Vol 17 No 11, November 2008
1674-1056/2008/17(11)/4268-05

Chinese Physics B

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Two-vibron bound states in the β–Fermi–Pasta–Ulam model*

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(Received 14 February 2008; revised manuscript received 24 April 2008)

This paper studies the two-vibron bound states in the β–Fermi–Pasta–Ulam model by means of the number conserving approximation combined with the number state method. The results indicate that on-site, adjacent-site and mixed two-vibron bound states may exist in the model. Specially, wave number has a significant effect on such bound states, which may be considered as the quantum effects of the localized states in quantum systems.

Keywords: discrete breathers, Fermi–Pasta–Ulam model, number state method, two-vibron bound states

PACC: 6320, 6320P, 6320R

1. Introduction

In past decades, discrete breathers (DBs) or intrinsic localized modes (ILMs), which are expected to play fundamental roles in both energy storage and transport in various low dimensional materials, have been the subject of intense theoretical researches.[1−5] Experimentally, they have been observed in various physical systems ranging from electronic and magnetic solids to microengineered structures including Josephson junctions and optical waveguide arrays.[6−12] In most of those cases, quantum dynamics is important, for example, quantum effects must be taken into account in molecular crystals. So the quantum counterparts of DBs or quantum breathers (QBs) have attracted intensive attentions in both theoretical[13−17] and experimental[18−20] researches owing to many important applications, for instance, studies of quantum modes on small lattices for quantum devices based on quantum dots.[21] Using numerical exact diagonalization (NED) based on the Einstein phonon basis, we point out that eigenstates in the form of multiphonon bound states are natural equivalents of DBs solutions of classical nonlinear systems.[15] Particularly, the two-vibron bound states (TVBS), which were studied in the Klein–Gordon (KG) lattice[22−24] and Bose–Hubbard (BH) model,[13,14,25] show that such bound states may be the simplest quantum equivalents of breather solutions in classical systems. Furthermore, the formation of TVBS has been observed in molecular adsorbates such as H/Si (111)[26,27], H/C (111)[28] and so on.

Several methods have been developed to investigate the quantum aspects of the DBs as well as QBs in quantum nonlinear systems:[13−16,22,29] the number state method (NSM),[13,14] the NED,[15] 'pseudofield' operator method[16] and so on. The NSM has been widely used to study the translationally invariant systems whose Hamiltonian conserves the number of bosons. In this paper, we will study the TVBS in the quantum version of β–Fermi–Pasta–Ulam (FPU) model by using NSM combined with number conserving approximation which is compatible with rotating wave approximation at the classical level. Originally introduced to shed light on fundamental problems such as thermal conductivity, equipartition of energy, and ergodicity in solids, the FPU chain plays an important role in the nonlinear systems.[30,31] However, the quantum dynamics of FPU model is less investigated and need a detailed inspection.

The present paper is organized as follows. In Section 2, the quantization scheme is first introduced. Then, the quantum dynamics of the quantized β-FPU is obtained within the NSM. The results and analysis are performed in Section 3. Section 4 gives the conclusion of our results.

*Project supported by the Key Project of Hunan Provincial Educational Department of China (Grant No 04A058).

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2. Model and method

The classical β-FPU model describes the nearest-neighbour interactions for a one-dimensional chain. Its Hamiltonian can be written as

$$H = \sum_n \frac{p_n^2}{2m} + \frac{k_2}{2}(x_n - x_{n-1})^2 + \frac{k_4}{4}(x_n - x_{n-1})^4, \quad (1)$$

where m is the mass of an atom, k_2 and k_4 are the nearest-neighbour harmonic and anharmonic force constants, respectively. It is known that this model can support DBs or ILMs.[32] In order to quantize Eq.(1), we write the momentum and position operators of the nth atom as

$$p_n = \mathrm{i}\sqrt{\frac{\hbar m\omega}{2}}(a_n^+ - a_n),$$
$$x_n = \sqrt{\frac{\hbar}{2m\omega}}(a_n^+ + a_n). \quad (2)$$

Here $\omega = \sqrt{2k_2/m}$, a_n^+ and a_n are boson creation and annihilation operators respectively, which satisfy the canonical commutation relations: $[a_m, a_n^+] = \delta_{m,n}$, $[a_m, a_n] = 0$ and $[a_m^+, a_n^+] = 0$. $\lambda = \hbar k_4/(k_2 m\omega)$ is introduced as a dimensionless parameter representing relative magnitude of anharmonic coefficient. Within the number conserving approximation and periodic boundary condition we get the effective Hamiltonian of the β-FPU model

$$\hat{H}_{\mathrm{eff}} = \hbar\omega\Bigg\{\frac{N}{2}\left(1+\frac{3}{4}\lambda\right) + \left(1+\frac{3}{2}\lambda\right)\sum_n a_n^+ a_n - \frac{1}{4}(1+3\lambda)\sum_n a_n^+(a_{n+1}+a_{n-1}) + \frac{3}{8}\lambda\sum_n\left[a_n^+ a_n^+ a_n a_n + \frac{1}{2}a_n^+ a_n^+(a_{n+1}a_{n+1} + a_{n-1}a_{n-1})\right] + \frac{3}{8}\lambda\sum_n\left[a_n^+ a_n(a_{n+1}^+ a_{n+1} + a_{n-1}^+ a_{n-1}) - (a_n^+ a_n^+ a_n a_{n+1} + a_n^+ a_n^+ a_n a_{n-1} + \mathrm{h.c.})\right]\Bigg\}, \quad (3)$$

where N is the total number of atoms. It is worth noting that the same procedure has also been adopted by Refs.[29, 33] in the same model, and Ref.[29] gave a more detailed description of it. In the following, we will employ the NSM to proceed with our analysis in the model.

The NSM has been widely used to study the BH model.[13,14,25,34] The number operator is

$$\hat{N}_1 = \sum_{j=1}^{N} a_j^+ a_j, \quad (4)$$

which has eigenvalue n. Under the periodic boundary conditions, Hamiltonian (3) is invariant under the action of the translation operator $\hat{T}$ with eigenvalue $\exp(\mathrm{i}\cdot k\cdot a)$, where $k = 2\pi\upsilon/(N\cdot a)$, a is the lattice constant, and υ is an integer. $\hat{T}$ is defined by the property $\hat{T}a_j^+ = a_{j+1}^+\hat{T}$ so that $\hat{T}[n_1 n_2 \ldots n_N] = [n_N n_1 \ldots n_{N-1}]$, n_i denotes the quanta at the site i, and $\sum_{i=1}^N n_i = n$. Taking advantage of the fact that $\hat{H}_{\mathrm{eff}}$, $\hat{N}_1$ and $\hat{T}$ are commutative with each other, for $n = 2$ and N odd, we can construct a general eigenfunction of both $\hat{H}_{\mathrm{eff}}$, $\hat{N}_1$ and $\hat{T}$ as

$$|\Psi\rangle = \frac{1}{\sqrt{N}}\Bigg\{\sum_{j=1}^{N}(\mathrm{e}^{\mathrm{i}\cdot k\cdot a}\hat{T})^{j-1}[c_1|20\ldots0\rangle + c_2|110\ldots0\rangle + c_3|1010\ldots0\rangle + \ldots + c_{\frac{N+1}{2}}|10\ldots010\ldots0\rangle]\Bigg\}. \quad (5)$$

To ensure that $\langle\Psi\mid\Psi\rangle = 1$, it is necessary that $c_1, c_2, \ldots$ are normalized as

$$\sum_{j=1}^{(N+1)/2}|c_j|^2 = 1. \quad (6)$$

Requiring that $\hat{H}_{\mathrm{eff}}|\Psi\rangle = E|\Psi\rangle$ we get the matrix equation

$$H_{\mathrm{eff}}c = Ec, \quad (7)$$

where $H_{\mathrm{eff}} = \left[\frac{N}{2}\left(1+\frac{3}{4}\lambda\right)\boldsymbol{I} + Q(k)\right]$, $\boldsymbol{I}$ is $[(N+1)/2]\times[(N+1)/2]$ identity matrix, $c = \mathrm{col}(c_1, c_2, \ldots, c_{(N+1)/2})$, and $Q(k)$ is the $[(N+1)/2]\times$

$[(N+1)/2]$ matrix

$$Q(k) = \begin{pmatrix} u & v^* & & & & \\ v & w & x^* & & & \\ & x & y & x^* & & \\ & & \ddots & \ddots & \ddots & \\ & & & x & y & x^* \\ & & & & x & z \end{pmatrix}, \tag{8}$$

where $u = 2 + \frac{15}{4}\lambda + \frac{3}{4}\lambda\cos(k \cdot a)$, $v = -\sqrt{2}\left(\frac{1}{4} + \frac{9}{8}\lambda\right)(1 + \mathrm{e}^{\mathrm{i}\cdot k\cdot a})$, $w = 2 + \frac{15}{4}\lambda$, $x = -\frac{1}{4}(1 + 3\lambda)(1 + \mathrm{e}^{\mathrm{i}\cdot k\cdot a})$, $z = 2 + 3\lambda - \frac{1}{2}(1 + 3\lambda)\cos\left(\frac{k\cdot a}{2}\right)\left[\cos\left(\frac{N\cdot k\cdot a}{2}\right) + \mathrm{i}\cdot\sin\left(\frac{N\cdot k\cdot a}{2}\right)\right]$, $y = 2 + 3\lambda$. We can calculate the eigenvalues and the corresponding eigenvectors exactly by the standard method from a numerical library.[35]

3. Energy spectrum and TVBS

In the present section, for simplicity, we mainly examine the energy spectrum and the corresponding eigenvectors of $Q(k)$ for both the cases of attractive ($k_4 < 0$) and repulsive ($k_4 > 0$) nonlinearity, as shown in Figs.1 and 2, respectively. Each circle in Figs.1 and 2 represents a single eigenvalue of $Q(k)$ in the lattice Brillouin zone (BZ). When the anharmonic part of the lattice energy is negligible, no matter in the case of attractive or repulsive nonlinearity, the eigen-spectrum is composed of quasi-continuum band, as shown in Figs.1(a) and 2(a). For a macroscopic system, such band covers a dense range of energy and forms a continuous band. However, if the nonlinearity can not be negligible, even if it is weak, a discrete band can be found at the edge of BZ for attractive nonlinearity, while it is found at the centre of BZ for repulsive nonlinearity, as shown in Figs.1(b) and 2(b), respectively. And for both strong attractive and repulsive nonlinearity, the discrete band completely splits from the quasi-continuum band, as shown in Figs.1(c) and 1(d) and 2(c) and 2(d). Similar phenomena have also been discovered in other nonlinear models.[13,14,22,23,25,36] However, the difference between our results and those obtained in the KG lattice[22,23] and BH[13,14,25] models is obvious: at the centre of BZ the width of gap (defined as the minimum of the absolute value of binding energy with respect to q) is much larger than that at the edge of BZ, as displayed in Figs.1(d) and 2 (b–d). We note that in both the BH models[13,14] and the quantum KG models,[22,23] there is only on-site nonlinearity with a linear intrasite coupling. However, the nonlinear term of the β-FPU model is nonlinear quartic interactions which make it possible to form different types of TVBS in the β-FPU model.

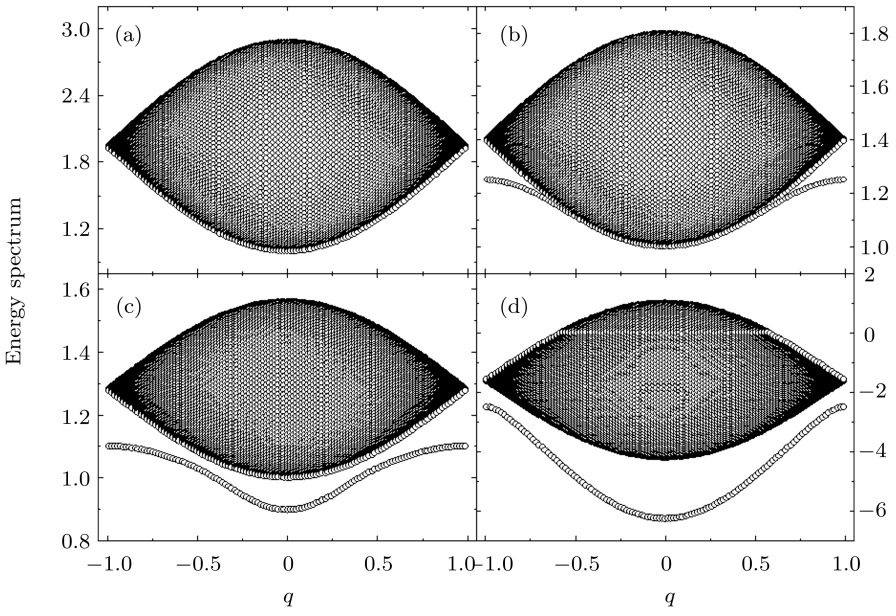


Fig.1. Energy spectrum of $Q(k)$ for different values of λ: (a) $\lambda = -0.02$, (b) $\lambda = -0.2$, (c) $\lambda = -0.24$, (d) $\lambda = -1.2$. The chain is composed of $N = 123$ sites. The Y-axis is measured in units of $\hbar\omega$ while X-axis bears the dimensionless $q = k \cdot a/\pi$ in first Brillouin zone.

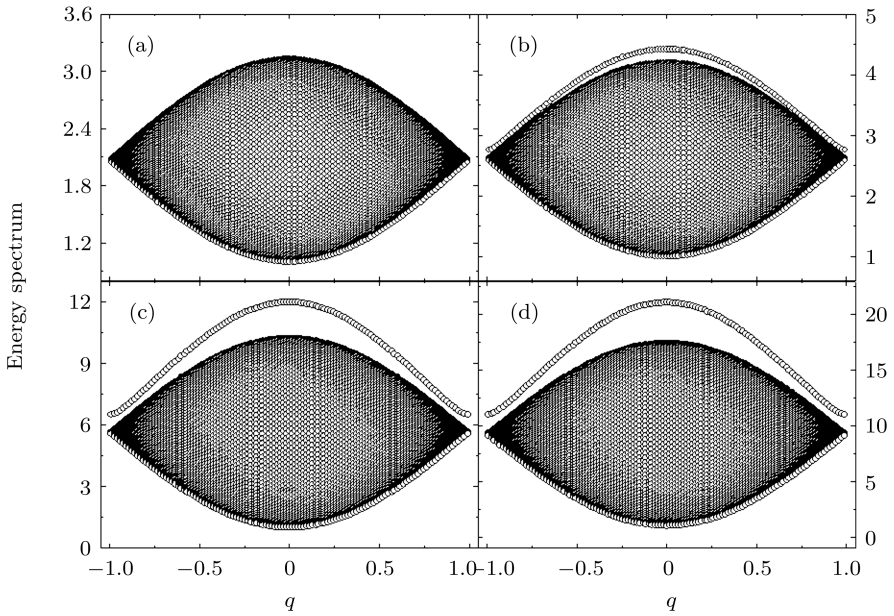


Fig.2. The same as Fig.1, but for repulsive nonlinearity: (a) $\lambda = 0.02$, (b) $\lambda = 0.2$, (c) $\lambda = 1.2$, (d) $\lambda = 2.4$.

To investigate the quantum counterparts of ILMs or DBs in the model, we now analyse the eigenvectors of each eigenvalue in Figs.1 and 2. The examination of the corresponding eigenvectors of the discrete band shows that there exist three different cases (see Fig.3). The first case is: at the centre of BZ, for repulsion (corresponding to the case of Fig.2(b–d)) and strong enough attraction (Fig.1(d)), $|c_1|$ is comparable to $|c_2|$ but much larger than others (corresponding to Fig.3(a)). In this case, the system prefers to be in mixed TVBS where there is a high probability of finding two quanta on the same site or the adjacent site. The second case is: at the centre of BZ and for not strong enough attraction, such as the case of Fig.1(c), $|c_1|$ is much larger than the others (as shown in Fig.3(b)). This means that the system prefers to be in on-site TVBS where the two quanta sit at the same site. And in the third case: $|c_2|$ is much larger than others (displayed in Fig.3(c)) at the edge of BZ for both cases of repulsive and attractive nonlinearity (Figs.1(b–d) and 2(c–d)). Physically, the bound state corresponding to this case is adjacent-site TVBS. Namely, there is a high probability of finding two quanta on the adjacent site. For both strong attractive and repulsive nonlinearity, from the centre to the edge of BZ, $|c_1|$ decreases while $|c_2|$ increases, which is an interesting thing. It means that wave number has a significant effect on the quantum localized states, and it may result from the quantum effects of the localized modes in quantum systems. This localization of energy clearly corresponds to the breather solution of the classical nonlinear system, so the discrete band was also called soliton band.[13] And in contrast to the eigenvectors of discrete band, the corresponding eigenvectors of quasi-continuum band do

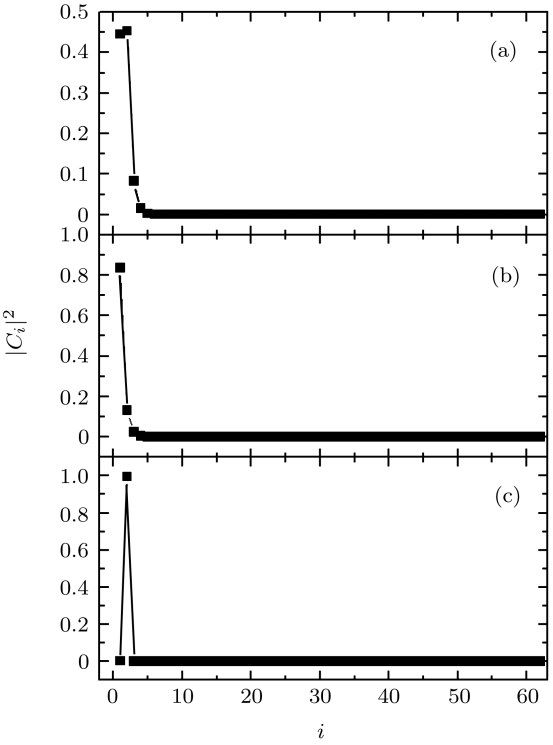


Fig.3. Three cases of bound states: (a) $\lambda = 1.2$, $q = 0$, (b) $\lambda = -0.24$, $q = 0$, (c) $\lambda = 1.2$, $q = 122/123$.

not hold the localized properties, so the quasi-continuum band corresponds to two free vibron states.

It is interesting to note that an analytical method of TVBS was developed for the model in Ref.[29]. Their results show that there only exist two different bound states: on-site and adjacent-site TVBS. However, our results indicate that three different bound states may exist in the model. When the nonlinearity is large enough, only the mixed TVBS and adjacent-site TVBS exist for both the attractive and repulsive nonlinearity, as analysed above. Furthermore, the phenomenon that different parts of BZ correspond to different types of TVBS has also been obtained, which was not reported in Ref.[29]. We note that in Ref.[29] the authors made some approximations in order to proceed with their analysis, which may drop out some information. In addition, the NSM can be simply used to discuss the more quanta cases in the model, while the analytical method in Ref.[29] will confront some difficulties.

4. Conclusions

We quantize the β-FPU model within the boson quantization rules combined with the number conserving approximation. Then by using the NSM, we obtain the energy spectrum of the quantized β–FPU model at two quanta level. Our results confirm that when the nonlinearity is significant, a discrete band will split from the quasi-continuum band. Such behaviour has also been discovered in other nonlinear models.[13,14,22,23,25,36] Differently, by analysing the corresponding eigenvectors of the discrete band, we find that three types of bound states (the mixed TVBS, adjacent-site TVBS and on-site TVBS) may exist in the β-FPU model. We believe that the difference is rooted in the existence of nonlinear quartic interactions. Also, it is somewhat different from the analysis in Ref.[29], where only two types of TVBS were reported. Finally, it should be mentioned that our analysis also reveals an interesting phenomenon: different parts of BZ correspond to different TVBS.

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