Dynamics of Narrow Bright Solitons in an Array of Attractive Atoms in a Bose-Einstein Condensate

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We study the dynamics of a narrow bright soliton in a one-dimensional lattice of condensed attractive atoms when the soliton width is comparable to the lattice spacing. If a momentum is imprinted to a stationary state, the soliton can have oscillations around a site or it can undergo a random motion along the array. The motion is very sensitive to the atomic background distribution, and a thermal cloud or quantum field fluctuations can induce a random motion of the soliton.

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In a Bose-Einstein condensate (BEC) of dilute atomic gases, the field fluctuations are small with respect to the field expectation value and a spatial coherence is present in the whole condensate. In this situation, we can replace the quantum field $\hat{\Psi}$ with a mean-field Ψ solution of the Gross-Pitaevskii equation [1]. Coherence of the BEC has been observed in many instances $[2-7]$. In a one-dimensional vertical array, coherence yields Bloch oscillations [8]. The corresponding theory is given in Ref. [9]. When the interparticle interaction is attractive, there is a competition between the atom-atom interaction and the Josephson coupling of neighboring sites of the optical lattice. The first one tends to cluster the atoms in the same well, whereas the second one tends to spread them. The minimal energy state is a bright soliton whose width decreases with the interaction strength and increases with the amount of the Josephson coupling. When the soliton width is larger than the spacing of the optical lattice, the momentum is a constant of motion [9]. Conversely, when the width is of the order of the lattice spacing, the energy varies with the packet position at the lattice periodicity [10,11] [Peierls-Nabarro potential (PN)] and the momentum is not conserved.

Here we study in detail the dynamics of a narrow soliton in an array under the tight binding approximation. We use a discrete nonlinear Schrödinger equation (DNLSE). By a rescaling of time, the DNLSE has only a free parameter, that is, the coefficient of the nonlinear term. We consider nonlinearities large enough to confine the soliton ground state within a small number of populated sites of the optical lattice. First, we consider an infinite array. At the initial time, a momentum p_0 is imprinted to a soliton with minimal energy. We find numerically the parameter region where the soliton is not able to jump the PN barrier. This region is wider than that evaluated by energetic considerations. The position of the trapped soliton can have damped oscillations or oscillations with beating. Lowering the interactions, the system goes out of the trapping region and jumps along the array sites. Near the trapping region and with an infinite array, the soliton has initially a random trajectory, but eventually it loses energy and is again captured by a site of the optical lattice. The behavior of the soliton for long times depends sensitively on the boundary conditions. During the motion, a fraction of atoms goes away from the soliton. If the number of sites is sufficiently small and there is an infinite potential at the borders, the lost atoms are reflected by the borders and perturb the dynamics of the soliton. We observe that the soliton motion is very sensitive to this background. This leads one to conjecture that a thermal atomic background or quantum field fluctuations can induce a random motion of the soliton.

A one-dimensional array can be created by the interference of two tilted laser beams. The period of the potential is $d = \lambda/[2 \sin(\theta/2)]$, where λ and θ are the wavelength and the angle between the two beams, respectively. We consider a harmonic potential $m\omega_{\perp}^2 x_{\perp}^2/2$ in the radial directions. If the nonlinear interaction is small with respect to the external potential, the radial and longitudinal coordinates are separable and the system can be described by the one-dimensional equation $i \frac{\partial \psi}{\partial \tau_0} = H_0 \psi + g |\psi|^2 \psi \equiv$ $-\frac{1}{2}$ $\frac{\partial^2 \psi}{\partial r^2} + U_0 \cos r \psi + g |\psi|^2 \psi$, where $r \equiv k_l x_{\parallel}$, $U_0 \equiv$ V_0/C_0 , $g = k_l g_{1D}/C_0$, $g_{1D} \equiv 2aN\omega_{\perp}\hbar$, and $\tau_0 \equiv C_0 t/\hbar$, with $C_0 = \hbar^2 k_l^2 / m$. Here k_l , *N*, and *a* are the wave vector of the periodic potential, the number of atoms, and the *s*-wave scattering length, respectively. ψ is normalized to 1. If $g|\psi|^2$ and its evolution frequencies are small with respect to the gap between the first and second energy bands, only the states in the first energy band contribute to the dynamics. Let ψ_k^b be the corresponding Bloch states with the property $\psi_k^b(x) = \exp(2\pi i k)\psi_k^b(x - 2\pi)$. We choose their phase such that ψ_k^b is real at the center of a choose then phase such that φ_k is real at the center of a well, and introduce the states $\chi_n = \sum_k \psi_k^k (x - 2\pi n)/\sqrt{N_s}$, N_s being the number of wells. These states are orthonormal, and we can write the wave function as a superposition of χ_k , $\psi = \sum_k \psi_k \chi_k$. From the equation of motion for ψ , we obtain the equation for ψ_k , $i\dot{\psi}_n = -\sum_k (E_k/2)\psi_{k+n}$ $g\Sigma_{klm}\psi_{k+n}^* \psi_{l+n} \psi_{m+n} \Gamma_{klm}$, where $E_k \equiv -2 \int \chi_0^* H_0 \chi_k dx$ and $\Gamma_{klm} \equiv \int \chi_0^* \chi_k^* \chi_l \chi_m dx$. For sufficiently large values

of U_0 , the functions χ_k are localized in a well and $E_k \ll E_1$ for $k \neq 0$ or 1 and $\Gamma_{klm} \ll \Gamma_{000}$ for *k*, *l*, or *m* not equal to zero. For example, at $U_0 = 0.6$ we find numerically $E_1 =$ 5.26×10^{-3} , $E_2 = -6.90 \times 10^{-5}$, $E_3 = 1.48 \times 10^{-6}$, $\Gamma_{000} = 3.20 \times 10^{-1}$, $\Gamma_{001} = -1.20 \times 10^{-3}$, $\Gamma_{011} =$ 4.04×10^{-5} , and $\Gamma_{0-11} = -2.04 \times 10^{-6}$. With $|g| \sim$ 10^{-2} , we have narrow solitons with most atoms in one or two adjacent wells. It is evident that only the terms with E_1 and Γ_{000} (tight binding approximation) contribute significantly to the dynamics. We can use the DNLSE,

$$
i\frac{\partial\psi_n}{\partial\tau} = -\frac{1}{2}[\psi_{n+1} + \psi_{n-1}] + \Lambda|\psi_n|^2\psi_n, \qquad (1)
$$

with the rescaling $\tau \equiv E_1 \tau_0$ and $\Lambda \equiv g \Gamma_{000}/E_1$. The term with E_0 gives only an energy shift and it has been omitted. The tight binding limit gives results [9] in agreement with the experiment of Ref. [8], where the soliton width is much larger than the array spacing. With narrow solitons the nonlinear interaction could populate the higher energy bands, and, in this case, the tight binding approximation would break down. In order to neglect the higher energy bands, the matrix elements of $g|\psi|^2$ between the first band states and the higher ones have to be much smaller than the energy gaps. This requirement is not incompatible with the presence of narrow solitons. Indeed, we can have narrow distributions with a sufficiently small $|g|$ merely increasing U_0 . Short solitons are present with $|\Lambda| > 1$; here we always consider $|\Lambda|$ < 4. For $U_0 = 0.6$ and $|\Lambda|$ < 4, we can eliminate adiabatically the higher energy bands. This gives quintic terms in the discrete equation whose contribution is negligible with respect to the contribution of the cubic terms. The creation of a one-dimensional condensate with attractive interaction was reported in Refs. [12,13] for a 7 Li condensate. The radial confinement was provided by a single laser beam with a wavelength of 1.064μ m. The periodic potential can be created with two tilted beams. With a lattice spacing of 2 μ m, we have C_0 = 89.2 \times 10³h. For $U_0 = 0.6$, V_0 is $0.6 \times U_0 = 47.3 \times$ $10³$ *h*. This value can be easily obtained with the setup used in the experiments. The time rescaling is $t = 2.1 \times$ $10^{-3}\tau$. With $\omega_{\perp} = 2\pi \times 800 \text{ s}^{-1}$ [12] and for $|\Lambda| = 4$, we have $N|a| \approx 2 \times 10^{-7}$. With a magnetic field of about 100 G or 600, it is possible to have a small negative scattering length [12,13]. With $a = -0.1$ nm, we have $N \approx 2000$. The number of atoms in the experiment of Ref. [13] was 6×10^3 . An even radial excitation can be created with energy $2\hbar\omega_{\perp}$. Also in this case, the radial excitations can be adiabatically eliminated and give a negligible quintic term in the discrete equation. The three-body recombination rate represents the main contribution to atom loss. With the loss rate constant reported in Ref. [14], we obtain an average loss rate γ_l of about 5 s⁻¹. This quantity can be reduced decreasing the number of atoms or increasing the array spacing and the radial dimensions. The loss rate is proportional to the square of the density; thus with 500 atoms γ_l is about 0.3 s⁻¹. With

larger spatial dimensions C_0 decreases; thus the dynamics is slower, but γ_l is much smaller and it is possible to observe the dynamics for larger τ . Furthermore, the results of Ref. [15] suggest that with the tuned scattering length $a = -0.1$ nm the three-body loss rate constant could be reduced by a factor of about 2×10^{-3} [16] with respect to the value reported in Ref. [14].

The DNLSE is invariant with respect to the transformations $\psi_n \to \psi_n^* e^{i\pi n}$ and $\Lambda \to -\Lambda$, whence the presence of soliton solutions for positive Λ (repulsive atomic interactions) at the upper edge of the energy band. The creation of a soliton with anomalous dispersion is reported in Ref. [17]. The invariance is broken when the neglected terms in the discrete equation are considered. In the following, we consider always a negative Λ and a negative scattering length.

In Ref. [9] the dynamics is studied by a variational approach with a Gaussian ansatz. If the Gaussian width is sufficiently larger than the lattice spacing, some sums over the site index can be replaced by integrals. For narrow solitons such a replacement cannot be performed and energy depends on the position [10]. The number of minimal energy states is equal to the number of sites. If $|\Lambda|$ is very large, almost all the atoms are localized at a single site. All the minimal energy solitons have the barycenter at a lattice site and they are separated by the PN barrier. The energy of ψ_n is $E = \sum_n \left[-\frac{1}{2} \psi_n^* (\psi_{n+1} + \psi_{n-1}) + \frac{\Lambda}{2} |\psi_n|^4 \right].$

Now let a momentum p_0 be imprinted onto a soliton with minimal energy. At the initial time the soliton has a symmetric distribution centered at a site and the wave function is real; we call it $\psi_n^{(m)}$. When a momentum p_0 is applied, the wave function becomes $\psi_n^{(m)} e^{ip_0 n}$. Notice that $p₀$ is adimensional. If the soliton jumps to another site, at an intermediate time its barycenter is in the middle point of two adjacent sites. Suppose that the corresponding density distribution is symmetric with respect to this point. Let $\psi_n^{(s)}$ be the state that has the minimal energy E_s among the states which are symmetric with respect to the middle point of two neighboring sites. Then, the initial energy has to be larger than E_s in order to have a jump. We have evaluated the energy of the ground states E_m and of the saddle points E_s using the imaginary time evolution method (collapse method). Starting from a function that is symmetric with respect to a site or with respect the middle point of two sites, the collapse method leads to $\psi_n^{(m)}$ or $\psi_n^{(s)}$, respectively. In Fig. 1(a) (solid line) we have reported $(\Delta E)_w/|\Lambda|$ as a function of $|\Lambda|$, where $(\Delta E)_w \equiv E_s - E_m$ is the height of the potential walls. For $\Lambda \to 0$, we have $(\Delta E)_w/|\Lambda| \to$ 0; this limit corresponds to the case of Ref. [9]. For $\Lambda \rightarrow$ $-\infty$, we have $(\Delta E)_w/|\Lambda| \rightarrow 1/4$. In this limit, the minimal energy state has all atoms at the same site and the saddle point state has them in two neighboring sites with the same population. The corresponding energies are $\Lambda/2$ and $\Lambda/4$, respectively, and $(\Delta E)_w/|\Lambda| = 1/4$.

FIG. 1. (a) $(\Delta E)_w/|\Lambda|$ (solid line) and $(\Delta E)_{p_0}/|\Lambda|$ (dashed lines), for some values of p_0 , as functions of $|\tilde{\Lambda}|$. The values of p_0 are π/n , where $n = 1, 2, 4, 8$, and 16 from right to left. The points of intersection of the dashed and dash-dotted lines give the values of Λ and p_0 for which we observe numerically the jump of the atomic density maximum. (b) Phase diagram Λ - p_0 for an infinite array. The solid line is the threshold evaluated numerically with the DNLSE; at its right the $|\Lambda|$ values yield trapping. The circles give the threshold evaluated including also the terms with E_2 , Γ_{100} , Γ_{010} , Γ_{001} , and Γ_{111} , for $U_0 = 0.6$. The dashed line is the threshold evaluated by energetic considerations. In the region between the plus symbols and the solid line, the soliton moves along the sites until it is again trapped in a site.

Let E_{p_0} be the initial energy of a soliton with momentum $p₀$. In order to have a jump between two wells, the quantity $E_{p_0} - E_m \equiv (\Delta E)_{p_0}$ must be larger than $(\Delta E)_w$. We have reported in Fig. 1(a) (dashed lines) the quantity $(\Delta E_{p_0})/|\Lambda|$ for some values of p_0 . For $|\Lambda| \le 1.5$, the PN barrier is practically negligible. The maximum energy of the soliton is obtained with $p_0 = \pi$. If $|\Lambda| > 4$, $(\Delta E)_{p_0 = \pi} < (\Delta E)_w$. Thus it is impossible to have a jump of a soliton merely by giving a momentum. Actually, we have seen numerically that the threshold for $|\Lambda|$ is overestimated. Even slightly below the threshold, the soliton is not able to jump to another site. During the motion, it loses atoms and undergoes damped oscillations inside a well. The points of intersection of the dashed and dash-dotted lines in Fig. 1(a) give the Λ and p_0 values for which we begin to observe the jump of atomic density maximum. In Fig. 1(b), we report the phase diagram Λ - p_0 . On the right of the solid line there are the values for which we do not observe jumps of the soliton. The dash line is the threshold evaluated by energetic considerations. The same threshold was reported in Ref. [18] by a variational approximation. It is given by the identity $(\Delta E)_{p_0} = (\Delta E)_{w}$. The circles give the threshold evaluated including in the discrete equation also the terms with E_2 , Γ_{100} , Γ_{010} , Γ_{001} , and Γ_{111} , with $U_0 = 0.6$. The discrepancy between the two results is very small and further reduces slightly increasing U_0 .

For $|\Lambda| > 1.5$, at the initial time more than 95% of the atoms are in three neighboring sites. If the soliton is trapped, to study its dynamics we can consider the site n_M with maximum population and the two adjacent ones. The soliton is described by three complex numbers. Since the phase is arbitrary, there are five parameters. Three parameters can be the soliton position *x*, its width σ , and the fraction of atoms N_{sol} in the three sites. Namely, $x \equiv$ $\sum'(n - n_M)|\psi_n|^2/N_{\text{sol}}, \quad \sigma = \sqrt{\sum'(n - n_M)^2|\psi_n|^2/N_{\text{sol}} - x^2}$ and $N_{\text{sol}} = \sum' |\psi_n|^2$, where Σ' is the sum over the three sites. We can write the wave function of the soliton as $\psi_n =$ $\zeta_n e^{ipn+i\delta^2 n^2/2}$ for $n = n_M - 1$, n_M , and $n_M + 1$, where ζ_n are positive numbers. The quantities p , δ , x , σ , and N_{sol} have a bijective mapping with the wave function of the soliton. We have evaluated these quantities in the region to the right of the solid line of Fig. 1(b). They undergo damped oscillations and the soliton goes into a stationary state. In contrast to the trapping effect discussed in Ref. [9], the quantity δ goes to zero and the final state is a real wave function beside a global phase factor. Near the solid line, for $p_0 < 0.5\pi$, we observe a pulsation of the position oscillations. Also the momentum *p* has a beating of the oscillations, with a phase $\pi/2$ with respect to *x*. In our simulations we have used a sufficiently high number of sites in order to neglect the boundary conditions.

To the left of the solid line in Fig. 1(b), the soliton has sufficient energy to jump to another site. Near the threshold and with an infinite array, the atomic cloud remains trapped at a site after a small number of jumps. When the momentum is increased or the nonlinear interaction is lowered, the number of jumps grows and a random trajectory in the

FIG. 2 (color online). Evolution of the atomic density distribution for $\Lambda = -2.46$ and $p_0 = 0.6\pi$ with 150 sites. We have included in the discrete equation also the terms with E_2 , Γ_{100} , Γ_{010} , Γ_{001} , and Γ_{111} , with $U_0 = 0.6$.

FIG. 3 (color online). The same as in Fig. 2, but with (a) 250 and (b) 500 sites.

array appears. This motion is damped, and eventually the soliton is again trapped on a site. Sufficiently far from the solid line, the random trajectory is replaced by one with decreasing velocity, until the soliton reaches constant speed (averaged over the lattice spacing) or stops again at a site. In Fig. 1(b) we denote with $+$ symbols some values of Λ and p_0 which give a motion with subsequent trapping in a time of $t = 800$. The values of Λ between the + symbols and the solid line give a final trapped soliton. By decreasing $|\Lambda|$, the time with motion grows.

Figure 2 reports the space-time evolution of the density distribution for $\Lambda = -2.46$ and $p_0 = 0.6\pi$, for 150 sites. We have integrated the discrete equation including also the terms with E_2 , Γ_{100} , Γ_{010} , Γ_{001} , and Γ_{111} , with $U_0 = 0.6$. The density is represented in logarithmic scale in order to magnify the background atomic distribution. The largest fraction of atoms is lost at the initial stage of motion. Almost all of them move in the direction opposite to the soliton. The escaped atoms are reflected by the end caps and hit the soliton at $t \sim 200$. Notice that the end caps can be realized by off-resonant lasers [12]. This atomic background distribution perturbs the soliton and sustains the random motion for long times. The number of atoms in the soliton fluctuates, but after a transient of $\Delta t \sim 25$ its average does not decrease during the evolution. The trajectory is very sensitive to the initial conditions. It changes also with a variation of 0.1% of the momentum. In Fig. 3 we report the same distribution, but with (a) 250 and (b) 500 sites. It is evident that a small background has important effects of the soliton dynamics. The density of the lost atoms is less than 1%. Note that at $t \sim 300$ in Fig. 3(a) the background induces a soliton motion opposite to the background direction. The soliton behaves as a particle with negative mass. In our simulations the background is produced during the motion, but at finite temperature also a thermal cloud is present. Our simulations suggest that this cloud can have important effects on the dynamics. Furthermore, with a sufficiently small number of atoms in the soliton, quantum fluctuations could be relevant and induce a random walk of the soliton.

In conclusion, for a narrow soliton in a one-dimensional array with an initial momentum, we have found a parameter region where it is trapped on a site. Energetic considerations overestimate the threshold of the interaction strength above which there is trapping. Near the threshold, the soliton position undergoes oscillations with pulsations. Below the threshold, the soliton has sufficient energy to jump to other sites. In a region of the parameter space, the soliton has a random motion on the array, until it is again captured by a site at a finite time. A small background distribution can sustain the motion preventing the soliton from being captured at a site. Our results lead one to conjecture that at finite temperature the thermal background can induce a random motion of a soliton. It would be interesting to study this temperature-induced diffusion of the barycenter. Even at very low temperatures and for a sufficiently small number of atoms, a diffusion could be given by quantum fluctuations of the field. This would be analogous to the macroscopic quantum tunneling of a collective variable [19].

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