

## Rise and Fall of a Bright Soliton in an Optical Lattice

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We study an ultracold atomic gas with attractive interactions in a one-dimensional optical lattice. We find that its excitation spectrum displays a quantum soliton band, corresponding to  $N$ -particle bound states, and a continuum band of other, mostly extended, states. For a system of a finite size, the two branches are degenerate in energy for weak interactions, while a gap opens above a threshold value of the interaction strength. We find that the interplay between degenerate extended and bound states has important consequences for both static and dynamical properties of the system. In particular, the solitonic states turn out to be protected from spatial perturbations and random disorder. We discuss how such dynamics implies that our system effectively provides an example of a quantum many-body system that, with the variation of the bosonic lattice filling, crosses over from integrable nonergodic to nonintegrable ergodic dynamics, through nonintegrable-nonergodic regimes.

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*Introduction and summary of the results.*—Solitary waves in classical fluids may arise when wave dispersion effects are compensated by nonlinear interactions [1]. The study of their mathematical properties has defined important areas in mathematical research [2–4], with far reaching implications for pure and applied modern science [5–9]. Although quantum mechanics is an intrinsically linear theory, solitons may emerge also in quantum fluids: in this case, nonlinearities arise as a result of effective cooperative phenomena occurring in quantum-many-particle systems. Indeed, solitons were demonstrated to emerge in different quantum-mechanical contexts, ranging from quantum material science to particle physics [10–15].

In this work, we are primarily motivated by the recent investigations in quantum fluids as provided by ultracold atoms trapped in one-dimensional optical potentials. In these systems, bright solitons may emerge for attractive atom-atom interactions [3] (see also Ref. [16]) and they have been observed in several experiments [17–20]. From a conceptual point of view, however, bosonic systems with attractive interactions must be treated with care: because of the Bose statistics, the lowest energy state can be macroscopically occupied with a density that is *magnified* by interactions. Important progress has been achieved describing the bosonic fluid through a famous integrable theory as proposed by the Lieb-Liniger model, which is amenable to

an exact analysis [21]. Relying on that, it was demonstrated that the ground state energy may display instabilities that can be nonetheless cured by a suitable choice of interactions and density [22]. Indeed, the limits of vanishing interaction with a finite density, leading to mean-field results for a large number of bosons [23], or of vanishing density with finite interactions [24], have been thoroughly explored. In particular, by analyzing the solutions of the mean-field Gross-Pitaevskii equation it was found [25,26] that a critical value of the attraction exists for which the ground state density undergoes to a transition from a uniform profile to a bright-soliton-type one (as implied by the onset of modulational instabilities in the condensate). In the same limit, it was exactly demonstrated using the Bethe-ansatz solution that density-density and higher-order correlation functions display a qualitative change of behavior in correspondence to the critical value predicted by the mean-field theory.

In this work we focus on a bosonic system described by the Bose-Hubbard model (BHM) [27,28] (1) confined in a one-dimensional lattice, where density and interactions strength are *both* finite. We perform a numerical study of energy bands and quantum correlations using the density matrix renormalization group (DMRG) method [29–33]. Among different aspects implied by the lattice, here we exploit the energy-band structure of the system, featuring

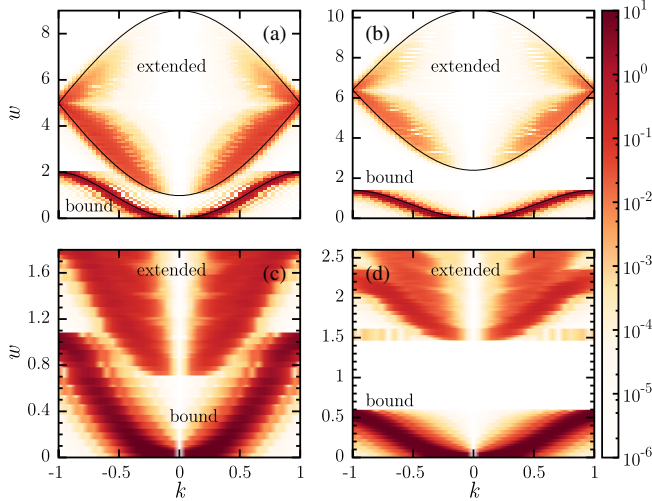


FIG. 1. Dynamical structure factor  $S(k, \omega)$  for a chain of  $L = 30$  sites. Upper row: analytical results for  $N = 2$  particles for  $U = 2 < U_c$  (a) and  $U = 5 > U_c$  (b). The black lines, obtained from the exact solution for  $N = 2$ , outline two bands of bound (lower) and scattering (upper) states [39,40]. Lower row:  $S(k, \omega)$ , numerical results for  $N = 5$  particles. In panels (c) and (d) interaction are set to  $U = 0.75 < U_c$  and  $U = 1.2 > U_c$ , respectively.

characteristic bendings, foldings, and energy gaps. Such effects can indeed define new physical regimes in our system with peculiar bound states of solitonic type (see Refs. [34–36]).

For finite attractive interactions we find that  $N$ -body bound states are formed; for weak interactions, however, these bound states are degenerate with a second band of other states, mostly extended or involving lower-order bound states. By increasing the interaction strength, the bound states get more and more energetically favorable, until a critical interaction strength  $U_c$  for which the band of bound states is completely separated by an energy gap from the rest of the spectrum.

The calculation of the dynamical structure factor, which is defined below by Eq. (2), provides the portrait of the band structure of the system, displaying a two-branch dispersion at low energies as shown in Fig. 1. Such quantity is experimentally detectable by means in ultracold-atom experiments by Bragg scattering methods [37,38]. We characterize the nature of ground and excited states in the spectrum by monitoring the density-density correlations functions, which display a different spatial behavior for extended and  $N$ -particle bound states, see Fig. 2.

The changing of band structure and the opening of a gap, which follows the variation of the interaction, has important consequences for the dynamics of the system. We devise a protocol in which we prepare a quantum soliton in the middle of the chain and then we let it expand under the guidance of Hamiltonian (1). For  $U = 0$  only extended states are naturally available in the dynamics; for  $0 < U < U_c$  the extended and bound states are available; for  $U > U_c$ , at low energies,

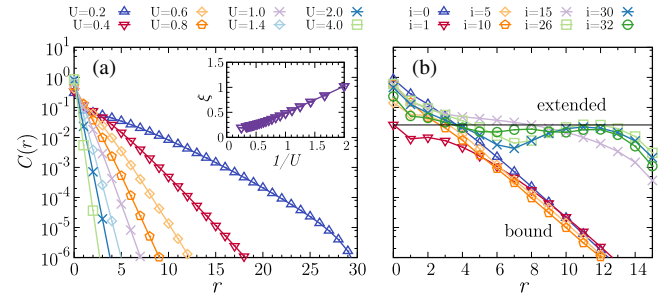


FIG. 2. Density-density correlation function  $C(r)$  for  $N = 5$  particles in a chain of  $L = 61$  sites. Panel (a):  $C(r)$  for the ground state as a function of  $U$ . Inset: the correlation length  $\xi$ . Panel (b):  $C(r)$  calculated over several excited states for  $U = 0.6 < U_c$ ,  $i$  labels the  $i$ th excited state ( $i = 0$  correspond to the ground state) for a chain of  $L = 30$  sites.

solely bound states exist. As a striking feature, in this latter regime the density keeps more and more the localized shape of the initial state and only a small fraction of the state spreads over the lattice. The crossover between the two regimes is purely mesoscopic since  $U_c$  scales like the inverse of the number of particles (see Supplemental Material [41]). We note that the expansion velocity experiences a crossover from a large value for  $U < U_c$  to a smaller value for  $U > U_c$ . These features, that have been predicted for two particles [39], clearly emerge in Fig. 4. Even though no quantum phase transition occurs in the system, we find that the expansion velocity close to  $U_c$  displays a universal scaling. Such a feature illustrates the subtle interplay between interactions and particle number in the dynamics of attractive bosons in a lattice.

We also find that the occurrence of degenerate scattering and bound states in the spectrum implies nontrivial time evolution of correlations: the large-distance asymptotic density-density correlations are not a function solely of the energy, but they strongly depend on the choice of the initial state. Indeed, not even a random perturbation is able to turn the time asymptotics of solitonic bound states into those of scattering states, see Fig. 3. Such a result indicates

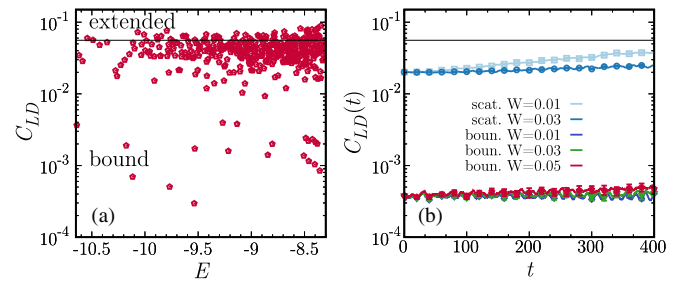


FIG. 3. Panel (a): expectation of  $C_{LD}$  for several eigenstates  $\phi_n$  as a function of their energy  $E$ , for  $N = 5$  particles in a chain of  $L = 21$  sites. Interaction is set to  $U = 0.5 < U_c$ . The black line at  $C_{LD} = (N/L)^2 \approx 0.056$  is a guide to the eye. Panel (b): time evolution of  $C_{LD}$ , from scattering or bound state with adjacent energy eigenvalues.

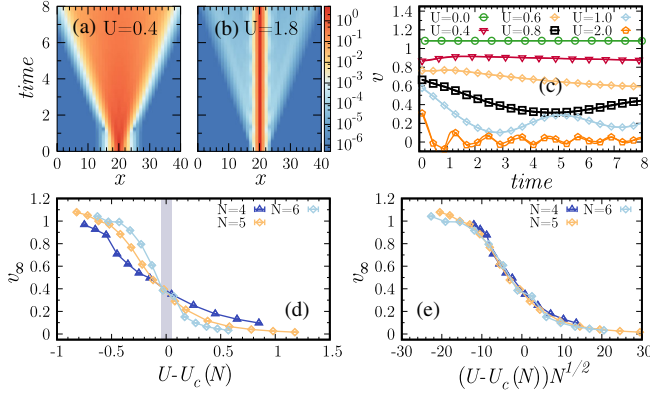


FIG. 4. Upper row (a)–(b): expansion of a soliton composed by  $N = 5$  particles, pinned to the center of a chain with  $L = 41$  sites for different regimes. Panel (c): expansion velocity  $v(t)$  for different interaction strengths. The black line divides the gapless (upper) regions from the gapped (lower) ones. Panel (d)–(e): asymptotic expansion velocity  $v_\infty$  as a function of  $U - U_c(N)$  and of  $[U - U_c(N)]\sqrt{N}$ .

that bright solitons in the lattice are robust to external perturbations. This specific lack of ergodicity has implications at a fundamental level to study the interplay between thermalization and integrability, see Fig. 5.

*The model.*—We employ the BHM describing  $N$  interacting bosons in a one-dimensional lattice. The Hamiltonian reads

$$\hat{H} = -J \sum_{j=1}^L (a_j^\dagger a_{j+1} + \text{h.c.}) - \frac{U}{2} \sum_{j=1}^L \hat{n}_j (\hat{n}_j - 1), \quad (1)$$

where the operators  $n_i = a_i^\dagger a_i$  count the number of bosons at site  $i$ ; the operators  $a_i, a_i^\dagger$  obey the canonical commutation relations  $[a_i, a_j^\dagger] = \delta_{ij}$ , and  $L$  is the number of sites. The parameters  $J, U$  in Eq. (1) are the hopping amplitude and the strength of the on-site interaction, respectively. Throughout this Letter, we consider only attractive interactions; both energies and the parameter  $U$  are in units of  $J$ . Times are in units of  $\hbar/J$ . Equation (1) describes a closed system and therefore it neglects three-body losses. We will also always (unless stated otherwise) consider open boundary conditions:  $a_1^\dagger a_L = a_L^\dagger a_1 = 0$ . The BHM (1) is not

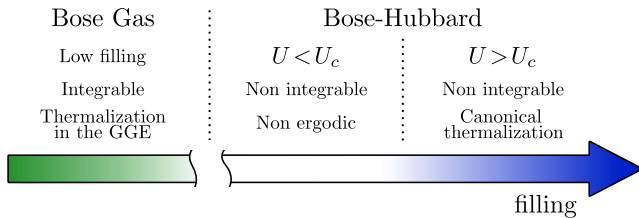


FIG. 5. Schematic diagram of the system as a function of the filling at varying interaction strength.

solvable by the coordinate Bethe ansatz. The failure results because of finite probabilities that a given site is occupied by more than two particles, whose interaction cannot be factorized in terms of two-body scattering [45–47]. Nevertheless, the plane-wave ansatz of the coordinate Bethe ansatz works well in the so-called two-particle sector, for which such probabilities are vanishing [39,40]. Despite the fact that the BHM is not integrable, its continuous limit is the Bose-gas integrable field theory [48] (see Supplemental Material [41]). We note that a similar logic works also for discretization for the classical nonlinear-Schrödinger equation [49].

*Bound versus scattering states.*—Information on the available excitations in the system as a function of their momentum  $k$  and energy  $\omega$  is provided by the dynamical structure factor  $S(k, \omega)$ :

$$S(k, \omega) = \sum_{\alpha \neq 0} \sum_r |\langle \alpha | e^{-ikr} \hat{n}_r | 0 \rangle|^2 \delta(\omega - \omega_\alpha), \quad (2)$$

where  $\hat{n}_r$  is the number operator acting on the site  $r$ ,  $|0\rangle$  is the ground state, and  $\alpha$  labels the states with increasing energy (i.e.,  $\alpha = 1$  is the first excited state). The peaks of  $S(k, \omega)$  reconstruct the energy bands of the system [50,51]. We observe that for small  $U$  a low-energy band separates from the rest of the spectrum. Corroborated by the exact results obtained for the BHM in the two-particle [39,40] and three-particle [50,51] sectors (see Supplemental Material [41]), we conclude that for a general number of particles the lower band is always made of  $L$  bound states. Such a conclusion is further supported by the study of correlation functions presented below. Remarkably, because of the lattice bending of the energy bands, we observe that for  $U < U_c$  the two bands of bound and extended states are partially overlapping [see Figs. 1(a), 1(c)]. For  $U > U_c$  the two bands are fully separated by an energy gap which linearly grows with the interaction strength [see Figs. 1(b), 1(d)]. Further details on  $U_c$  and a full study of the energy bands can be found in the Supplemental Material [41]. We point out that the regime of degeneracy between extended and bound states cannot be captured by either mean-field or continuous Lieb-Liniger model since both theories describe the solitonic states with a single parameter (the interaction  $U$ ), without reference to any specific feature of the energy bands.

In order to characterize bound states, we study the density-density correlation function (the system being translationally invariant, the density itself does not display fruitful features):  $C(r) = \langle n_{L/2} n_{L/2+r} \rangle$ . From our numerical analysis we confirm that the ground state is a bound state:  $C(r) \sim \exp(-r/\xi)$  with correlation length  $\xi$  decreasing with increasing  $U$ —Fig. 2(a). For excited states, the lowest excitation branch is, indeed, made of bound states characterized by  $C(r)$  decaying exponentially with a single  $\xi$  depending solely on  $U$ . On the other hand, for states



belonging to the second branch, at intermediate distances,  $C(r)$  approaches a plateau  $\sim n_{as} = (N/L)^2$ , before dropping down when approaching the walls of the box. We thus can conclude that the higher branch contains extended states. This strong difference in the correlations in the two bands can be quantified by studying the density-density correlations at large distance, as defined by the correlator  $C^{\text{LD}} = \sum_{i=2}^{L/4} C(i)/\mathcal{N}$ , where  $\mathcal{N}$  is the number of sites over which this function has its support. While for scattering states  $C^{\text{LD}} \approx n_{as}$ , see Fig. 2(c), for bound states the magnitude of the correlations is several orders of magnitude smaller because of the faster decay of the corresponding  $C(r)$ . Such a feature provides a clear indicator of the nature of the states (extended or bound).

We proceed to study the stability of these states through a suitable dynamical protocol. Specifically, we address the evolution of bound and scattering excited states,  $|\psi^B\rangle$  and  $|\psi^S\rangle$ , respectively, with adjacent energy eigenvalues in the spectrum for  $U < U_c$ , after having perturbed the system by adding a random-noise source in it. The dynamics is then governed by a Hamiltonian which depends both on the interaction strength  $U$  and on the intensity of the perturbation,  $W$ :  $\mathcal{H}(W, U) = \mathcal{H}(U) + \sum_i \epsilon_i n_i$ , where  $\epsilon_i$  is a random variable chosen uniformly in the interval  $[-W, +W]$ . In Fig. 3(b) we note that (within the time scale available in our numerical simulations)  $C^{\text{LD}}(t)$  remains almost constant in the course of the evolution, meaning that bound and scattering states are not mixed by random disorder. This is a strong evidence, on the timescale considered, of the soliton stability and robustness.

*Dynamical expansion of pinned solitons.*—Finally, we devise a specific dynamical protocol to evidence the features of the band structure shown in Fig. 1.

A soliton is pinned in a given site  $i_0$  of the lattice, by initially breaking the lattice translational symmetry with an attractive potential  $\mathcal{H}_i(\mu, U) = \mathcal{H}(U) + \mu(U)n_{i_0}$ , and then let it expand. The pinning energy  $\mu(U)$  is chosen such that the energy injected in the system by the perturbation is equal to the width of the bound-state band (see Supplemental Material [41]). In this way, while for small  $U$  we populate both scattering and bound states, for  $U > U_c$  when the gap separates the two bands, mostly bound states are populated.

The dynamical evolution is governed by  $\mathcal{H}(U)$  obtained by removing the pinning potential. In Figs. 4(a)–4(c) we show the expansion dynamics of the density for three cases:  $U < U_c$ ,  $U \approx U_c$ , and  $U > U_c$ . Increasing the interaction strength, we see that the density profile stays closer and closer to the shape of the initial state, only its small fraction spreading into the chain. This can be seen more quantitatively by studying the expansion velocity:  $v(t) = (d/dt)\sqrt{R^2(t) - R^2(0)}$ , with  $R^2(t) = (1/N)\sum_{i=1}^L n_i(t)(i - i_0)^2$ . In Figs. 4(d)–4(e) we show, respectively,  $v(t)$  and its asymptotic value  $v_\infty$  at large times.

While for  $U < U_c$  no oscillations are visible within the simulation time considered, at increasing  $U \geq U_c$  the velocity displays typical oscillations with period scaling as  $\hbar/U$ .

The asymptotic expansion velocity  $v_\infty$  is identified by fitting it to a phenomenological expression,  $v(t) \approx v_\infty + \cos(At)/t^B$ , where  $A$  and  $B$  are fitting parameters. The inspection of  $v_\infty$  in Fig. 4(e) further shows the difference between the two regimes.

Interestingly enough, close to  $U_c$ , we find that  $v_\infty$  displays scaling behavior; the results are not affected by the size of the system. While there is no criticality in the system, the observed feature is due to a diverging timescale associated with the soliton thermalization: as critical slowing down implies scaling, here, the scaling is due to the fact that the soliton cannot equilibrate to the state with uniform density.

*Conclusions.*—In this work, we studied the spatial correlations and dynamical properties of attractive bosons in one-dimensional lattices. The presence of the lattice induces a characteristic energy band structure, for which bright solitons display specific properties with distinctive correlation functions. Such features can affect the dynamics of the system substantially. We have demonstrated how a bright solitonic bound state can be created in the system and, by studying the expansion dynamics, we have provided a way to test its stability against external perturbations.

Our work can be relevant for fundamental studies on the ergodicity of quantum systems. Thermalization in quantum many-body systems is usually expressed in terms of the well-known eigenstates thermalization hypothesis (ETH) [52,53]: if the expectation values of local observables for individual eigenstates are a smooth function of energy, then the system behaves ergodically and one can replace, for such observable, the long-time average by the Gibbs ensemble average with no memory of the specific initial state except its energy. The bimodal distribution of correlations in Figs. 3(a) and 3(b) with coexistence, for  $U < U_c$ , of the two families of states at the same energy leads to a clear violation of the ETH. Our understanding of the system can be summarized in Fig. 5, where three regimes may occur.

(I) Since lattice spacing  $\Delta$  results to be vanishing proportionally to the filling factor  $\nu = N/L$ , at sufficiently small  $\nu$ , our bosonic system is integrable (described by the Bose-gas field theory [48,54]). According to the general theory, in this limit the system is expected to thermalize to a generalized Gibbs ensemble. (II) By increasing the filling factor, the system does not remain integrable, being described by the Bose-Hubbard model. For such system, when bound states and scattering states coexist with equal energies (i.e., for  $U < U_c$ ), the long-times asymptotic states strongly depend on the initial states. (III) At larger filling, the system is far from integrability, as the Bose-Hubbard corrections to the

Bose gas grow stronger. In this case, the solitonic band is nearly flat, making the coexistence between bound and scattering states impossible. In this limit, therefore, the system is ergodic. Such a scenario indicates that going from (I) to (III), the integrability, controlled by the filling (instead of the perturbation added to the Hamiltonian, in the framework of more standard approaches), is destroyed by entering an intermediate regime, in which the system keeps some trace of integrability in that the dynamics is not ergodic. In this sense then, we contribute to the search of a quantum analog of the KAM theorem [55] which is one of the key challenges in contemporary research (see Refs. [56–58]). We note that the scenario emerging in our work is in line with the findings of Rigol [59]. As a follow up of the present study, it would be interesting to study whether more complex bound states and observables at higher energies can provide different types of intermediate thermalizations.

We believe that our analysis is within the current activity in atomic physics quantum technology. Ultracold atoms with tunable interactions have been already loaded in one-dimensional optical lattices in several experiments [60–63]. A specific protocol allowing us to address bound and scattering states selectively at a given mean energy can be implemented by quenching the interaction from repulsion or attraction and evolving with the target Hamiltonian. Atomtronic circuits can also provide appropriate tools to explore the dynamics of the system [64–67].

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