

## Nonlinear dynamics of a dipolar Bose-Einstein condensate in an optical lattice

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The dynamics of Bose-Einstein condensates in optical lattices with the long-range dipole-dipole interactions, the short-range on-site interactions, and hopping terms is reduced to the generalized discrete nonlinear Schrödinger equation. We present the different types of solitary excitations which appear in different parameter regions. We anticipate that these excitations will be observable and discuss how the model parameters can be tuned in experiments.

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The dynamics of an ultracold dilute gas of Bosonic atoms in an optical lattice can be described by the Bose-Hubbard model [1]. The model predicts a phase transition from a superfluid phase to a Mott insulator observed for ultracold atoms in the optical lattice [2]. On the other hand, the dynamics of Bose-Einstein condensates (BECs) trapped in a spatially periodic potential can be mapped, in tight-binding approximation, to a discrete nonlinear Schrödinger equation [3]. It gives a link between the condensate dynamics and the physics of discrete nonlinear media [4,5]. Though various aspects of the BEC dynamics in the optical lattice have appeared separately in the literature (e.g., the intrinsic localized modes as well as the envelope soliton [6], the discrete soliton, the breathers and the dynamical phase diagram [3], the dynamical superfluid-insulator transition [7], etc.), in all these references the nonlinear Schrödinger equation included only nonlinearities caused by short-range on-site interactions. However, the nonlinearity caused by the long-range dipole-dipole interaction has an important influence on the properties of BEC (see, e.g., some recent publications on the nonlinearity caused by the long-range interaction in BECs [10–12]). The immediate motivations of the present paper are twofold; from one side, we develop a procedure for handling, all together, the long-range dipole-dipole interaction, the short-range on-site interaction, and the hopping term and want to show that the dynamics of dipolar bosons in the optical lattices can be described by the general discrete nonlinear Schrödinger equation. This will allow us to get a better understanding, both at the classical and at the quantum level, of the interplay between on-site–intersite interactions as well as integrability-nonintegrability and discrete-continuum properties of BEC in optical lattice [13]. From the other side, we show that the system of dipolar BECs in the optical lattice give us a different tool to study the different solitary excitations as the physical parameters of the system of dipolar BECs in optical lattice varied. Such a highly controllable system may be crucial in answering some unresolved questions in the theory of quantum nonlinear dynamics.

We consider a dilute gas of bosons in the optical lattice with the following Hamiltonian [1]:

$$\begin{aligned}
 H = & \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2}{2m} \nabla^2 + V_{opt} \right] \Psi(\mathbf{r}) \\
 & + \int d\mathbf{r} d\mathbf{r}' \Psi^\dagger(\mathbf{r}) \Psi^\dagger(\mathbf{r}') V_{int} \Psi(\mathbf{r}') \Psi(\mathbf{r}) \\
 & + \int d\mathbf{r} \Psi^\dagger(\mathbf{r}) V_{ext} \Psi(\mathbf{r}), \quad (1)
 \end{aligned}$$

where  $\Psi^\dagger(\mathbf{r})$  and  $\Psi(\mathbf{r})$  are the boson field operators that annihilate and create a particle at the position  $\mathbf{r}$ ,  $V_{opt} = V_0 \sin^2(2\pi z/\lambda)$  is the optical lattice potential,  $\lambda$  is the light wave length,  $V_{ext}$  is an external potential such as the gravity in the Yale experiment [4] or magnetic traps [5],  $V_{int}$  includes on-site and nearest-neighbor interactions. In the case of polarized dipoles the interaction potential is  $V_{int} = d^2(1 - 3\cos^2\theta)/(\mathbf{r} - \mathbf{r}')^3 + (4\pi\hbar^2 a/m)\delta(\mathbf{r} - \mathbf{r}')$  where the first term  $V_{dd}$  is the dipole-dipole interaction characterized by the dipole  $d$  and the angle  $\theta$  between the dipole direction and the vector  $\mathbf{r} - \mathbf{r}'$ , and the second term is the short-range interaction given by the  $s$ -wave scattering length  $a$  [10].

The boson field operators of  $\Psi(\mathbf{r})$  and  $\Psi^\dagger(\mathbf{r})$  can be expanded over Wannier functions  $w(\mathbf{r} - \mathbf{r}_n)$  of the lowest energy band, localized on this site. This implies that the energies involved in the system are small compared to the excitation energies of the second band,  $\Psi(\mathbf{r}) = \sum_n C_n w(\mathbf{r} - \mathbf{r}_n)$ ,  $\Psi^\dagger(\mathbf{r}) = \sum_n C_n^\dagger w^*(\mathbf{r} - \mathbf{r}_n)$ . The Wannier functions  $w(\mathbf{r} - \mathbf{r}_n)$  are assumed to be strongly localized around the site  $n$ . It is normalized in the  $n$ th well and orthonormal with different site bands. For the weakly overlapped condensates, each BEC wave function, centered at the minima of the potential, can be expanded by the Wannier functions and using this approach, the general discrete nonlinear Schrödinger equation can be obtained for dipolar BEC in the optical lattice such as follows. If we only consider nearest-neighbor sites of  $n$  (which is a good approximation for the BEC in one-dimensional optical lattice as the large lattice constant and a similar approximation has been adopted in Ref. [8]), Eq. (1) can be expressed as

$$\begin{aligned}
H = & \sum_n [\varepsilon_0 C_n^\dagger C_n + \varepsilon_{ext} C_n^\dagger C_n + J_{nn+1} C_n^\dagger C_{n+1} + J_{nn-1} C_n^\dagger C_{n-1} \\
& + U_0 C_n^\dagger C_n^\dagger C_n C_n + U_1 (C_{n+1}^\dagger C_n^\dagger C_{n+1} C_n + C_{n-1}^\dagger C_n^\dagger C_{n-1} C_n) \\
& + U_2 C_n^\dagger C_n^\dagger (C_{n+1} + C_{n-1}) C_n], \quad (2)
\end{aligned}$$

where  $C_n$  is the annihilation operator of a particle at the lattice site  $n$ , which is considered as being in a state described by the Wannier function  $w(z-z_n)$  of the lowest energy band, localized on this site; where  $\varepsilon_0 = \int w^*(\mathbf{r}-\mathbf{r}_n) [-(\hbar^2/2m)\nabla^2 + V_{opt}] w(\mathbf{r}-\mathbf{r}_n) dz$ ,  $\varepsilon_{ext} = \int w^*(\mathbf{r}-\mathbf{r}_n) V_{ext} w(\mathbf{r}-\mathbf{r}_n) dz$ ,  $J_{nn\pm 1} = \int w^*(\mathbf{r}-\mathbf{r}_n) [-(\hbar^2/2m)\nabla^2 + V_{opt} + V_{ext}] w(\mathbf{r}-\mathbf{r}_{nn\pm 1}) dz$ , here  $\varepsilon_{ext}$  describes an energy offset of each lattice site,  $J_{nn\pm 1}$  is the hopping term which describes the nearest-neighbor tunneling, we choose  $J = -J_{nn+1} = -J_{nn-1}$ ,  $U_0 = (4\pi\hbar^2 a)/m$  is the short-range on-site interaction given by the  $s$ -wave scattering length  $a$ . When  $a > 0$  (or  $< 0$ ),  $U_0 > 0$  (or  $< 0$ ) corresponds to the repulsive (or attractive)

potential.  $U_1 = 2\langle n+1n | V_{dd} | nn+1 \rangle = 2\langle n-1n | V_{dd} | nn-1 \rangle$  and  $U_2 = 4\langle nn | V_{dd} | nn+1 \rangle = 4\langle nn | V_{dd} | nn-1 \rangle = 4\langle nn | V_{dd} | n+1n \rangle = 4\langle nn | V_{dd} | n-1n \rangle$  are the nearest-neighbor dipole-dipole interactions, where  $\langle nj | V_{dd} | lm \rangle = \int d\mathbf{r} d\mathbf{r}' w^*(\mathbf{r}-\mathbf{r}_j) V_{dd} w(\mathbf{r}'-\mathbf{r}_l) w(\mathbf{r}-\mathbf{r}_m)$ . This is a many-centers integral which represents the diagonal or nondiagonal term of dipole-dipole interaction [9]. The three and four centers integrals are small and can be neglected. For the two centers integral, the largest terms are  $\langle n+1n | V_{dd} | nn+1 \rangle$ ,  $\langle n-1n | V_{dd} | nn-1 \rangle$ ,  $\langle nn | V_{dd} | nn+1 \rangle$ , and  $\langle nn | V_{dd} | nn-1 \rangle$ , etc. The effects of the terms  $\langle n+1n | V_{dd} | nn+1 \rangle$ ,  $\langle n-1n | V_{dd} | nn-1 \rangle$  provide only the energy shift and are similar to that of the on-site interaction term. So, the terms  $\langle n+1n | V_{dd} | nn+1 \rangle$ ,  $\langle n-1n | V_{dd} | nn-1 \rangle$  can be combined with the on-site interaction term  $U_0$  when we consider the dynamics of the BEC in the optical lattice. But for the terms  $\langle nn | V_{dd} | nn+1 \rangle$  and  $\langle nn | V_{dd} | nn-1 \rangle$ , they lead to off-diagonal mixing terms which have different and important influence on the dynamics of BECs in the optical lattice as we can see from the following. Thus, in the following, we consider only the off-diagonal mixing terms for the two-centers integral.

We now consider a coherent state  $|\alpha(t)\rangle$  of the atomic matter field in a potential well [2]. Evaluating the atomic field operator  $C_n$  for such a state, we find then the macroscopic matter wave field,  $\psi_n = \langle \alpha(t) | C_n | \alpha(t) \rangle$ . Using the time-dependent variation principle, we can get the equation of motion for BEC in the optical lattice,

$$\begin{aligned}
i \frac{\partial \psi_n}{\partial t} + J \psi_{n+1} + J \psi_{n-1} - \varepsilon_n \psi_n - U_0 |\psi_n|^2 \psi_n \\
- U_{dd} (\psi_{n+1} + \psi_{n-1}) |\psi_n|^2 = 0, \quad (3)
\end{aligned}$$

where  $\varepsilon_n = \varepsilon_0 + \varepsilon_{ext}$  is the total energy of each lattice site,  $U_{dd} = U_2$  is the coefficient which denotes the dipole-dipole interaction.

Dynamics of BEC with repulsive on-site interaction ( $U_0 > 0$ ): Using the substitution  $\psi_n \rightarrow [2J/(U_0 + 2U_{dd})]^{1/2} \varphi_n \exp[-i(\varepsilon_0 - 2J + J\lambda^2)t]$ ,  $\lambda^2$  is the background

amplitude, we can obtain the following general discrete nonlinear Schrödinger equation [13]:

$$\begin{aligned}
i \frac{\partial \varphi_n}{\partial t} + (\varphi_{n+1} + \varphi_{n-1} - 2\varphi_n) - \epsilon (\varphi_{n+1} + \varphi_{n-1}) |\varphi_n|^2 \\
+ 2(\epsilon - 1) |\varphi_n|^2 \varphi_n + 2\rho^2 \varphi_n = 0, \quad (4)
\end{aligned}$$

where  $\epsilon = 2U_{dd}/(U_0 + 2U_{dd})$ ,  $\rho^2 = (\lambda^2 - \varepsilon_{ext}/J)/2$ ,  $t \rightarrow Jt$ .

When  $\epsilon = 1$ , Eq. (4) is reduced to the integrable Ablowitz-Ladik model which can be solved by the inverse scattering technique, and it leads to the so-called dark soliton solution with Bloch oscillations in a constant electric field [14]. When  $0 < \epsilon < 1$ , Eq. (4) is nonintegrable and only the approximate solution can be obtained by the multiple scale expansion method [13]. As it was shown in Ref. [13], there are singular points in Eq. (4) when  $(U_0 + 2U_{dd})/2U_{dd} = (\lambda^2 - \varepsilon_{ext}/J)/2$ . At the singular points, the dispersive term becomes zero and the given site is decoupled from its neighbors. Near these singular points or far from them, the dynamic behaviors of  $\varphi_n$  are quite different.

When the excitations are in the vicinity of the singular points, there are soliton solutions which can be described by the *Toda lattice* model and the solution of Eq. (4) in the small-amplitude limit is

$$\varphi_n = \kappa^n \epsilon^{-1/2} (1 - \gamma^2 \mu a_n) \exp(-i\gamma\chi_n + i\omega_0 t), \quad (5)$$

where  $\epsilon \ll 1$ , and  $\gamma \ll 1$  is a small parameter,  $a_n = a_n(\tau)$  and  $\chi_n = \chi_n(\tau)$  are two real functions of the time  $\tau = 2\gamma t \sqrt{2(\epsilon^{-1} - 1 + \kappa)}$ ,  $\omega_0 = 2[(\lambda^2 - \varepsilon_{ext}/J)/2 - \epsilon^{-1}]$ ,  $\mu = \kappa \operatorname{sgn}(\epsilon - 1 + \kappa)$ . Substituting Eq. (5) in Eq. (4) and gathering all the terms of orders up to  $\gamma^3$ , we arrive at the following *Toda system*:  $da_n/d\tau = a_n(c_n - c_{n-1})$ ,  $dc_n/d\tau = a_{n+1} - a_n$ , where  $c_n = \sqrt{2}[\epsilon^{-1} - 1 - \kappa](\chi_n - \chi_{n+1})$ . We can find that small-amplitude dark pulses near the singular points can be viewed as exact solitons of the Toda lattice. When  $\kappa = 1$ ,  $\mu = 1$ , the system has a stable in-phase dark soliton near the singular points. When  $\kappa = -1$ ,  $(U_0 + 2U_{dd})/2U_{dd} < 1/2$ ,  $\mu = 1$ , the system has an out-of-phase dark soliton. When  $\mu = -1$ ,  $\kappa = -1$ ,  $(U_0 + 2U_{dd})/2U_{dd} > 1/2$ , the system has an out-of-phase bright soliton. In addition, when  $(U_0 + 2U_{dd})/2U_{dd} = 1/2$ , the system will have strong dispersive character.

When the excitations are far from the singular points, the dynamics of BEC in the optical lattice can be described by the small-amplitude limit. The solution can be sought using the multiscale expansion technique [13,15]. The general concept of multiscales have wide applicability to various problems that involve phenomena that occur in relation to different scales. As the action of the nonlinear terms, there often exists various oscillations with different time scales in discrete nonlinear media. In the method of multiscale expansion applied in general discrete nonlinear Schrödinger equation [13,14], these oscillations are classified as the fast and slow processes and the corresponding variables with different time scales are introduced in an obvious way. The first step of the method of multiscale expansion is to introduce new variables  $a_n(t)$  and  $\Phi_n(t)$  related to the amplitude and phase of  $\varphi_n(t)$  as

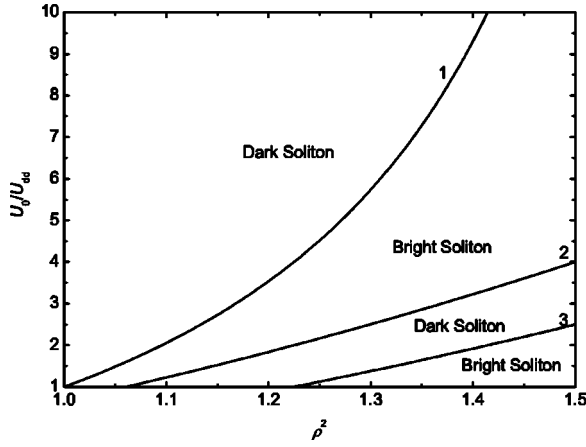


FIG. 1. The different parameter regions ( $P_1, \rho^2$ ) showing the different solitary excitations of BECs in the optical lattice, where curve 1 is  $P_1 = (8\rho^2 - 6)/(3 - \rho^2)$ , curve 2 is  $P_1 = 8\rho^2/3$ , and curve 3 is  $P_1 = 2\rho^2 - 2$ ; “dark soliton” and “bright soliton” represent regions where the dark and bright solitons exist, respectively.

$$\varphi_n(t) = [\rho + a_n(t)]e^{-i\Phi_n(t)}, \quad (6)$$

where  $a_n(t) = \gamma^2 a^{(0)}(T, X; \tau) + \gamma^4 a^{(1)}(T, X; \tau) + \dots$ ,  $\Phi_n(t) = \gamma\Phi^{(0)}(T, X; \tau) + \gamma^3\Phi^{(1)}(T, X; \tau) + \dots$ . The small parameter  $\gamma$  ( $\gamma \ll 1$ ), just introduced, is related to the smallness of the deviation  $a_n(t)$ . Besides this, the above approach assumes that the terms in the expansion are related to three different scales, i.e., the fast variables  $X = \gamma n$  of space and  $T = \gamma t$  of time. A slow variable  $\tau = \gamma^3 t$  of time. Analyzing Eq. (4) in all orders over  $\gamma$  up to  $\gamma^5$  terms, and using the compatibility condition, we can find that the leading term  $a^{(0)}$  satisfies the following KDV equation [13]:  $-4\rho\sqrt{1 - \epsilon\rho^2}(\partial a^{(0)}/\partial\tau) - \frac{1}{3}(1 - \epsilon\rho^2)[3 - (3\epsilon + 1)\rho^2](\partial^3 a^{(0)}/\partial^3 Z) + 8\rho^2(3 - 4\epsilon\rho^2)a^{(0)}(\partial a^{(0)}/\partial Z) = 0$ , and it can be written as [15]  $a^{(0)}(z, t) = -(12\nu^2 G_2/G_1)\text{sech}^2[\nu(z - V\tau)]$ , where  $\nu$  is an arbitrary parameter,  $G_1 = -\frac{1}{3}(1 - \epsilon\rho^2)[3 - (3\epsilon + 1)\rho^2]$ ,  $V = -2\nu^2 G_2/C$ ,  $G_2 = -8\rho^2(3 - 4\epsilon\rho^2)$ ,  $C = -4\rho\sqrt{1 - \epsilon\rho^2}$ . We can find the soliton solution of Eq. (4) in the small amplitude approximation,

$$\psi_n = (\rho - (12\nu^2 G_2/G_1)\text{sech}^2[\nu\{z - V(\tau)\}])e^{-i\Phi_n(t)}. \quad (7)$$

We get the following three curves with the  $J, U_0$ , and  $U_{dd}$ :  $P_1 = (8\rho^2 - 6)/(3 - \rho^2)$ , curve 1;  $P_1 = 8\rho^2/3 - 2$ , curve 2;  $P_1 = 2\rho^2 - 2$ , curve 3; where  $P_1 = U_0/U_{dd}$  represents the ratio of the nearest-neighbor interaction and on-site interaction. The above three curves divide the parameter space ( $P_1, \rho^2$ ) into four regions in which the dark and bright soliton solutions exist, as it is shown in Fig. 1. In this figure, in the region between  $P_1 > (8\rho^2 - 6)/(3 - \rho^2)$ , the  $G_1 < 0, G_2 < 0$ , the BEC in the optical lattice has dark soliton solution. When  $8\rho^2/3 - 2 < P_1 < (8\rho^2 - 6)/(3 - \rho^2)$ , the  $G_1 > 0, G_2 < 0$ , the BEC in the optical lattice has bright soliton. When  $2\rho^2 - 2 < P_1 < 8\rho^2/3 - 2$ , the  $G_1 > 0, G_2 > 0$ , the BEC in the optical lattice has dark soliton solution. When  $P_1 < 2\rho^2 - 2$ , the  $G_1 < 0, G_2 > 0$ , the BEC in the optical lattice has bright soliton solution. In addition to the above cases, the curve  $P_1 = 2\rho^2 - 2$  itself determines the amplitude of the singular points. Close to this line the dynamics of small-amplitude excitations fol-

low *Toda lattice equations*. The curve  $P_1 = 8\rho^2/3 - 2$  makes the nonlinear term become zero, and this implies that any localized pulse will spread out in the background radiation (no solitary excitations). On the other hand, the curve  $P_1 = (8\rho^2 - 6)/(3 - \rho^2)$  represents the dispersionless excitations, and this case will give shock wave soliton solutions when the nonlinearity is not zero.

Up to now, we found that for the repulsive interaction, the equation of motion of dipolar BECs has the singular points when the hopping term, the short-range on-site interaction, the long-range dipole-dipole interaction, and the external field satisfy the corresponding relations. By modifying these experimental parameters, the different types of solitons appear near or far away from these singular points.

Dynamics of BEC with attractive on-site interaction ( $U_0 < 0$ ): Without any external potential and for the small kinetic energy, Eq. (3) is reduced to

$$i\frac{\partial\psi_n}{\partial t} + (\psi_{n+1} + \psi_{n-1}) - \frac{U_0}{J}\psi_n^\dagger\psi_n\psi_n - \frac{U_{dd}}{J}(\psi_{n+1} + \psi_{n-1})\psi_n^\dagger\psi_n = 0. \quad (8)$$

Equation (8) is nonintegrable, and a first-order adiabatic approximation solution can be obtained by perturbation method. Treating the term  $\nu\psi_n|\psi_n|^2$  as a perturbation, where  $U_0 < 0, \nu = -U_0/J > 0$ , and using the adiabatic approximation, a soliton retains its functional form in the presence of perturbation [16–18], the solution to the first order of  $\nu$  can be written as

$$\psi_n = \frac{1}{\sqrt{\mu}} \sinh \beta \text{sech}[\beta(n - x)] e^{i\alpha(n-x) + i\sigma}, \quad (9)$$

where  $dx/dt = (2 \sinh \beta \sin \alpha)/\beta$ ,  $d\beta/dt = 0$ ,

$$\frac{\partial\alpha}{\partial t} = \nu \frac{\partial}{\partial x} \sum_{s=1}^{\infty} \frac{4\pi^2 s \sinh^2 \beta}{\beta^3 \sinh(\pi^2 s/\beta)} \cos(2\pi s x),$$

$$\frac{d\sigma}{dt} = 2 \cos \alpha \cos \beta + \frac{2\alpha}{\beta} \sin \alpha \sinh \beta, \quad (10)$$

where  $U_{dd} < 0, \mu = -U_{dd}/J > 0$ . This solution is a bright soliton but the role of the dipole-dipole interaction may follow from a refinement of the general consideration described above. We conclude that for the attractive interaction, the equation of motion of dipolar BECs can be treated by perturbation methods and the bright soliton solution can be found.

For observation of the above excitations, one of the possible physical realizations of a gas of dipolar BECs can be provided by electrically polarized gases of polar molecules or by applying a high dc electric field to atoms [19]. In order to induce the dipole moment of the order 0.1 D (1 D =  $3.336 \times 10^{-30}$  Cm in SI units) and the corresponding scattering length  $a_d \sim 10\text{--}100$  Å, one needs an electric field of the order of 10 V/cm and the corresponding  $s$ -wave scattering length  $\sim 10\text{--}1000$  Å. Nevertheless, the influence of dipole forces on excitation of a dipolar BEC might be in this case also observable using not as high electric fields. Another

possibility is using magnetic atomic dipoles [20–22]. For example, the chromium atoms have a magnetic moment  $\mu=6\mu_B$ , which is equivalent to an electric dipole moment of  $d=0.06$  D, and an effective scattering length  $a_d=-5$  Å. This could be enough to observe the influence of dipole-dipole interaction on the elementary excitations of chromium BEC, provided the  $s$ -wave scattering length is not anomalously large, and it takes a value in the range of a few tens of Å.

In fact, the dipole-dipole interaction leads to interesting properties and significantly modifies the ground-state and collective excitations including nonlinear solitary excitations of trapped condensates. The dipole-dipole interactions are also responsible for spontaneous polarization and spin waves in spinor condensates in optical lattices and may lead to self-bound structures in the field of a traveling wave. Sources of cold dipolar bosons include atoms or molecules with permanent magnetic or electric dipole moments. Other candidates could be atoms with electric dipoles, induced either by large dc electric fields or by optical admixing the permanent dipole moment of a low-lying Rydberg state to the atomic ground state in the presence of a moderate dc electric field. Since the interactions in a gas of dipolar bosons are easily tunable by modifying the wavelength and intensity of the lattice and by changing the magnitude of the external fields in the experiment. We can easily manifest the effect of the dipole-dipole

term for realizing various kinds of solitary excitations such as bright and dark solitons.

In summary, we found that, due to the long-range dipole-dipole interaction, the dynamics of dipolar bosons in optical lattices can be described by the general discrete nonlinear Schrödinger equation. As the long-range dipole-dipole interaction, the system of dipolar bosons in optical lattices with repulsive on-site interaction possesses singular points. In the vicinity of the singular points, the dynamics of dipolar bosons in optical lattices are described by the Toda lattice equation while away from the singular points they are described by the KDV equation. In addition we find different regions in which stable bright or dark soliton excitations will exist and on the boundaries of these regions the system becomes effectively dispersionless and the formation of shock waves becomes possible. These different excitations are observable when we modify the wavelength and intensity of the lattice and change the magnitude of the external fields in the experiment.

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