# Quantum $q$-breathers in a finite Bose-Hubbard chain: The case of two interacting bosons

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We study the spectrum and eigenstates of the quantum discrete Bose-Hubbard Hamiltonian in a finite one-dimensional lattice containing two bosons. The interaction between the bosons leads to an algebraic localization of the modified extended states in the normal-mode space of the noninteracting system. Weight functions of the eigenstates in the space of normal modes are computed by using numerical diagonalization and perturbation theory. We find that staggered states do not compactify in the dilute limit for large chains.

## I. INTRODUCTION

The study of discrete breathers in different physical systems has had remarkable developments for the past two decades.[1–4] These excitations are generic time-periodic and spatially localized solutions of the underlying classical Hamiltonian lattice with translational invariance. Their spatial profiles localize exponentially for short-range interaction. Recent experimental observations of breathers in various systems include such different cases as bond excitations in molecules, lattice vibrations, and spin excitations in solids, electronic currents in coupled Josephson junctions, light propagation in interacting optical waveguides, cantilever vibrations in micromechanical arrays, cold atom dynamics in Bose-Einstein condensates loaded on optical lattices, among others.[5–13] In many cases, quantum dynamics is important. Quantum breathers consist of superpositions of nearly degenerate many-quanta bound states, with very long times to tunnel from one lattice site to another.[4,14–29] Remarkably, quantum breathers, though being extended states in a translationally invariant system, are characterized by exponentially localized weight functions, in full analogy to their classical counterparts.

Recently, the application of these ideas to the normal-mode space allowed us to explain many facets of the Fermi-Pasta-Ulam (FPU) paradox,[30] which consists of the nonequipartition of energy among the linear normal modes in a nonlinear chain. There, the energy is localized around the initial normal mode which is excited. Introducing the notion of $q$-breathers,[31–33] which are time-periodic excitations localized in the normal-mode space, the FPU paradox and some related problems were successfully explained. Despite the fact that the interaction in the normal-mode space is long ranged, it is selective and purely nonlinear; thus, $q$-breathers localize exponentially in the normal-mode space.

In this paper, we address the properties of quantum $q$-breathers. We study a one-dimensional quantum lattice problem with two quanta. By defining an appropriate weight function in the normal-mode space, we explore the localization properties of the eigenstates of the system. We observe localization of the weight function as a function of the wave number, which we interpret as a signature of quantum $q$-breather excitations. By using a numerical diagonalization

of the Hamiltonian and nondegenerate perturbation theory, we find algebraic decay of the weight function in the normal-mode space, at variance to the exponential decay found for $q$-breathers in the case of a classical nonlinear system. Another intriguing difference is based on the interference effects of two interacting quanta. For the general case, the quantum $q$-breather states approach the noninteracting eigenstates in the dilute limit of large chains. However, states with Bloch momentum close to $\pm\pi$ keep their finite localization in that limit.

In Sec. II, we describe the model and introduce the basis we use to write down the Hamiltonian matrix. In Sec. III, we review results on the properties of two-quanta bound states—the simplest versions of a quantum breather. In Sec. IV, we consider the case of extended states. We introduce a weight function to describe localization in the normal-mode space, and obtain analytical results using perturbation theory. We present our numerical results obtained by diagonalization of the Hamiltonian matrix, comparing them to analytical estimations. We conclude in Sec. V.

## II. MODEL

We study a one-dimensional periodic lattice with $f$ sites described by the Bose-Hubbard (BH) model. This is a quantum version of the discrete nonlinear Schrödinger equation, which has been used to describe a great variety of systems.[34] The BH Hamiltonian is given by[35]

$$\hat{H} = \hat{H}_0 + \gamma\hat{H}_1, \tag{1}$$

where

$$\hat{H}_0 = -\sum_{j=1}^{f} b_j^+(b_{j-1} + b_{j+1}), \tag{2}$$

$$\hat{H}_1 = -\frac{1}{2}\sum_{j=1}^{f} b_j^+ b_j^+ b_j b_j. \tag{3}$$

Here, $b_j^+$ and $b_j$ are the bosonic creation and annihilation operators which satisfy the commutation relations $[b_i, b_j^+] = \delta_{ij}$, $[b_i^+, b_j^+] = [b_i, b_j] = 0$. $\gamma$ is the parameter controlling the

strength of the interaction, and the chain of length $f$ is subject to periodic boundary conditions. The chain is translational invariant and the Hamiltonian (1) commutes with the number operator $\hat{N} = \Sigma_{j=1}^{f} b_j^+ b_j$, whose eigenvalue is denoted by $n$. We consider the simplest nontrivial case of $n=2$. It is of direct relevance to studies and observations of bound two-vibron states.[36–47]

In order to describe the quantum states, we use a number state basis[35] $|\Phi_n\rangle = |n_1, n_2, \ldots, n_f\rangle$, where $n_i$ represents the number of bosons at site $i$ ($n = \Sigma n_i$). As an example, $|0200000\rangle$ corresponds to a state with two bosons on the second site and zero bosons elsewhere. For a given number of bosons, each eigenstate is a linear combination of number states with fixed $n$. In addition to the number of quanta $n$, there are $n-1$ further quantum numbers which define the relative distance between the bosons. For $n=2$ that reduces to defining one further relative distance $j-1$ between the two quanta, which can take $(f+1)/2$ different values in our case:

$$|\Psi_2\rangle = \sum_{j=1}^{(f+1)/2} v_j |\Phi_2^j\rangle. \quad (4)$$

Due to translation invariance, the eigenstates of $\hat{H}$ are also eigenstates of the translational operator $\hat{T}$, where $\tau = \exp(ik)$ is its eigenvalue with $k = 2\pi\nu/f$ being the Bloch wave number and $\nu \in [-(f-1)/2, (f-1)/2]$. Due to periodic boundary conditions, $\hat{T}|n_1, n_2, \ldots, n_f\rangle = |n_f, n_1, n_2, \ldots, n_{f-1}\rangle$. For the sake of simplicity, we deal with an odd number of sites $f$. Thus, we can construct number states which are also Bloch states:

$$|\Phi_2^j\rangle = \frac{1}{\sqrt{f}} \sum_{s=1}^{f} \left( \frac{\hat{T}}{\tau} \right)^{s-1} |1 \underbrace{0 \cdots 0}_{j-1} 1 \cdots \rangle. \quad (5)$$

With this basis, we can derive the eigenenergies for each given Bloch wave number $k$ from $\hat{H}_k |\Psi_n\rangle = E|\Psi_n\rangle$ after computing the eigenvalues of the matrix with the same structure as in Ref. 35 for the case of the BH system:

$$\hat{H}_k = - \begin{pmatrix} \gamma & q\sqrt{2} & & & & \\ q^*\sqrt{2} & 0 & q & & & \\ & q^* & 0 & q & & \\ & & \ddots & \ddots & \ddots & \\ & & & q^* & 0 & q \\ & & & & q^* & p \end{pmatrix}, \quad (6)$$

with $q = 1 + \tau$ and $p = \tau^{-(f+1)/2} + \tau^{-(f-1)/2}$. By varying the Bloch wave number in its irreducible range, we obtain the eigenenergy spectrum shown in Fig. 1.

## III. BOUND STATES: LOCALIZATION IN REAL SPACE

In Figs. 1(a)–1(c), we show that as the interaction parameter is increasing, an isolated ground-state eigenvalue $E_2(k)$ appears for each $k$ that corresponds to a bound state.[35] For this isolated ground state, there is a high probability of finding two quanta on the same site. In the limit $f \to \infty$, the



FIG. 1. Energy spectrum of the Bose-Hubbard model for different values of the interaction $\gamma$: (a) $\gamma=0.1$, (b) $\gamma=1.0$, and (c) $\gamma=10$. Here, $f=101$.

bound-state eigenvalue has the analytical expression[35,48]

$$E_2(k) = -\sqrt{\gamma^2 + 16\cos^2 k/2}, \quad (7)$$

and the corresponding (unnormalized) eigenvector $\mathbf{v} = (v_1, v_2, \ldots)$ is[48]

$$\mathbf{v} = \left( \frac{1}{\sqrt{2}}, \mu, \mu^2, \mu^3, \ldots \right), \quad (8)$$

where

$$\mu = -\frac{[\gamma + E_2(k)]e^{ik/2}}{4\cos(k/2)}. \quad (9)$$

A suitable weight function of this isolated ground state has the form

$$C_j \equiv |v_j|^2 = |\mu|^{2(j-1)} = e^{2\lambda(j-1)}, \quad j > 1, \quad (10)$$

where $C_1 = 1/2$ and $\lambda = \ln|\mu|$. Since $|\mu|^2 < 1$ for $\gamma \neq 0$, the weight function shows exponential decay when the distance between the two bosons increases. That result corresponds to the exponential localization of classical discrete breathers.[1–4]

However, note that for $|k| \to \pi$, we have $\mu \to 0$ independent of the value of $\gamma \neq 0$. Thus, one obtains compact localization. Note that it is said that a state is compact in a certain basis, if it occupies a certain subspace, but has exactly zero overlap with the rest.

The compact localization for $|k| \to \pi$ is not observed in the classical limit and relies on the fact that the Schrödinger equation is a linear wave equation which admits (destructive) interference effects.

## IV. QUANTUM $q$-BREATHERS: LOCALIZATION IN NORMAL-MODE SPACE

All the other states (except the bound state) form the two-quanta continuum. Their energies for $\gamma = 0$ correspond to the sum of two single-particle energies with the constraint that the sum of their momenta equals the Bloch momentum $k$. One arrives at

$$E^0_{k,k_1} = -2[\cos(k_1) + \cos(k_1 + k)], \qquad (11)$$

where $k_1 = \pi \nu_1 / [(f+1)/2] - k/2$ is the conjugated momentum of the relative coordinate (distance) of both quanta and $\nu_1 = 1, \ldots, (f+1)/2$. $E^0_{k,k_1}$ has a finite spread at fixed $k$ (see Fig. 1). However, for $k = \pm \pi$, the spectrum becomes degenerate. Thus, for $|k \pm \pi| \ll 1$, the eigenenergies are very close (almost degenerate). Remarkably, the bounds of the spectrum for $\gamma \neq 0$ are very well described by the $\gamma = 0$ result. Increasing $\gamma$ at fixed $k$, the eigenenergies will slightly move, but never cross. Thus, a continuation of an eigenstate at $\gamma = 0$ to $\gamma \neq 0$ will preserve its relative ordering with respect to the other eigenenergies.

For $\gamma \neq 0$, these quantum $q$-breather states will be deformed. In analogy to the study of the fate of normal modes in classical nonlinear systems,[31–33] we will study the changes of the two-quanta continuum. For finite $f$ and $\gamma$, the new states will be spread in the basis of the $\gamma = 0$ continuum. For

$f \to \infty$, one expects that the new states become again identical with the $\gamma = 0$ states, since the two quanta will meet on the lattice with less probability as $f$ increases. Thus, we will test the compactification of the new states in the $\gamma = 0$ eigenstate basis both for $\gamma \to 0$ and for $f \to \infty$.

We compute the weight functions in the normal-mode space in order to probe the signature of quantum $q$-breathers. For this purpose, we start by using perturbation theory to set up these weight functions, where $H_1$ is the perturbation. We fix the Bloch momentum $k$ and choose an eigenstate $|\Psi^0_{\tilde{k}_1}\rangle$ of the unperturbed case $\gamma = 0$. Upon increase of $\gamma$, it becomes a new eigenstate $|\Psi_{\tilde{k}_1}\rangle$, which will have overlap with several eigenstates of the $\gamma = 0$ case. We expand the eigenfunction of the perturbed system to the first-order approximation

$$|\Psi_{\tilde{k}_1}\rangle = |\Psi^0_{\tilde{k}_1}\rangle + \gamma \sum_{k'_1 \neq \tilde{k}_1} \frac{\langle \Psi^0_{k'_1}|\hat{H}_1|\Psi^0_{\tilde{k}_1}\rangle}{E^0_{\tilde{k}_1} - E^0_{k'_1}} |\Psi^0_{k'_1}\rangle. \qquad (12)$$

The perturbation of strength $\gamma$ is local in the matrix representation (6); thus, the relevant perturbation parameter is $\gamma / f$. This has to be compared to the typical spacing of unperturbed eigenenergies. For Bloch wave numbers far from $\pm \pi$, the spacing is of order $1/f$, so the approximation should work for $\gamma < 1$. For Bloch wave numbers close to $\pm \pi$, the approximation breaks down if $\gamma \gtrsim \pi - |k|$.

The off-diagonal ($k_1 \neq \tilde{k}_1$) weight function at the first order is given by

$$C(k_1; \tilde{k}_1) \equiv |\langle \Psi^0_{k_1}|\Psi_{\tilde{k}_1}\rangle|^2 = \frac{|\langle \Psi^0_{k_1}|\hat{H}_1|\Psi^0_{\tilde{k}_1}\rangle|^2}{|E^0_{\tilde{k}_1} - E^0_{k_1}|^2}. \qquad (13)$$

$E^0_{k_1}$ and $E^0_{\tilde{k}_1}$ are the eigenenergies of the unperturbed system. With $\Delta = k_1 - \tilde{k}_1$, the weight function can be rewritten in the following form:

$$C(k_1; \tilde{k}_1) = \frac{A^2 \gamma^2}{64(f+1)^2 \cos^2\left(\dfrac{k}{2}\right)\sin^2\left(\dfrac{\Delta}{2}\right)\left[\sin\left(\dfrac{2\tilde{k}_1 + k}{2}\right)\cos\left(\dfrac{\Delta}{2}\right) + \cos\left(\dfrac{2\tilde{k}_1 + k}{2}\right)\sin\left(\dfrac{\Delta}{2}\right)\right]^2}, \quad k_1 \neq \tilde{k}_1, \qquad (14)$$

where $A$ is a constant. For $\gamma = 0$, $|\Psi_{\tilde{k}_1}\rangle = |\Psi^0_{\tilde{k}_1}\rangle$, and the weight function is compact. For $|\Delta| \ll 1$,

$$C(k_1; \tilde{k}_1) \approx \frac{\gamma^2}{(f+1)^2 \dfrac{\Delta^2}{2} \cos^2\left(\dfrac{k}{2}\right)\left[\sin\left(\dfrac{2\tilde{k}_1 + k}{2}\right) + \dfrac{\Delta}{2} \cos\left(\dfrac{2\tilde{k}_1 + k}{2}\right)\right]^2}, \quad k_1 \neq \tilde{k}_1. \qquad (15)$$
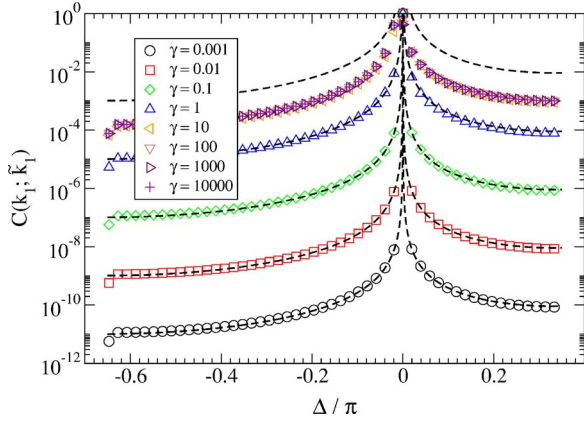
FIG. 2. (Color online) Weight function for different values of the interaction $\gamma$. Here, $f=101$, $k=0$, and $\widetilde{k}_1 = \frac{2}{3}\pi$. Dashed lines are results using formula (14) with $A^2 = 3.8$.
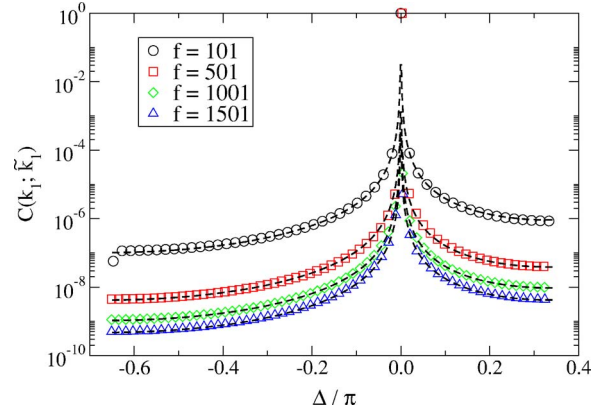


FIG. 4. (Color online) Weight function for different sizes of the system. Here, $\gamma = 0.1$, $k=0$, and $\widetilde{k}_1 \approx \frac{2}{3}\pi$ for all curves. Dashed lines are results using formula (14) with $A^2 = 3.8$.

From this formula, we obtain several interesting results. First of all, the decay of the weight function with increasing $\Delta$ means that we have localization in the normal-mode space. For $2\widetilde{k}_1 + k \neq 0, 2\pi$, we have

$$C \sim \frac{\gamma^2}{(f+1)^2} \frac{1}{\Delta^2}. \qquad (16)$$

We find algebraic decay $\sim 1/\Delta^2$ of the weight function, and for $\gamma \to 0$ or $f \to \infty$, the weight function compactifies. For $2\widetilde{k}_1 + k = 0, 2\pi$, we have

$$C \sim \frac{\gamma^2}{(f+1)^2} \frac{1}{\Delta^4}. \qquad (17)$$

Here, we find algebraic decay $\sim 1/\Delta^4$ of the weight function that also compactifies when $\gamma \to 0$ or $f \to \infty$. Finally, for $k$ close to $\pm\pi$ and large $f$, $C \sim \gamma^2/\Delta^2$. Thus, we find that the $f$ dependence drops out for staggered states $|k \pm \pi| \ll 1$, and these states do not compactify for $f \to \infty$. That is a remarkable quantum interference property, since both simple intuition (see above) and classical theory predict the opposite.

In Fig. 2, we show numerical results obtained by diago-

nalization of the Hamiltonian for different values of $\gamma$. We find localization in the normal-mode space, which can be interpreted as a quantum $q$-breather. When increasing $\gamma$, the quantum $q$-breather becomes less localized, and for large values of the interaction (from $\gamma = 10$ onward), results do not change. The dashed lines are the results using formula (14) with $A^2 = 3.8$, a value that was obtained by fitting the numerical results for the lowest $\gamma$ (=0.001). We can see good agreement with numerical results up to $\gamma = 1$, beyond which perturbation theory does not fit anymore. In Fig. 3, we show that the weight function is more localized for $k=0$ and less localized for $k \to -\pi$.

While probing the influence of the size of the nonlinear quantum lattice on the localization phenomenon, we find in Fig. 4 that as the size increases, the states compactify as we expected. In Fig. 5, we see the $1/\Delta^2$ decay for eigenstates fulfilling $2\widetilde{k}_1 + k \neq 0, 2\pi$ ($k=0$), and in Fig. 6 the $1/\Delta^4$ decay for eigenstates fulfilling $2\widetilde{k}_1 + k = 0, 2\pi$ (also $k=0$). Both results agree with the analytical results using perturbation theory.

In Fig. 7, we observe the predicted independence of the localization phenomenon from the size of the system when $k$
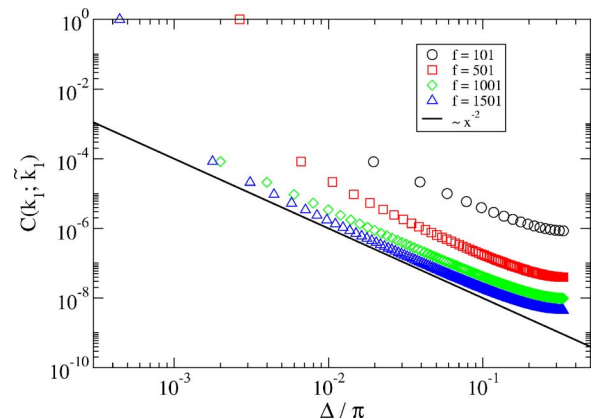


FIG. 3. (Color online) Weight function for different values of the Bloch wave number $k$. Here, $\gamma = 0.1$, $f=101$, and $\widetilde{k}_1 + k/2 = \frac{2}{3}\pi$. Dashed lines are results using formula (14) with $A^2 = 3.8$.
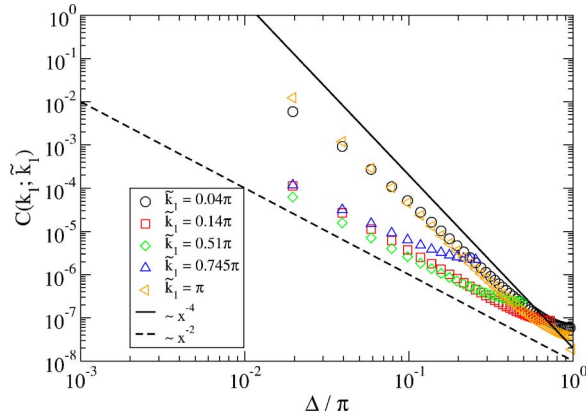


FIG. 5. (Color online) The same as in Fig. 4 in log-log scale.

FIG. 6. (Color online) Weight function for eigenstates with different $\widetilde{k}_1$. Here, $\gamma=0.1$, $f=101$, and $k=0$.



FIG. 7. (Color online) Weight function for different sizes of the system close to the band edge $k=-\pi$. Here, $\gamma=0.001$ and $\widetilde{k}_1+k/2=\frac{2}{3}\pi$. The dashed line is the result using formula (14) with $A^2=3.8$.

is close to $-\pi$. It is interesting that in this case, the weight function does not compactify in the dilute limit $f\rightarrow\infty$ as one would expect from simple grounds. The reason is that the larger $f$, the closer we can tune the Bloch wave number to $\pm\pi$, where the perturbation expansion breaks down.

## V. CONCLUSIONS

In this work, we studied the properties of quantum $q$-breathers in a one-dimensional chain containing two quanta modeled by the Bose-Hubbard Hamiltonian. To explore localization phenomena in this system, we computed appropriate weight functions of the eigenstates in the normal-mode space using both perturbation theory and numerical diagonalization. We observe localization of these weight functions that is interpreted as a signature of quantum $q$-breathers. The localization is stronger when the size of the system increases. Unlike the classical case where the localization is exponential, we found here algebraic localization. This is a long-range behavior, which follows from the fact that the interaction $\gamma$ induces a linear perturbation of the eigenstates which is local in real space and also local in the matrix representation in Eq. (6). That induces a mean-field-type interaction between the normal modes and naturally leads to algebraic localization. Note that the matrix (6) is formally analogous to a semi-infinite tight-binding chain with a defect at one end. Nevertheless, it appears in our context when starting with a translationally invariant system, but with many-particle states which include interaction.

Since the effective interaction strength drops in the dilute limit of large chains, we observe stronger localization (except for the case of staggered states). The crucial difference to the classical model is that while the linear classical dynamics coincides with the single-particle quantum problem, nonlinearity in the classical model effectively deforms the single-particle dynamics (and adds many other features such as chaos, etc). The interaction in the quantum problem takes the wave function into the new Hilbert space of many-body wave functions, which is still a linear space, but higher dimensional. Another feature of that quantum interaction is the fact that staggered states do not compactify in the dilute limit
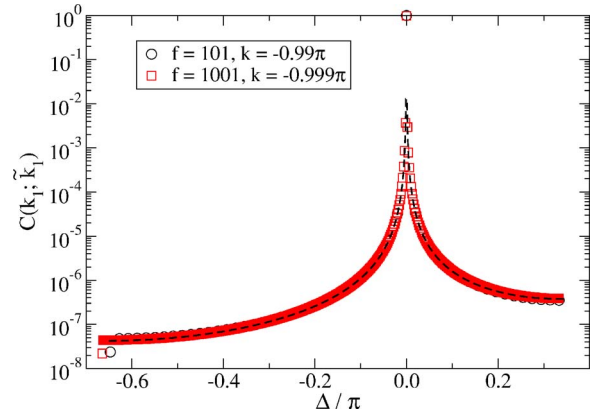
of large chains. That property is based on the interference of quantum states and is not observed in the corresponding classical nonlinear equation. A similar (yet weaker) signature of quantum interference is the observed change of the power of the algebraic decay from 2 (generic) to 4 when choosing particular values of the wave number $k_1$, which depend on the Bloch wave number $k$. And yet another signature of quantum $q$-breathers is the fact that they keep a finite localization in the limit $\gamma\rightarrow\infty$ as seen in Fig. 2 and at variance to their classical counterparts, which turn from exponentially localized to completely delocalized in that limit. The reason is that in this strong-interaction limit, extended two-boson states correspond to their noninteracting counterparts which are projected onto the basis space which does not contain doubly occupied chain sites, while strong nonlinearity in the classical problem completely deforms periodic orbits of the noninteracting system.

We are aware of the fact that the quantum problem studied here is a linear one (in terms of differential equations). Its correspondence to a classical nonlinear system can be observed in the limit of many bosons when treating the many-particle quantum states within a Hartree approximation, which projects onto product states. Often the classical description is also achieved using suitable (e.g., coherent state) representations. The presented results have an unambiguous meaning in the chosen basis of the noninteracting system. Yet, they will of course in general depend on the chosen basis. Therefore, it remains a puzzling question how to restore exponential localization of classical $q$-breathers from the algebraic decay of quantum $q$-breathers with two bosons in the limit of larger numbers of bosons. The fate of quantum $q$-breathers in higher dimensional lattices is another interesting open question, which will be left to future work.

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