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Localization of Bose-Einstein condensates in optical lattices

Research Article

Roberto Franzosi[1,2*], Salvatore M. Giampaolo[3,4], Fabrizio Illuminati[3,4], Roberto Livi[5], Gian-Luca Oppo[6], Antonio Politi[7]

1 *C.N.I.S.M. UdR di Firenze, Dipartimento di Fisica, Università degli Studi di Firenze, Via Sansone 1, I-50019 Sesto Fiorentino, Italy*

2 *I.P.S.I.A. C. Cennini, Via dei Mille 12/a, I-53034 Colle di Val d'Elsa (SI), Italy*

3 *Dipartimento di Matematica e Informatica, Università degli Studi di Salerno, Via Ponte don Melillo, I-84084 Fisciano (SA), Italy*

4 *INFN Sez. di Napoli, Gruppo collegato di Salerno, Via Ponte don Melillo, I-84084 Fisciano (SA), Italy*

5 *Dipartimento di Fisica, Università di Firenze and INFN, Sez. di Firenze, Via G. Sansone 1 Sesto Fiorentino, I-50019, Italy*

6 *Department of Physics, University of Strathclyde, 107 Rottenrow, Glasgow G4 ONG, Scotland, U.K.*

7 *Istituto dei Sistemi Complessi, Consiglio Nazionale delle Ricerche, Via Madonna del Piano 10 Sesto Fiorentino, I-50019, Italy*

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Abstract: The dynamics of repulsive bosons condensed in an optical lattice is effectively described by the Bose-Hubbard model. The classical limit of this model, reproduces the dynamics of Bose-Einstein condensates, in a periodic potential, and in the superfluid regime. Such dynamics is governed by a discrete nonlinear Schrödinger equation. Several papers, addressing the study of the discrete nonlinear Schrödinger dynamics, have predicted the spontaneous generation of (classical) breathers in coupled condensates. In the present contribute, we shall focus on localized solutions (quantum breathers) of the full Bose-Hubbard model. We will show that solutions exponentially localized in space and periodic in time exist also in absence of randomness. Thus, this kind of states, reproduce a novel quantum localization phenomenon due to the interplay between bounded energy spectrum and non-linearity.

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*E-mail: franzosi@fi.infn.it

1. Introduction

Localization of atoms in optical lattices is among the macroscopic quantum-effects that have been theoretically studied and experimentally observed in Bose-Einstein condensates (BECs). Localized states of BECs along an optical lattice are the consequence of the nonlinear character of the classical equations of motion of these systems. These kinds of solutions have been predicted on the bases of the analogy between the Gross-Pitaevskii equation, that describe the superfluid (classical) dynamics of BECs, and the nonlinear Schrödinger equation used in nonlinear optics [1–8]. In continuous-space models the localized solution have the form of gap solitons and matter-wave solitons [5–7]. While in nonlinear classical lattice-Hamiltonians, solutions have the form of discrete breathers. The latter are, in fact, periodic in time, and exponentially localized in space, solutions distinctive of nonlinear discrete systems. The superfluid regime for a system of BECs in an optical lattice is described by a discrete nonlinear Schrödinger equation (DNSE). In recent papers [23, 24], by numerically integrating the DNSE, the spontaneous generation of breathers in BECs in optical lattices were predicted. In particular, in [23] a technique to obtain localization of BECs by means of boundary dissipations, that is by removing atoms at the optical lattice ends, was presented.

The present paper focuses on exact (numeric) localized solutions of the full (quantum) Bose-Hubbard model (BHM). We show that the solutions are energy-eigenstates and are exponentially localized in space and periodic in time. Furthermore, we proceed by a dynamic variational method in order to determine an analytic approximation to the maximally excited state. We compare the results derived with those obtained by exact diagonalization. In order to derive such analytic approximation, we follow the route adopted in previous papers [25, 26], by introducing a macroscopic trial state of the form $e^{iS/\hbar}|x\rangle$, where S is a time-dependent phase and $|x\rangle$ is an SU(M) coherent state. The requirement that the trial state satisfies the Schrödinger equation, on average, means that S is an effective action. By a variational on S, one can derive an approximation to the maximally excited energy eigenstate of the system. By comparing the atomic density distribution of the approximate state with the one of the exact solution we show that, in a wide range of the Hamiltonian parameters, the approximated state (named semiclassical solution) provides an excellent approximation to the exact maximally excited state.

Quantum localized states in a BHM of repulsive atoms, can be realized by virtue of the combination of two features of this Hamiltonian: it has a non-linear dependence from the site occupation number operators and it has a bounded energy spectrum. The last condition, in fact, guarantees the existence of an upper-bounded energy spectrum with spatially bounded states. Whereas the first property makes it possible to have a perceptible separation in the energy spectrum between the higher levels. A further important aspect is the lack of invariance for spatial system translation. The open boundary conditions make the central lattice site, where the states localize, special. Thus, finite-size systems are required in order to observe a finite energy separation between the maximum Hamiltonian-eigenstate and the others. When translational symmetry is preserved, as would be the case for periodic boundary conditions, no localized states can be realized. In fact, the symmetry makes all of the Hamiltonian-eigenstates, that differ for cyclic permutation of the site indices, degenerate. Thereby, a maximum energy eigenstate will be a generic superposition of all these states, since there is not reason to favor any of them over others. It is characterized by a flat distribution of the atomic density along the lattice. We will show in the following sections that, for finite lattice size and a wide range of values of the non-linear parameter, the highest-energy levels of the repulsive-BHM are characterized by a level (with maximum energy) separated by the quasi-degenerate multiplet of the close lower levels.

2. Bose-Einstein condensates in an optical lattice

The second-quantized Hamiltonian

$$\hat{H} = \int d\mathbf{r}\hat{\psi}^{+}(\mathbf{r})\left[-\frac{\hbar^2}{2m}\nabla^2 + V_{ext}(\mathbf{r})\right]\hat{\psi}(\mathbf{r}) + \frac{4\pi\hbar^2 a_s}{2m}\int d\mathbf{r}\hat{\psi}^{+}(\mathbf{r})\hat{\psi}^{+}(\mathbf{r})\hat{\psi}(\mathbf{r})\hat{\psi}(\mathbf{r}) \tag{1}$$

describes the quantum dynamics of an ultracold dilute gas of bosonic atoms. Here V_{ext} is the external trapping potential and the boson-field operators $\hat{\psi}(\mathbf{r})$ ($\hat{\psi}^{+}(\mathbf{r})$) annihilate (create) atoms at $\mathbf{r} = (r_x, r_y, r_z)$ in a given internal state. The nonlinear self-interaction term depends on the s-wave scattering length a_s and on the atomic mass m. We consider repulsive atoms, i.e. $a_s > 0$. In the case of a one-dimensional optical lattices, the external trapping potential reads

$$V_{ext}(\mathbf{r}) = \hbar^2\omega^2 \sin^2\frac{k_L r_x}{4E_r} + m\Omega^2\frac{r_y^2 + r_z^2}{2},$$

where k_L is the laser mode which traps the atoms and

$$E_r = \frac{\hbar^2 k_L^2}{2m}$$

is the recoil energy. In the x-direction one has an optical lattice structure of length L, while the trapping frequency Ω is assumed to be strong enough to confine the atomic condensate in the y and z directions by harmonic wells. Thus, the physics is effectively one-dimensional.

In the presence of a periodic external potential, we can derive from (1) an effective quantum (Bose-Hubbard) Hamiltonian that describes, within the second quantization formalism, the boson dynamics along the optical lattice. In order to derive this effective dynamics we follow Ref. [14]. Since the one-dimensional potential V_{ext} is periodic, the "single atom" eigenstates of Hamiltonian in Eq. (1) are Bloch functions [14] $\Phi_q^{(n)}(\mathbf{r})$, labelled by the quasi-momentum q and the band index n. Already for shallow optical potentials, that is for values of $\frac{\hbar^2\omega^2}{4E_r}$ of the order of a few (~ 5) recoil energies E_r, the energy separation between the two lowest bands is much larger than their spread (see [13]). In Ref. [13] it is also shown that, for moderate optical potential depths, a good approximation for the lowest energy gap is given by $\hbar\omega$, where ω is the longitudinal oscillation frequency of a particle trapped in the harmonic approximation of the potential V_{ext} close to a minimum. As done in [14], let us assume that only the fundamental energy band is involved into the dynamics and we describe the system using Wannier functions. Kohn, in [15], has shown that, by properly choosing the branch points of the Bloch's functions, for each band there exists one and only one Wannier function that is real and decays exponentially with the distance. The lowest-band Wannier functions $u_j(\mathbf{r})$ defined by Kohn in Ref. [15], are localized at the minima $(x_j, 0, 0)$ of the optical potential, where

$$x_j = \frac{j\pi}{k_L}, \quad j = 1, \ldots, M$$

and

$$M = L \times \frac{k_L}{\pi},$$

and result to be

$$u_j(\mathbf{r}) = W^{-\frac{1}{2}} \sum_q e^{-iqx_j} \Phi_q^{(0)}(\mathbf{r}),$$

where W is a normalization constant. We express the field operators as (see [14])

$$\hat{\psi}(\mathbf{r}, t) = \sum_{j=1}^{M} u_j^*(\mathbf{r}) \hat{a}_j(t), \tag{2}$$

where the boson operator $\hat{a}_j$ ($\hat{a}_j^+$) destroys (creates) an atom at the lattice site j.

By substituting Eq. (2) into Eq. (1) we obtain

$$H = \sum_{jklm} U_{jklm} \hat{a}_j^\dagger \hat{a}_k^\dagger \hat{a}_l \hat{a}_m - \frac{1}{2} \sum_{jk} T_{jk} a_j^\dagger \hat{a}_k,$$

where

$$U_{jklm} = \frac{4\pi\hbar^2 a_s}{2m} \int d\mathbf{r} u_j^*(\mathbf{r}) u_k^*(\mathbf{r}) u_l(\mathbf{r}) u_m(\mathbf{r})$$

is the strength of the on-site interaction and

$$T_{jk} = -2 \int d\mathbf{r} u_j^* \left[\frac{\mathbf{p}^2}{2m} + V_{ext} \right] u_k$$

is the hopping amplitude. Already for moderate optical potential depth

$$\frac{\hbar^2\omega^2}{4E_r^2} \gtrsim 5,$$

the numerical values of the off-diagonal elements of the interaction matrix U_{jklm} and the tunneling matrix T_{jk} between sites (other than nearest neighbors) are negligible with respect to $U_{jjjj} \equiv U$ and $T_{jj+1} = T_{j+1j} \equiv T$ respectively (see Ref. [13]). Thus, one obtains the effective one-dimensional M-site Bose-Hubbard Hamiltonian

$$H = \sum_{j=1}^{M} \left[U n_j (n_j - 1) + \xi_j n_j \right] - \frac{T}{2} \sum_{j=1}^{M-1} \left(a_j^+ a_{j+1} + \text{h.c.} \right), \tag{3}$$

where the boson operators satisfy the boson commutation relations $[\hat{a}_k, \hat{a}_j^+] = \delta_{k,j}$.

3. Classical dynamics in the SU(M) coherent states picture

Originally introduced in order to describe the superfluid/Mott-insulator transition in lattice systems [12], the Bose-Hubbard model is nowadays used to describe the dynamics of systems of cold bosonic-atoms on an optical lattice [13]. In Ref. [14] it has been predicted, and then experimentally verified in [16], that the dynamics of an ultracold dilute gas of bosonic atoms in an optical-lattice/periodic-potential is well described by the Bose-Hubbard model.

Hamiltonian in Eq. (3) commutes with $\hat{N} = \sum_k \hat{n}_k$ and can be expressed in terms of the set of operators $\hat{E}_{kr} = \hat{a}_k^\dagger \hat{a}_r$ which, in turn, give a dimension-independent realization of the SU(M) algebra. Thus, one can choose an irreducible unitary representation of the SU(M) (Lie-)algebra with

the same dimension of the space spanned by the system's states:

$$D(M,N) = \frac{(M+N-1)!}{[N!(M-1)!]}.$$

This fact suggest to describe the system dynamics in terms of SU(M) generalized coherent states. Of course, being H a quadratic form of operators $\hat{E}_{kr}$, this description is exact only in the superfluid ($\Lambda \to 0$) limit where the linear dependence is recovered. Nevertheless, a description in terms of coherent states, permites a drastic reduction of degrees of freedom and analytic or numeric computations are allowed. Let us underline that, accordingly to the fact that Hamiltonian (3) conserves the total number of atoms, such coherent states are eigenvectors of $\hat{N}$.
A detailed derivation of the SU(M) coherent states can be found in Refs. [17–19]. We will just summarize a few facts about them. They are defined as

$$|\mathrm{x}, N\rangle = \frac{1}{\sqrt{N!}} \left(\sum_{j=1}^{M} x_j \hat{a}_j^\dagger \right)^N |0, \ldots, 0\rangle, \tag{4}$$

where M and N are the numbers of lattice sites and atoms respectively. The complex coherent state variables $x_j \in \mathbb{C}$, for $j = 1, \ldots, M$, are constrained on the unit-sphere, i.e. $\sum_{j=1}^{M} |x_j|^2 = 1$ [17–19]. The following identities hold

$$\begin{aligned}
\hat{a}_j |\mathrm{x}, N\rangle &= \sqrt{N} x_j |\mathrm{x}, N-1\rangle, \\
\hat{a}_j^\dagger |\mathrm{x}, N\rangle &= \frac{1}{\sqrt{N+1}} \partial_{x_j} |\mathrm{x}, N+1\rangle, \\
\hat{a}_j^\dagger \hat{a}_k |\mathrm{x}, N\rangle &= x_k \partial_{x_j} |\mathrm{x}, N\rangle, \\
\langle \mathrm{x}, N | \hat{a}_j^\dagger \hat{a}_k |\mathrm{x}, N\rangle &= N x_k x_j^*,
\end{aligned} \tag{5}$$

and will be used below to derive a semiclassical description for the dynamics of the system. The classical equations of motion involve the order parameters x_j, which are just complex numbers. They will be derived by a time dependent variational principle (TDVP) [20, 20, 21]. By solving such equations, we will obtain $x_j(t)$ for $j = 1, \ldots, M$, and from these, the state of the quantum system via Eq. (4). The TDVP procedure [20, 20, 21] is based on a suitable choice of the quantum trial state for the system. Thus we can make the ansatz

$$|\Phi(t)\rangle = \exp\left(\frac{iS(t)}{\hbar} \right) |\mathrm{x}(t)\rangle, \tag{6}$$

where $|\mathrm{x}(t)\rangle$ is a time-dependent SU(M) coherent state, whereas $\exp\left(\frac{iS(t)}{\hbar}\right)$ is a phase factor.
In the following we derive a closed set of dynamical equations for the variables $x(t)$ and the expression for $S(t)$. In particular, we will show that $S(t)$ is an effective semiclassical action. In Eq. (6), and hereafter, we drop the explicit dependence on N in the coherent states of Eq. (4). The TDVP method amounts to constraining the time evolution of $|\Phi(t)\rangle$ by using, instead of the full, just the weaker form of the Schrödinger equation $\langle\Phi|(i\hbar\partial_t - H)|\Phi\rangle = 0$ (note the explicit dependence on time t has been dropped). Using Eq. (6) one obtains the identity $S = \int dt (i\hbar\langle \mathrm{x}|\partial_t|\mathrm{x}\rangle - \langle \mathrm{x}|H|\mathrm{x}\rangle)$, which is indeed an (effective) action. The equations of motion for the dynamical variables x_j can be derived from the action $S = \int dt (i\Sigma_j \dot{x}_j x_j^* - \mathcal{H})$, where $\mathcal{H}(\mathrm{x}, \mathrm{x}^*) := \langle \mathrm{x}|H|\mathrm{x}\rangle$ is the classical Hamiltonian. Thus, the set of variables $\{x_j\}_j$ result canonical (complex) variables that satisfy the Poisson brackets

$$\{x_j^*, x_\ell\} = \frac{i\delta_{j\ell}}{\hbar N}$$

and describe the condensate through population $|x_j|^2$ and phase $\arg(x_j)$ of each site. The explicit form of the classical Hamiltonian is

$$\begin{aligned}
\mathcal{H} = &\sum_{j=1}^{M} \left[UN(N-1)|x_j|^4 + \xi_j N |x_j|^2 \right] - \\
&+ \frac{T}{2} N \sum_{j=1}^{M'} \left(x_j^* x_{j+1} + \text{c.c.} \right),
\end{aligned} \tag{7}$$

whereas the corresponding equations of motion are

$$i\frac{dx_j}{d\tau} = \left[\Lambda(N-1)|x_j|^2 + \epsilon_j \right] x_j - \frac{1}{2}\left[x_{j-1} + x_{j+1} \right]. \tag{8}$$

We have introduced the parameters $\Lambda = \frac{2U}{T}$, $\epsilon_j = \xi_j$, and time has been rescaled via $\tau = \frac{Tt}{\hbar}$ so that τ is a dimensionless quantity. Finally, let us also emphasize that Eq. (8) is a discrete version of the Gross-Pitaevskii equation [2].

4. Classical and quantum breathers

A technique to obtain localization of BECs in optical lattices via boundary dissipations was introduced in [23]. In [23, 24], we have numerically integrated the set of equations Eqs. (8) with boundary dissipation terms. Fig. 1 shows two typical evolutions of the atomic density along the optical lattice with losses at the ends of the trapping potential. In Fig. 1a two static breathers have been excited via progressive losses of atoms at the boundaries, whereas in Fig. 1b the atomic losses have generated a single localized state.

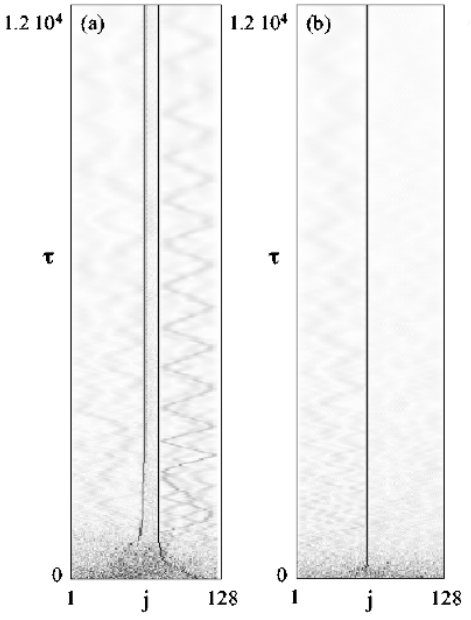

Figure 1. Time evolution of the atomic density for $\gamma_1 = \gamma_M = 0.3$, $\epsilon_j = 0$ for all j, $M = 128$, (a) $\Lambda(N(0) - 1) = 89.6$ and (b) $\Lambda(N(0) - 1) = 44.8$, where $N(0)$ is the initial number of atoms.

The static breathers are stable solutions; exponentially localized in space and periodic in time. They have a simple mathematical form which can be derived as follows. These static solutions satisfy Eqs. (8) with a time dependence characterized by only one frequency ω. Let us reformulate Eqs. (8) by introducing the variables of site population and phase. By substituting the new variables

$$n_j = |x_j|^2, \quad \phi_j = -\frac{i}{2} \ln\left(\frac{x_j}{x_j^*}\right), \tag{9}$$

into Eqs. (8) we get

$$\begin{aligned} \dot{n}_j &= -\left[\sqrt{n_{j+1}n_j}\sin(\Delta\phi_j) - \sqrt{n_j n_{j-1}}\sin(\Delta\phi_{j-1})\right], \\ \dot{\phi}_j &= -\left[\Lambda(N-1)n_j - \mu\right] \\ &\quad + \frac{1}{2}\left[\sqrt{\frac{n_{j+1}}{n_j}}\cos(\Delta\phi_j) + \sqrt{\frac{n_{j-1}}{n_j}}\cos(\Delta\phi_{j-1})\right], \end{aligned} \tag{10}$$

where we have assumed $\epsilon_j = 0$, $\Delta\phi_j := \phi_{j+1} - \phi_j$, and μ is a Lagrange multiplier introduced for taking into account the conserved quantity $\sum_j n_j = N$. The solution for a static breather requires $\dot{n}_j = 0$, which corresponds to the π-state configuration

$$\phi_j - \phi_{j+1} = \pm\pi. \tag{11}$$

Thus, the second of Eqs. (10) becomes

$$\dot{\phi}_j = -(\Lambda n_j - \mu) - \frac{1}{2}\left[\sqrt{\frac{n_{j+1}}{n_j}} + \sqrt{\frac{n_{j-1}}{n_j}}\right]. \tag{12}$$

By setting $\dot{\phi}_j = \omega = (\mu - \chi)$ in the latter equation, we get the algebraic set of equations

$$-2(\chi - \Lambda n_j) + \left[\sqrt{\frac{n_{j+1}}{n_j}} + \sqrt{\frac{n_{j-1}}{n_j}}\right] = 0, \tag{13}$$

where the solutions n_j have to be worked out in a self-consistent way together with χ which is fixed by the constrain $\sum_j n_j = N$. We have solved numerically Eqs. (13) by Newton's method, for $\Lambda = 1, 10, 100$, $N = 7$ and $M = 9$. The atomic density distributions of the classical breathers obtained in this way, have been compared with the analogous quantity derived by the quantum breathers of the Bose-Hubbard Hamiltonian.

In analogy with the classical case, a static quantum breather, is characterized by a single frequency, namely it is an Hamiltonian's eigenstate. For this reason, the full quantum spectrum of Bose-Hubbard Hamiltonian has been numerically calculated for several of the Λ values, by a full diagonalization method. We have found that in a wide range of values of Λ, there exist eigenstates which are exponentially localized along the lattice. For any given value of Λ, the quantum-breather state corresponds to the highest energy eigenstate. Furthermore, we have found that the higher energy levels have the structure shown in the inset of Fig. 2, with the highest level separated by a multiplet of levels, nearly degenerate. It is worth emphasizing that the energy difference between the highest level and the near multiplet, goes to zero very fast when increasing the relevant physical parameter ΛN. Already for $\Lambda N \simeq 10^4$ this energy difference is no more appreciable. Whereas we have been able to observe localized quantum states, for values of ΛN in the interval $[1, 10^3]$. The energy gap between the highest level and the multiplet of levels also depends on M. And by increasing the lattice size this difference rapidly decreases. In other words, our results can be observed in systems with sizes small enough that the translation symmetry breaking produces tangible consequences. When the latter symmetry is restored, quantum states with localization around whatever lattice site are, of course, equivalent, and the maximum energy eigenstate is a superposition of these states. In this case no localization can be seen.

The atomic density distribution of the quantum breathers has been calculated for several values of Λ. We have compared these distributions to the ones of the classical breathers obtained by numerically solving Eqs. (13) with

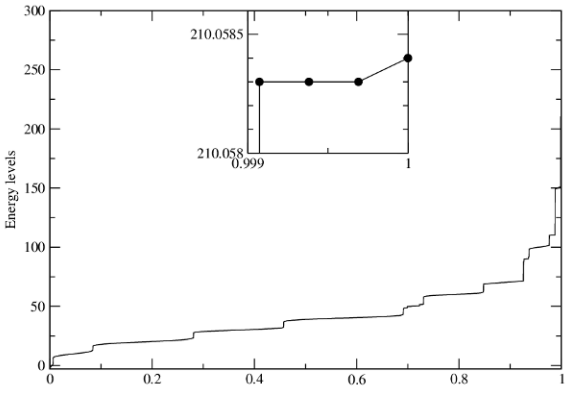

Figure 2. Energy spectrum for $\Lambda = 10$, $N = 7$, and $M = 9$. The inset magnifies the four highest levels.

the same values of Λ. A good agreement between these quantities is evident in Fig. 3; which summarizes the results obtained for $\Lambda = 1, 10, 100$, $N = 7$ and $M = 9$.

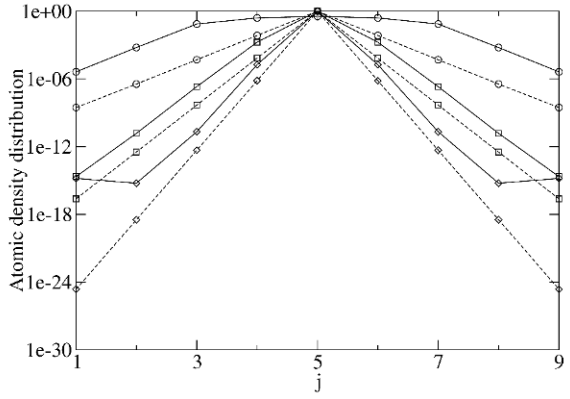

Figure 3. The figure compares the atomic density distributions for the maximum energy eigenstates (continuous lines) and the static breathers obtained by solving Eqs. (13) (dashed lines) for $N = 7$ and $M = 9$, and $\Lambda = 1$ (circles), $\Lambda = 10$ (squares), and $\Lambda = 100$ (diamonds).

5. Concluding remarks

In the last few years, Bose-Einstein condensates have become one of the most versatile test-beds for unexpected behavior of quantum physics. A variety of macroscopic quantum effects have been theoretically investigated and experimentally observed in BECs. Breather states in DNSE have been studied for the last few decades. Since the equations of motion that describe the dynamics of BECs in optical lattices, in the superfluid limit, belong to the class of DNSEs, one also expects, to observe breathers in such systems.

In the present paper we have focused our attention on the Bose-Hubbard model which describes the quantum dynamics of BECs in optical lattices. We have given an effective description of its dynamics by describing the system states in term of $SU(M)$ coherent states. Although the system's equations of motion are reformulated as classical Hamiltonian equations, they describe quantum dynamics of the system pretty well. Moreover, we have numerically diagonalized the full Bose-Hubbard Hamiltonian and we have shown that the breathers can also be observed in the quantum regime.

We have shown that they are the highest-energy eigenstates and exists for a wide range values of Hamiltonian parameters. These quantum breathers, as well as the classical ones, are exponentially localized in space and periodic in time. Remarkably, these kinds of states exists in the absence of randomness. Thus they reproduce a novel quantum localization phenomenon, essentially due to the interplay between bounded energy spectrum and non-linearity.

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