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Biphonons in the β-Fermi–Pasta–Ulam model

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Abstract

Discrete breathers or intrinsic localized modes are nonlinear localized states that appear in several classical extended systems, such as for instance the Fermi–Paste–Ulam (FPU) model. In order to probe the quantum states that correspond to discrete breathers, we quantize the β-FPU model using boson quantization rules, retain only number conserving terms, and analyze the two-quanta sector of the model. For both attractive and repulsive nonlinearity, we find the occurrence of biphonons in two forms, on-site and nearest-neighbor site, and analyze their properties. We comment on the use of this model as a minimal model for extended molecular and biomolecular systems.

Keywords: Fermi–Pasta–Ulam model; Discrete breathers; Quantum breathers; Biphonons

1. Introduction

The one dimensional nonlinear model introduced by Fermi, Pasta and Ulam in 1955 has proved to be a workhorse of nonlinear dynamics during the last half century [1]. In addition to showing that the use of computers can lead to new physics, it has assisted in generating a wealth of new results on solitons, integrable systems, thermal conductivity, etc. The same model was also used for the introduction of the concept of intrinsic localized modes or discrete breathers (DBs), i.e. the nonlinear localized modes that appear in discrete lattices with nonlinearity [2]. Discrete breathers appear in a variety of lattice models where we have the coexistence of nonlinearity with discreteness, i.e. weak interaction between different constituent parts of the system [3]. The existence theorem of MacKay and Aubry placed on solid mathematical ground the existence of DBs in nonlinear lattices with on-site nonlinearity [4], while some mathematical and physical aspects of discrete breathers in FPU-type lattices have also been investigated [5,6]. Numerous features of DBs in lattices have been studied through the use of the exact numerical construction procedure introduced by Aubry and coworkers [7,8].

The presence of DBs in classical models raises the issue of quantum aspects of these modes in the models, as well as the investigation of quantum breathers in physical systems. Regarding model systems, one may use a semiclassical approach and quantize classical DBs using the Bohr–Sommerfeld procedure [7]. An alternative approach is to perform direct quantization in the model Hamiltonian and derive as well as classify the resulting states; in the present work, we will use the latter approach. Specifically, we will consider the classical β-FPU model, quantize it using boson quantization rules, and subsequently analyze the two-quanta sector of this model in the context of the boson conserving approximation. Our analysis is analogous to the approach followed in the context of a model with an on-site ϕ^4 potential that, within a number preserving approximation, leads to a quantum version of the Discrete Nonlinear Schrödinger (DNLS) equation [10–12]. In the following sections, we will first introduce the basic model as well as the quantization rules, and discuss the linear modes of the system. Subsequently, we will perform an analytical investigation of the two-boson sector of the number preserving model and show the regime of existence as well as the nature of two-boson bound states. Analysis of the regime of validity of these findings follows, by comparison with other works as well as the possible applications of the findings in real systems.

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2. The β Fermi–Pasta–Ulam model and its quantization

We consider a one dimensional system of identical particles, each of mass M described through the Hamiltonian:

$$H = \sum_n \frac{p_n^2}{2M} + \frac{C}{2}(x_n - x_{n-1})^2 + \frac{b}{4}(x_n - x_{n-1})^4, \tag{1}$$

where x_n is the position and p_n is the momentum of the n-th particle, while C, b denote the strength of the linear and nonlinear acoustic nearest-neighbor coupling, respectively. This Hamiltonian corresponds to the classical β-FPU model and has been investigated in numerous works ever since its initial introduction in 1955. It is known that, in a certain parameter regime, the model can support mobile DBs or ILMs [2]. These modes are nonlinear vibrational modes that are localized in space and periodic in time; their quantum counterparts are expected to be bound states of arbitrary numbers of phonons. In order to quantize Eq. (1), we may introduce phonon creation and annihilation operators, either in real space, viz. $a_n^\dagger$, a_n respectively, or in momentum space, i.e. $a_q^\dagger$, a_q respectively. The position and momentum operators of the Hamiltonian in the discrete position are:

$$p_n = \mathrm{i}\sqrt{\frac{\hbar M\omega}{2}}(a_n^\dagger - a_n) \tag{2}$$

$$x_n = \sqrt{\frac{\hbar}{2M\omega}}(a_n^\dagger + a_n) \tag{3}$$

while, in terms of collective modes in the momentum representation, they are written as follows:

$$p_q = \mathrm{i}\frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{\mathrm{i}qnR_0}\sqrt{\frac{\hbar M\omega_q}{2}}(a_{-q}^\dagger - a_q) \tag{4}$$

$$x_q = \frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{\mathrm{i}qnR_0}\sqrt{\frac{\hbar}{2M\omega_q}}(a_q^\dagger + a_q) \tag{5}$$

where R_0 is the lattice spacing and N is the total number of oscillators. The frequencies ω and ω_q will be specified below.

2.1. Quantization schemes and analysis of linearized modes

In order to estimate the error that may be introduced due to the quantization in terms of local modes or within the number conserving approximation, we compare the spectrum of the linear part of Eq. (1) quantized in terms of (i) local modes labeled by the site index n and (ii) extended, collective modes labeled by q. For that purpose, we rewrite Eq. (1) for $b = 0$ as follows:

$$H = \sum_n \frac{p_n^2}{2M} + ax_n^2 - \frac{a}{2}x_n(x_{n+1} + x_{n-1}); \tag{6}$$

using Eqs. (2) and (3) with $\omega = \sqrt{\frac{2C}{m}}$ and, after some algebra, Eq. (6) becomes

$$H = N\frac{\hbar\omega}{2} + \hbar\omega\sum_n a^\dagger a_n$$

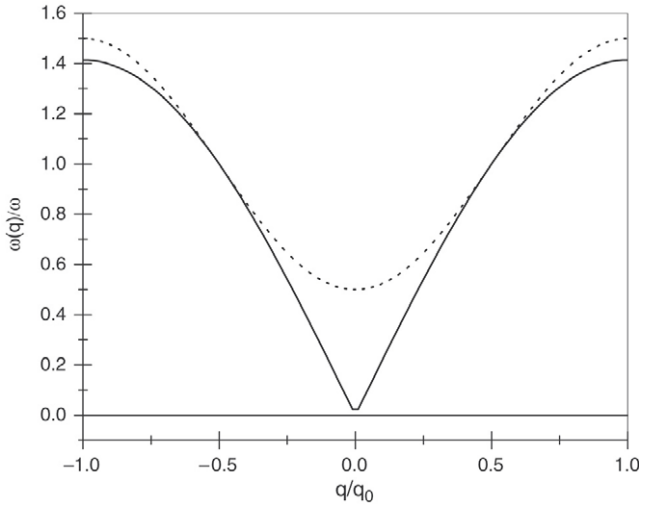

Fig. 1. Dispersion of linearized modes for the two quantization schemes with on-site (dotted line) and delocalized modes (continuous line), respectively. We note that the use of number conserving terms introduces a gap in the linear spectrum, when the latter is obtained through position representation operators.

$$-\frac{\hbar\omega}{8}\sum_n (a_n^\dagger + a_n)(a_{n+1}^\dagger + a_{n-1}^\dagger + \text{h.c.}). \tag{7}$$

Disregarding number nonconserving terms (NNC) and performing the Fourier transformation of the oscillator operators as $a_q = \frac{1}{\sqrt{N}}\sum_q \mathrm{e}^{\mathrm{i}qnR_0}a_n$, we arrive at the final expression:

$$H = N\frac{\hbar\omega}{2} + \sum_q \hbar\tilde{\omega}a_q^\dagger a_q, \tag{8}$$

where $\tilde{\omega} = \omega(1 - \frac{1}{2}\cos qR_0)$. Quantization in terms of collective modes of Eqs. (4) and (5), on the other hand, results in a similar expression for the linear Hamiltonian, viz.

$$H = \sum_q \frac{\hbar\omega_q}{2} + \sum_q \hbar\omega_q a_q^\dagger a_q \tag{9}$$

but with $\omega_q = \omega\sqrt{(1 - \cos qR_0)}$. The comparison of the linear mode dispersion relations for the linearized Hamiltonians of Eqs. (8) and (9) are shown in Fig. 1. We observe that the use of local modes within the number conserving approximation introduces a gap in the linear spectrum at long wavelengths, while direct use of the q-space modes retains the acoustic nature of the Hamiltonian of Eq. (1). In the remainder of this work, we will consider only number conserving terms in the Hamiltonian, since we are primarily interested in coherent phenomena induced by resonant spectroscopy experiments [9].

2.2. Quantization of the nonlinear terms

We now proceed with the inclusion of the nonlinear terms of the Hamiltonian; we use the following auxiliary relations:

$$\sum_n (x_n - x_{n-1})^2 = \sum_n x_n^2 + \sum_n x_{n-1}^2 - 2\sum_n x_n x_{n-1}$$

which, by virtue of lattice periodicity and assuming $N \to \infty$, becomes

$$\sum_n (x_n - x_{n-1})^2 = 2\sum_n x_n^2 - 2\sum_n x_n(x_{n+1} + x_{n-1}).$$

Similarly,

$$\sum_n (x_n - x_{n-1})^4 = 2\sum_n x_n^4 - 4\sum_n x_n^3(x_{n+1} + x_{n-1}) + 3\sum_n x_n^2(x_{n+1}^2 + x_{n-1}^2).$$

Upon substitution of oscillator momentum and displacement relations as defined in Eqs. (2) and (3), we obtain a set of exact expressions that are further simplified by retaining only the number preserving terms:

$$\sum_n x_n^4 \approx 3\left(\frac{\hbar}{2M\omega}\right)^2 \sum_n (1 + 2a_n^{\dagger 2}a_n^2 + 4a_n^\dagger a_n),$$

$$\sum_n x_n^3(x_{n+1} + x_{n-1}) \approx 6\left(\frac{\hbar}{2M\omega}\right)^2 \sum_n a_n^\dagger(a_{n+1} + a_{n-1}) + 3\left(\frac{\hbar}{2M\omega}\right)^2 \sum_n [a_n^{\dagger 2}a_n(a_{n+1} + a_{n-1}) + \text{h.c.}]$$

$$\sum_n x_n^2(x_{n+1}^2 + x_{n-1}^2) \approx 2N\left(\frac{\hbar}{2M\omega}\right)^2 + 8\left(\frac{\hbar}{2M\omega}\right)^2 \sum_n a_n^\dagger a_n + 2\left(\frac{\hbar}{2M\omega}\right)^2 \sum_n \left[a_n^{\dagger 2}(a_{n+1}^2 + a_{n-1}^2) + \sum_{n,s=\pm 1} a_n^\dagger a_n a_{n+s}^\dagger a_{n+s} a_n\right].$$

Using these expressions, we arrive at the following quantized number conserving FPU Hamiltonian:

$$H = \varepsilon_0 + \hbar\bar{\omega}\sum_n a_n^\dagger a_n - J'\sum_n a_n^\dagger(a_{n+1} + a_{n-1}) + B\sum_n \left[a_n^{\dagger 2}a_n^2 + \frac{1}{2}a_n^{\dagger 2}(a_{n+1}^2 + a_{n-1}^2)\right] + B\left[\sum_{n,s=\pm 1} a_n^\dagger a_n a_{n+s}^\dagger a_{n+s}a_n - (a_n^{\dagger 2}a_n a_{n+s} + \text{h.c.})\right] \quad (10)$$

where

$$\varepsilon_0 = \frac{\hbar\omega N}{2}\left(1 + \frac{3b}{2a}\left(\frac{\hbar}{2M\omega}\right)\right), \quad \bar{\omega} = \omega\left(1 + \frac{3b}{a}\left(\frac{\hbar}{2M\omega}\right)\right) \quad (11)$$

$$J' = a\left(\frac{\hbar}{2M\omega}\right)\left(1 + \frac{3b}{a}\frac{\hbar}{M\omega}\right), \quad B = 3b\left(\frac{\hbar}{2M\omega}\right)^2. \quad (12)$$

Let us discuss briefly the physics of the terms appearing in the quantum Hamiltonian of Eq. (10); since the meaning of the linear terms is clear we comment only on the nonlinear terms. The on-site and intersite repulsion ($B > 0$) or attraction ($B < 0$) defined through the terms $a_n^{\dagger 2}a_n^2$ and $a^\dagger a_{n\pm 1}^\dagger a_{n\pm 1}a_n$, $a_n^{\dagger 2}a_{n\pm 1}^2$ correspond to simultaneous tunneling of two phonons (or vibrons) between neighboring sites, i.e. they describe the simultaneous creation of two vibrons at site n with a simultaneous annihilation of two vibrons at sites $n \pm 1$; these terms may give rise to direct bivibron tunneling. The term $a_n^{\dagger 2}a_n a_{n\pm 1}$ corresponds to the simultaneous creation of two vibrons on the same site, where one of them is annihilated at the same site while the other one tunnels to the neighboring site. Since this term effectively describes the single vibron tunneling, it may be treated in a mean field manner as an effective intersite transfer term and replaced by $a_n^{\dagger 2}a_n a_{n\pm 1} \approx \langle a_n^\dagger a_n\rangle a_n^\dagger a_{n\pm 1}$. Its Hermitian conjugate also has the same form. As a result of the use of the mean field approximation for these terms, the last two terms of the effective Hamiltonian of Eq. (10) may be included in a single vibron tunneling term in which J' is replaced by $J = J' + 2B\langle a^\dagger a\rangle$.

3. Two-vibron bound states

In the analysis of the bivibron solutions, we shall follow the well-known procedure introduced by Wortis in the analysis of two-magnon bound states and latterly utilized extensively in the examination of biexcitons and biphonons [13–15]. The first step is the choice of state vector in the form:

$$|\Psi\rangle = \sum_{m,n} \Psi_{m,n} a_m^\dagger a_n^\dagger |0\rangle, \quad \langle\Psi|\Psi\rangle = 1 \quad (13)$$

where $\Psi_{m,n}$ are the occupation probability amplitudes of the sites m and m, respectively. The boson nature of vibrons imposes the condition:

$$\Psi_{m,n} = \Psi_{n,m},$$

while the normalization condition yields

$$\sum_{m,n} |\Psi_{m,n}|^2 = 1.$$

Substitution of the state vector of Eq. (13) into the Schrödinger equation $H|\Psi\rangle = E|\Psi\rangle$, where H is the Hamiltonian of Eq. (10), as well as the use of the above intermediate expression lead to the following equation for bivibron amplitudes:

$$(E - 2\hbar\bar{\omega})\Psi_{m,n} + J'\sum_{s=\pm 1} \Psi_{m,n+s} + \Psi_{m+s,n} = 2B\left[\Psi_{m,n} + \frac{1}{2}\sum_{s=\pm 1}(\Psi_{m+s,n+s} - \Psi_{m+s,n} - \Psi_{m,n+s})\right]\delta_{m,n} + B\sum_{s=\pm 1}(2\Psi_{m,n}\delta_{m,n+s} - \Psi_{m+s,n}\delta_{m+s,n} - \Psi_{m,n+s}\delta_{m,n+s}). \quad (14)$$

Using lattice periodicity, we may express the amplitudes $\Psi_{m,n}$ in the following form:

$$\Psi_{m,n} = \frac{1}{\sqrt{N}}\Phi_{m-n}e^{i\frac{K(m+n)R_0}{2}},$$

where $K = k_1 + k_2$ denotes the total quasi-momentum associated with the motion of the bivibron center of mass

and belonging in the first Brillouin zone. Due to the indistinguishability of vibrons, $\Phi_{m-n} = \Phi_{n-m}$, i.e. Φ is the function of distance between two vibrons and may be written as $\Phi_{m-n} \equiv \Phi_l$, where $l = m - n$. As a result of lattice periodicity, the equation for the two-boson states of Eq. (14) may be written as follows:

$$(E - 2\hbar\bar{\omega})\Phi_l + 2J\cos\frac{KR_0}{2}\sum_{s=\pm1}\Phi_{l+s} - 2B\left(1 + \cos KR_0 - 2\cos\frac{KR_0}{2}\right)\Phi_l\delta_{l,0} - 2B\Phi_l(\delta_{l+1,0} + \delta_{l-1,0}) + 2B(\Phi_{l+1} + \Phi_{l-1})\cos\frac{KR_0}{2}\delta_{l,0} = 0. \quad (15)$$

The expression in Eq. (15) represents a system of linear algebraic equations for amplitudes Φ_l for each l and has the form of a two dimensional Schrödinger equation in the tight-binding approximation. This equation is equivalent to the one obtained by Pouthier in the approximate analysis of a Davydov-like Hamiltonian applied to the problem of amide I vibrational self-trapping [16]. Eq. (15) is quite complicated and, in order to proceed with its analysis, we now perform the mean field replacement of the single vibron tunneling term, as explained previously; we obtain:

$$(E - 2\hbar\bar{\omega})\Phi_l + 2J\cos\frac{KR_0}{2}\sum_{s=\pm1}\Phi_{l+s} - 2B(1 + \cos KR_0)\Phi_l\delta_{l,0} - 2B\Phi_l(\delta_{l+1,0} + \delta_{l-1,0}) = 0.$$

We proceed by expanding Φ_l in Fourier series:

$$\Phi_l = \frac{1}{\sqrt{N}}\sum_q f_q e^{iqlR_0}$$

and upon substitution in Eq. (15) we obtain:

$$(E - \varepsilon(K,q))f_q = 2B(1 + \cos KR_0)\frac{1}{N}\sum_{q'} f_{q'} + 4B\cos q\frac{1}{N}\sum_{q'}\cos q' f_{q'} \quad (16)$$

with

$$\varepsilon(K,q) = 2\hbar\bar{\omega} - 4J\cos\frac{KR_0}{2}\cos qR_0. \quad (17)$$

The function $\varepsilon(K,q)$ denotes the energy of two free vibrons. The final Eq. (16), which describes the eigenvalue problem for the two-boson sector of the Hamiltonian of Eq. (10), is an integral equation for the functions f_q and may be solved using standard techniques. Before proceeding with its solution, we first analyze the conditions for bivibron state existence.

4. Bivibron spectrum: Analytical considerations for free and bound states

In order for a bound state (BS) to exist, it must be outside the free state continuum lying between the minimum and maximum values of $\varepsilon(K,q)$ of Eq. (17). As a result, for a fixed total quasi-momentum K, the BS energy must lie either below the lower energy bound

$$2\hbar\bar{\omega} - \left|4J\cos\frac{KR_0}{2}\right|,$$

or above the higher energy bound

$$2\hbar\bar{\omega} + \left|4J\cos\frac{KR_0}{2}\right|.$$

In order to distinguish these two different branches of free two-phonon states, we may rewrite Eq. (17) as follows:

$$\varepsilon^{\pm}(K,q) = 2\hbar\bar{\omega} \pm 4J\cos\frac{KR_0}{2}\cos qR_0. \quad (18)$$

Introducing Eq. (18) into Eq. (16), the lower (upper) bivibron branch may be written, respectively, as follows:

$$(E^{\pm} - \varepsilon^{\pm}(K,q))f_q = 2B(1 + \cos KR_0)\frac{1}{N}\sum_{q'} f_{q'} + 4B\cos qR_0\frac{1}{N}\sum_{q'}\cos q' f_{q'}. \quad (19)$$

Eq. (19) may be recast in the more convenient form by dividing by $\cos\frac{KR_0}{2}$ and introducing the following notation:

$$\lambda_K = \frac{E - 2\hbar\bar{\omega}}{2J\cos\frac{KR_0}{2}}, \quad (20)$$

$$X = \frac{1}{N}\sum_q f_q, \quad Y = \frac{1}{N}\sum_q \cos q f_q, \quad (21)$$

$$A_K = \frac{2B}{J}\cos\frac{KR_0}{2}, \quad B_K = \frac{2B}{J\cos\frac{KR_0}{2}}. \quad (22)$$

The final form of Eq. (19) is then:

$$(\lambda_K \pm 2\cos qR_0)f_q = A_K X + B_K\cos qR_0 Y. \quad (23)$$

In terms of the newly introduced parameters, the lower free two-vibron branch is obtained for $\lambda_K < -2$, while for $\lambda_K > 2$ we have the corresponding upper branch. In other words, λ_K is negative for the lower branch and positive in the upper branch and, as a result, both conditions simplify to $|\lambda_K| > 2$.

From Eq. (23) we obtain the formal solution for the amplitude f_q:

$$f_q = \frac{A_K}{\lambda_K \pm 2\cos qR_0}X + \frac{B_K\cos qR_0}{\lambda_K \pm 2\cos qR_0}Y. \quad (24)$$

Multiplication of Eq. (24) by $\frac{1}{N}$ and summation over q results in the following homogeneous system of linear algebraic equations:

$$(1 - A_K I_0)X - B_K I_1 Y = 0 \quad (25)$$

$$(\lambda_K - A_K)X + 2Y = 0 \quad (26)$$

where

$$I_0 = \frac{1}{N}\sum_q \frac{1}{\lambda_K \pm 2\cos qR_0}, \quad (27)$$

$$I_1 = \frac{1}{N}\sum_q \frac{\cos q R_0}{\lambda_K \pm 2\cos q R_0} = \frac{1}{2}(1 - \lambda_K I_0). \tag{28}$$

The nontrivial solutions of the system of Eqs. (25) and (26) are obtained when the determinant is set equal to zero, leading to

$$(\lambda_K - A_K)B_K I_1 + 2(1 - A_K I_0) = 0. \tag{29}$$

The Eq. (29) that needs to be solved for the the unknown parameter λ_K cannot be handled very easily. It may be solved numerically but, since the numerical solution needs to be obtained for each value of the quasi-momentum K, this cannot be done straightforwardly either. Instead of following a direct numerical approach, in the present work we choose to find approximate analytical solutions of the equation that will give an understanding of the various biphonon regimes. A complete numerical solution will be given in the future.

Bivibron spectrum in the regime $\lambda_K < 0$

Let us investigate the energy regime below the free two-vibron band, where $\lambda_K < 0$; in this case integral I_0 becomes

$$I_0 = -\frac{1}{N}\sum_q \frac{1}{\lambda + 2\cos q R_0}$$

where, for convenience, we set $\lambda = -\lambda_K$. We use the correspondence rule $\frac{1}{N}\sum_q \ldots \to \frac{R_0}{2\pi}\int_{-\pi/R_0}^{\pi/R_0} \ldots \mathrm{d}q$ in order to turn summations into integrations and obtain

$$I_0 = -\frac{1}{\sqrt{\lambda_K^2 - 4}}.$$

The integral I_1 follows from the relation connecting it with I_0 of Eq. (28). Using these facts, we may write the determinant Eq. (29) as follows:

$$-(\lambda + A_K)B_K I_1 + 2(1 - A_K I_0) = 0. \tag{30}$$

We observe that Eq. (30) has solutions only for the case of attractive interaction, viz. only when $B < 0$. In the opposite case of $B > 0$, both I_0 and I_1 are negative, and Eq. (30) becomes a sum of positive terms and can never become zero.

Due to the fact that the parameters A_K and B_K are not independent, the only parameter determining the bivibron spectrum is $a = 2\frac{B}{J}$. We may now discuss for which values of a the eigenvalue Eq. (30) has physically meaningful solution(s). For that purpose, we consider the eigenvalue problem for only specific characteristic values of bivibron momentum and, in particular, we focus on the case $K = 0$. For this value of total bivibron momentum, Eq. (30) becomes

$$a(\lambda + a)(\lambda - \sqrt{\lambda^2 - 4}) + 4(a + \sqrt{\lambda^2 - 4}) = 0. \tag{31}$$

Although Eq. (31) cannot be solved explicitly for λ as a function of the parameter a, viz. $\lambda(a)$, one may, however, easily obtain the inverse relation of a as a function of λ, viz. $a = a(\lambda)$, due to the quadratic nature of the equation in a. Solution and numerical inversion leads to the results shown in Fig. 2, where it is shown that the bivibron spectrum for $K = 0$ consists of two bands that may be associated with the two types of pairing,

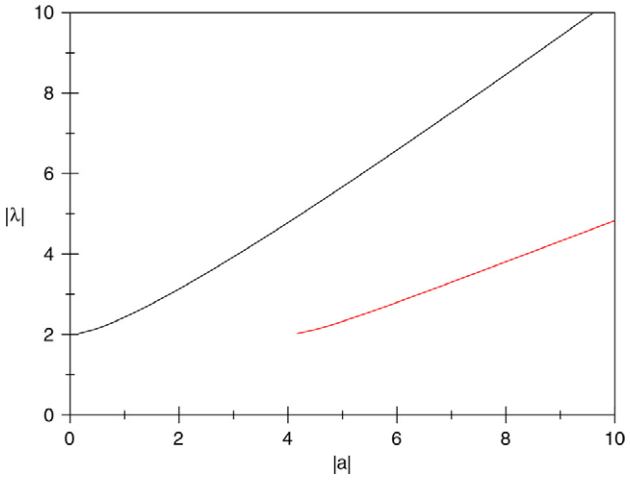

Fig. 2. Regimes of allowed values of $a = \frac{2B}{J}$ for the two types of bound biphonons: on-site (left-hand curve) and adjacent site (right-hand curve).

on-site and intersite, respectively. We note that the formation of either type of bound states demands a different minimal value of a. The first branch appears for values $a > 0.05$, while the second one appears for larger values, viz. $a > 4$.

The physical difference between the two branches can be understood through simple considerations of the eigenvalue Eq. (30); the term A_K plays an on-site role, while B_K plays an inter-site role. By setting the latter equal to zero, viz. $B_K \approx 0$, we obtain $A_K = -\sqrt{\lambda_K^2 - 4}$ and thus recover the results of reference [15] regarding a single on-site bivibron. The later exists only in the regime $a > 2$ and thus corresponds to the left-hand curve of Fig. 2. It is the inclusion of the inter-site term B_K that induces the appearance of the second branch.

In order to give a clearer picture of the bivibron spectrum, we concentrate on the regime for $\lambda_k \gg 2$. For this case, we may use the approximate expression $I_0 \to -1/\lambda \Rightarrow I_1 = 1/2(1+\lambda I_0) \to 0$, and consequently the eigenvalue Eq. (30) becomes

$$\frac{(\lambda + A_K)B_K}{\lambda^2} + 2\left(1 + \frac{A_K}{\lambda}\right) = 0. \tag{32}$$

In the limit of large λ, the eigenvalue problem becomes a simple quadratic equation in λ that may be solved easily and provides the following simple expression for the bivibron spectrum:

$$\frac{\varepsilon(K) - 2\hbar\bar{\omega}}{2J} = -a\cos\frac{K R_0}{2}\left(f_k \pm \sqrt{f_k^2 - 2}\right) \tag{33}$$

$$f_k = \left(\cos\frac{K R_0}{2} + \frac{1}{2\cos\frac{K R_0}{2}}\right). \tag{34}$$

Bivibron spectrum in the regime $\lambda_K > 0$

The regime for $\lambda_K > 0$ is obtained in an exactly similar manner to the preceding analysis; specifically, for attractive interaction ($a < 0$) we have $A_K < 0$ and $B_K < 0$, while the integral I_0 becomes

$$I_0 = \frac{1}{N}\sum_q \frac{1}{\lambda + 2\cos qR_0}$$

and the eigenvalue equation now becomes

$$-(\lambda + |A_K|)|B_K|I_1 + 2(1 + |A_K|I_0) = 0. \quad (35)$$

Since $I_1 < 0$, Eq. (35) cannot be satisfied as a sum of positive terms and, as a result, there is no upper branch bound states for attractive interaction. For repulsive interaction ($a > 0$), on the other hand, we follow exactly the analysis of the $\lambda_K < 0$ case and obtain the same two branches shown in Fig. 2. We thus find that the cases $\lambda_K < 0$ and $\lambda_K > 0$ lead each to two sets of bound states placed symmetrically below and above the free bivibron band, respectively.

The two-vibron band picture in the context of the present scheme is presented in Fig. 3 for two values of the parameter a, leading to bound biphonons for $a = 2$ (higher grey continuous and dotted lines (red in the web version)) and $a = 3$ (lower black continuous and dotted lines (blue in the web version)). The central dark-shaded region bounded by two continuous dark lines corresponds to the band of two free vibrons, while the two sets of lines below this band correspond to bound bivibron states. The continuous lines correspond to an on-site bound bivibron, while the dotted-lines correspond to next-neighboring bivibrons. We observe that the on-site bivibron always has lower energy than the nearest neighbor bivibron, while the latter may be inside the two-vibron band for some wavenumbers. Eq. (33) has two sets of solutions, one is always equal to $-a$ while the other is equal to $-2a\cos^2(KR_0/2)$; for $|KR_0| > \pi/2$, the former, representing the on-site bivibron, has lower energy than the latter, viz. the two-site bivibron. At $KR_0 = \pm\pi/2$, the two solutions collide and, in the regime $-\pi/2 < KR_0 < \pi/2$, they switch symmetry and the dispersive branch now becomes the on-site bivibron, thus retaining the lowest energy for the whole momentum range. This behavior is attributed to the approximate nature of the analytical solutions found, and it would be interesting to analyze the effect numerically through exact diagonalization. We note that the biphonon spectrum for repulsive interaction (not shown in the figure) is exactly symmetric to the present one for attractive interaction, but *above* the free two-phonon band.

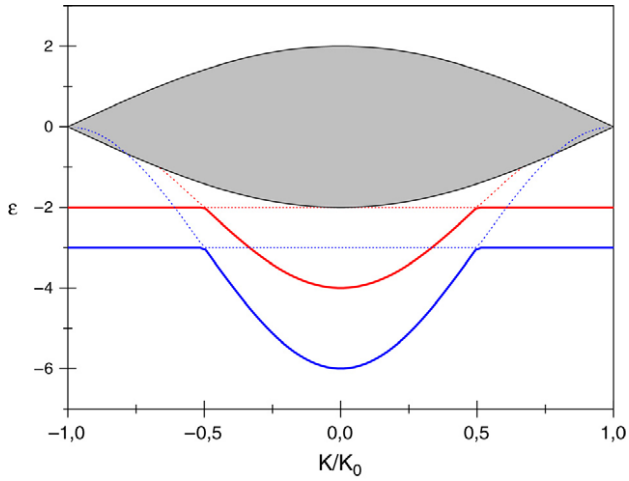

Fig. 3. Energy spectrum for $|\lambda| \gg 2$. The black lines and the dark region in between them correspond to free two-vibron states, i.e. delocalized two-vibron state. For attractive nonlinearity shown here, the two sets of lines correspond to the bound bivibron band and dotted lines to two-site bivibrons, while continuous lines correspond to on-site bivibrons. The nonlinearity parameter values used are $|a| = 2$ (grey curves (red in the web version)) and $|a| = 3$ (black curves (blue in the web version)).

5. Conclusions

The quantization of the β-FPU model with boson quantization rules and the subsequent analysis of the two-quanta sector within the boson conserving approximation leads to the appearance of biphonons. These states may be considered as the lowest states arising from the acoustic nonlinearity of the Hamiltonian and may be thought of as quantum counterparts of the classical FPU discrete breathers. Analytical calculations showed that two types of states may appear within the two-quanta sector, corresponding to on-site biphonons as well as adjacent-site biphonons. The latter states have higher energy than the former ones, as expected. The presence of two types of biphonons may result in higher mobility for the two-quanta states compared with the case where only a single on-site two-boson state existed. Our analysis shows that biphonon states appear in the number conserving β-FPU model below the band of free two-phonon states in the case of attractive nonlinearity, viz. for $b < 0$, while for repulsive nonlinearity they appear above the free band. We thus find that both attraction and repulsion may lead to effective binding of the single quanta states. We note that in quantum DNLS-like models [10–12], as well as quantum Klein–Gordon models [17], on the other hand, there is only on-site nonlinearity with a linear intrasite coupling. This fact generally favors the formation of single site multi-vibron states, and in the two-quanta sector does not lead to the formation of an intersite bivibron.

The introduction of the boson conserving approximation is compatible with the rotating wave approximation at the classical level. Within the latter, Sievers and Takeno showed the existence of classical discrete localized modes in the FPU model, viz. IMLs or DBs. The biphonon states found within the context of the number conserving FPU may be considered as the quantum analogs of these classical states. Clearly, there are many more quantum breather states that are labeled by the number of quanta they contain; a complete study for an arbitrary number of quanta may be performed numerically using techniques such as those in ref [17]. As we pointed out in the second section of the paper, quantization of the number conserving Hamiltonian using local variables introduces an artificial gap in the linear spectrum, leading to an effective on-site term in the Hamiltonian of Eq. (10). As a result, the biphonon states found here may not be very long-lived if used as initial states in the complete quantum FPU model. It is therefore worthwhile investigating via numerically exact procedures if quantum breather states can form in the quantum FPU model without the number conserving approximation, as well as what is the lifetime of the biphonon states found here.

The work presented here may be viewed as describing a minimal model for phenomena occurring in quasi-one dimensional chains of molecular crystals and biological materials. We note that multiphonon states have been observed, as well as analyzed semiclassically, in certain metal-oxide materials [18,19]. On the other hand, a multiphonon analysis was performed in an extension of the Davydov model for quasi-one dimensional macromolecules and applied to the case of $C = O$ stretching vibrations in acetanilide [16]. The latter model and analysis were further used in the fitting of infrared pump-probe experiments in a certain protein, except for the N–H vibrational states [20]. Although the Davydov model used in these works is much more sophisticated than the FPU models in terms of the details it encompasses, the latter is much simpler and, due to the straightforwardness of the calculations it involves, may assist in the understanding of these complex phenomena. In order to make the FPU model compatible with the physics of the aforementioned phenomena, we may introduce an on-site potential term in the Hamiltonian of Eq. (1) of the form $H' = H + \sum_N V(x_n)$, where H' is the new Hamiltonian and $V(x_n) \approx 1/2M\Omega_0^2 x_n^2 +$ higher terms, viz., a generally nonlinear on-site potential at the n-th oscillator site with linear frequency Ω_0. In the boson conserving Hamiltonian of Eq. (10), the new on-site term simply shifts the frequency term ω to

$$\bar{\omega} = \Omega_0 + \omega\left(1 + \frac{3b}{a}\left(\frac{\hbar}{2M\omega}\right)\right).$$

All results represented in Section 3 are still valid, except that the energy spectrum will be shifted by Ω_0; if additional nonlinear terms of the potential $V(x_n)$ are included, some changes may result, as we discuss below.

Let us now use the FPU model with on-site potential to analyze quasi-one dimensional chains of proteins or similar materials such as acetanilide. The bare frequency Ω_0 corresponds to the optical $C = O$ or N–H mode, while the linear coupling between adjacent masses corresponds to dipole–dipole coupling, as in the Davydov model. Let us first consider the case of $b = 0$, viz. only linear coupling terms; then no self-localization may occur, since the model is purely linear, *except* if the optical mode additionally has some anharmonicity. In the latter case, a localized mode may appear almost generically, but it will be only of the on-site type, viz. all bosons on the same site. If, however, we allow for the nonzero FPU nonlinear coupling, i.e. $b \neq 0$, then, as we saw in the previous sections, both on-site and next-nearest site biphonon states may appear, as a direct consequence of the attractive nonlinear intersite coupling. The possible presence of some on-site anharmonicity does not change this feature drastically. The acoustic-type nonlinear terms in the Hamiltonian of Eq. (10) enable the binding of delocalized phonon modes into states effectively localized in one or two adjacent sites. We observe that the FPU model provides an adequate qualitative picture for the experiments in ACN as well as proteins, and may be used as a minimal model to fit the results of these experiments. On the other hand, biphonons may be considered as the lowest quantum states corresponding to classically localized states, i.e. they can be thought of as the simplest quantum breather or quantum soliton states [21].

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