alpha}$ and $W_{\alpha\alpha'} = W_{\alpha\alpha'\alpha\alpha'}$)

$$i\dot{f}_\alpha(k) = E_\alpha(k) f_\alpha(k) + \hat{V}_\alpha \int f_\alpha(k)dk + \sigma W_{\alpha\alpha} Q_{\alpha\alpha\alpha}(k).$$

TABLE I. Parameters of the spectrum and hopping integrals (defined in the text) for $k = \pm 1$.

A	M_0	E_0	W_{00}	M_1	E_1	W_{11}	W_{01}
-1	-0.163	0.471	0.25	0.1	1.467	0.174	0.182
-5	-2.5	-2.076	0.358	0.3	2.5	0.234	0.274

Near the boundary of the BZ we can expand $E_\alpha(k) \approx E_\alpha + (k - k_0)^2/2M_\alpha$ where $E_\alpha = E_\alpha(k_0)$ is the energy of the αth band at the boundary of the BZ (see Fig. 1). Then, introducing $\hat{f}_\alpha(x, t) = e^{iE_\alpha t} \int dk e^{i(k-k_0)x} f_\alpha(k, t)$ and after straightforward algebra we obtain the nonlinear Schrödinger (NLS) equation with a delta impurity

$$i\frac{\partial \hat{f}_\alpha}{\partial t} + \frac{1}{2M_\alpha}\frac{\partial^2 \hat{f}_\alpha}{\partial x^2} - \sigma W_{\alpha\alpha}|\hat{f}_\alpha|^2 \hat{f}_\alpha = \hat{V}_\alpha \delta(x) \hat{f}_\alpha. \quad (4)$$

The wave function $\psi(x, t)$ is recovered from Eq. (4) by

$$\psi \simeq \frac{1}{\sqrt{2}} e^{-iE_\alpha t} \sum_n (-1)^n w_{\alpha n}(x) \hat{f}_\alpha(nL). \quad (5)$$

Stationary defect modes of (4) have the form: $\hat{f}_\alpha(x) = e^{-i\varepsilon_\alpha t}\phi_\alpha(x)$ with $\phi_\alpha(x)$ real. A detailed analysis and classification of defect modes of the NLS equation can be found in Ref. [11]. The applicability of the effective mass approximation and the requirement for the frequency of the mode to belong to a forbidden gap, imply the conditions: $|\varepsilon_\alpha| \ll E_{\alpha+1} - E_\alpha$ and $\varepsilon_\alpha M_\alpha < 0$ (Fig. 1).

We discuss below defect modes in the first lowest gap (i.e., for $\alpha = 0, 1$). For $\sigma M_\alpha < 0$ one obtains *cosh modes*

$$\phi_\alpha(x) = \frac{\sqrt{2|\varepsilon_\alpha|/W_{\alpha\alpha}}}{\cosh[\sqrt{2|M_\alpha\varepsilon_\alpha|}(|x| - x_\alpha)]}. \quad (6)$$

Here $x_\alpha = a \tanh[\mathrm{sign}(M_\alpha \hat{V}_\alpha)\sqrt{\varepsilon_*/\varepsilon_\alpha}]/\sqrt{2|M_\alpha\varepsilon_\alpha|}$, and $\varepsilon_* = -M_\alpha \hat{V}_\alpha^2/2$. This mode exists when $|\varepsilon_\alpha| > |\varepsilon_*|$. For $M_\alpha \hat{V}_\alpha < 0$ the cosh mode has only one maximum and otherwise it has a two-hump profile [11].

When $\sigma M_\alpha > 0$ there is another localized solution of Eq. (4)—a *sinh mode*—which corresponds to a smaller detuning $|\varepsilon_\alpha| < |\varepsilon_*|$ such that $\varepsilon_\alpha \sigma < 0$,

$$\phi_\alpha(x) = \frac{\sqrt{2|\varepsilon_\alpha|/W_{\alpha\alpha}}}{\sinh[\sqrt{2|M_\alpha\varepsilon_\alpha|}(|x| + x_\alpha)]}. \quad (7)$$

Now $x_\alpha = a \tanh(\sqrt{\varepsilon_\alpha/\varepsilon_*})/\sqrt{2|M_\alpha\varepsilon_\alpha|}$.

Since w_{1n} are odd functions and the defect potential is localized on its zero we have that $|\hat{V}_1| \ll |\hat{V}_0|$ ($\hat{V}_1 = 0$ in the limit $\ell = 0$). Thus $\hat{f}_0$ is subject to much larger influence of the defect than $\hat{f}_1$. We also notice that since $M_\alpha = \mathcal{O}(1)$ one has $|\varepsilon_*| \sim \hat{V}_\alpha^2$. On the other hand, the applicability of our approach implies that all the terms in Eq. (4)

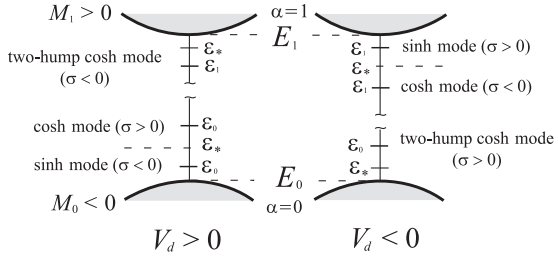

FIG. 1. Location of the impurity modes for $V_d > 0$, $V_d < 0$.

are of the same order and that $\lambda \gg \pi$. Thus $|\varepsilon_\alpha| \sim |\hat{V}_\alpha|/\lambda \sim 1/\lambda^2 \ll |E_\alpha| \sim 1$ and $\hat{V}_\alpha \ll 1$. Therefore, below we concentrate on cosh modes excited in the vicinity of the lowest band ($\alpha = 0$) and with $\sigma = 1$.

In Fig. 2 we plot both our analytical approximation for cosh modes given by Eqs. (5) and (6) and direct numerical solutions of Eq. (1) for different amplitudes of OL and defect parameters. The figure shows a very good accuracy of the one-band approximation. We have checked that decreasing the defect width by a factor of 10 does not appreciably change the shapes of the defect modes and their amplitudes differ only by 1%, which confirms the excellent accuracy obtained from the delta-approximation for $\ell \ll \pi$. The analytical approximation becomes worse for larger values of the defect strength, since in that case the modes are localized on very few lattice periods, and the tight-binding approximation should be used instead [10]. The approximation is worse for more complex modes: one-hump modes are better described in the tight-binding approximation than the two-hump modes, which is an evidence of the contribution of higher bands.

Two-hump modes display interesting features compared to their counterparts of the NLS equation, where they can be excited only in the case of attractive interactions [11]. Because of the possibility of the change of sign of the effective mass, such modes can also exist in the presence of the lattice for positive scattering length. Moreover, the modes have single maxima in their centers [Figs. 2(e)–2(h)], i.e., the term "two-hump" must be understood *de bene esse*. This happens because $\hat{f}_\alpha(x)$ are envelopes of Wannier functions.

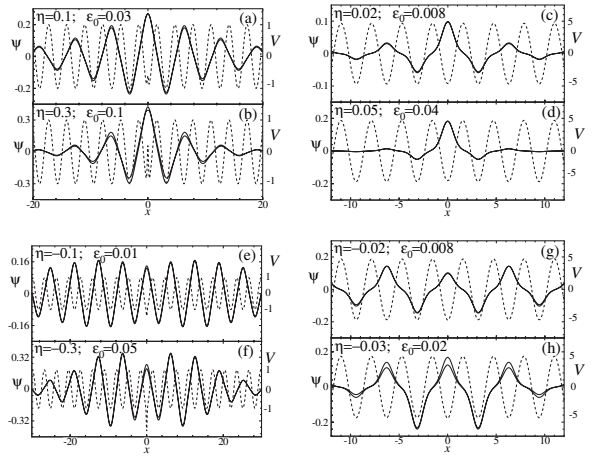

FIG. 2. Approximate analytical (thin lines) and numerical (thick lines) shapes of one-hump (a), (b), (c), (d) and two-hump (e), (f), (g), (h) cosh modes of the lowest band for $A = -1$ (a), (b), (e), (f), and for $A = -5$ (c),(d),(g),(h) with $\ell = 0.1$. Dashed lines show respective potentials (the scale is indicated on the right axes). Approximate data are computed using Table I. For $A = -5$ the defect, having amplitude of order of 0.1, is not visible.

In all the cases depicted in Fig. 2 the defect modes are transformed into the conventional gap solitons in the limit $\eta \to 0$, which also follows directly from (6) where $\varepsilon_* \to 0$ and $|x_\alpha| \to 0$.

To test the stability of cosh modes we have started by computing their evolution. Although for initial data we have used the approximate formulas, the shapes of these modes persist for several hundreds of units of time. Next we have imposed stronger perturbations by shifting the position of the defect. First, we shift the defect at $t = 10$ to the nearest minimum, $x_d = \pi$ and observe how the mode follows the defect and displaces its center to $x = \pi$. After some relaxation time the profile of the defect mode centered about $x = \pi$ is very similar to the initial one centered about $x = 0$ [Figs. 3(a) and 3(b)]. However, when the defect is shifted to $x_d = \pi/2$, the mode is gradually destroyed, since the new position does not correspond to a stable configuration [Figs. 3(c) and 3(d)].

The robust behavior of the mode shown in Fig. 3(a) suggests that it could be driven by moving the defect. Meanwhile, the mode is destroyed when it stays close to the local maxima of the potential. This suggests that the defect motion should be defined as a steplike function composed of two characteristic time intervals: a fast one, τ, in which the defect is shifted by one lattice period and a slow one, T, allowing the cosh mode to recover its shape on the new site. The mode dynamics shown in Fig. 3(b) can be interpreted as a tunneling of a part of atoms, between the two central minima, in a time τ_0, attracted by the shifted

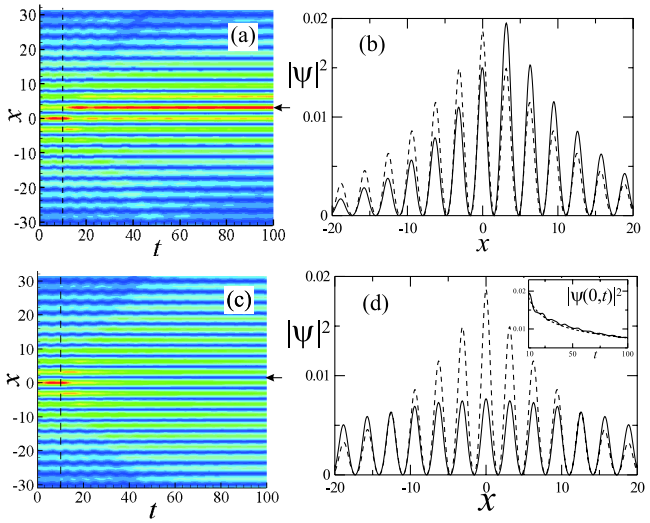

FIG. 3 (color online). (a), (b) Density plots of the dynamics of the cosh mode with $A = -1$, $\ell = 0.1$, $\eta = 0.1$, and $x_d = 0$. At $t = 10$ [dashed vertical lines in (a) and (c)] the defect is shifted to a position (a) $x_d = \pi$ and (c) $x_d = \pi/2$ indicated by the arrows. In (b) and (d) dashed and solid lines correspond to the initial ($t = 0$) and final ($t = 100$) profiles of the density of the mode. Inset in (d) shows dynamics of the amplitude of the central peak (solid line) after shifting of the defect: it is fitted by the law $\propto t^{-0.38}$ (dashed line).

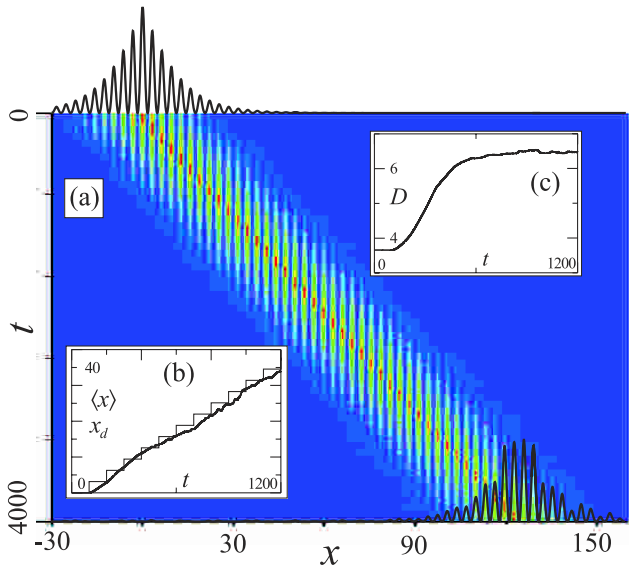

FIG. 4 (color online). [Color online] (a) Pseudocolor and amplitude plots of the motion of the driven defect mode. Initial parameters as in Fig. 3. (b) Defect position, $x_d(t)$ (thin line), and average coordinate of the center of the defect mode $\langle x\rangle(t)$ (thick line). (c) Evolution of the dispersion $D(t)$.

defect. Since this is a "single" tunneling process and the intermediate states are unstable the characteristic times should satisfy $\tau \ll \tau_0 \ll T$.

To estimate the Josephson tunneling time τ_0 we take into account that our approximation implies small differences in populations of neighbor wells and that we are near the boundary of the BZ, which means that the phase difference between atoms in adjacent cells is π. Thus we can use the results of Ref. [12] for the estimation of the half-period of the oscillations of a BEC in a double-well potential to obtain $\tau_0 \approx 3.67$ for $A = -1$. Hence, the defect must be shifted faster than $\pi/\tau_0 \approx 0.86$ and then stop for $T \gg 3.67$ to let the system relax to equilibrium.

Figure 4 shows numerical simulations of the driving of a defect mode with $x_d(t) = \pi\sum_{j=0}\theta(t - t_0 - 100j)$, where $\theta(t)$ is the Heaviside step function and t_0 is a time at which motion is started. Shown are also the mean dispersion or the width of the wave packet $D = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$ where $\langle x^n\rangle = \int x^n|\psi|^2dx/\int|\psi|^2dx$ [Figs. 4(b) and 4(c)].

In Fig. 4(c) we see that the dispersion of the wave packet grows in the interval $t \in (200, 600)$ after which the moving mode achieves a stationary profile. This reshaping occurs through the emission of radiation which also contributes to the appearance of small oscillations of $\langle x\rangle$ [see Fig. 4(b)] in this time interval.

A way to excite defect modes in real situations is to create a gap soliton with energy near the band edge in a homogeneous OL [4], then by increasing adiabatically the intensity of the transverse laser bean one could generate the defect mode. We have simulated this process numerically (see Fig. 5) starting from an envelope soliton with

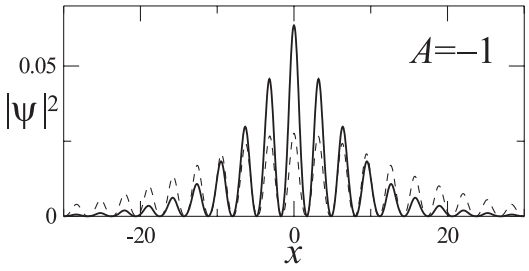

FIG. 5. Adiabatic excitation of the cosh mode from a gap soliton with $\varepsilon_0 = 0.01$, shown for $t = 0$ (dashed line) and $t = 10^3$ (solid line). The final values of the parameters are $\eta = 0.1$, $\varepsilon_* = 0.0034$, and $\varepsilon_0 \approx 0.027$.

energy $E_0 + \varepsilon_0$ and increasing η according to $\eta = 0.1\sin^2(5\cdot 10^{-4}\pi t)$ (with $\ell = 0.1$). The obtained final state is the cosh mode.

In this Letter we have shown that a BEC in a 1D optical lattice with an additional localized potential supports stable defect modes which in certain limits can be described by a nonlinear Schrödinger equation with a delta impurity. We have constructed these modes analytically and numerically and have shown that they can be driven along the lattice by a defect. Finally, we have shown that defect modes can be easily excited by adiabatically switching on the defect. Our results open new possibilities for controlling matter waves which we hope will stimulate further experiments with BECs in optical lattices.

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