# Tangent bifurcation of band edge plane waves, dynamical symmetry breaking and vibrational localization

S. Flach [1]

*Max-Planck-Institut für Physik Komplexer Systeme, Bayreuther Str.40 H.16, D-01187 Dresden, Germany*

## Abstract

We study tangent bifurcation of band edge plane waves in nonlinear Hamiltonian lattices. The lattice is translationally invariant. We argue for the breaking of permutational symmetry by the new bifurcated periodic orbits. The case of two coupled oscillators is considered as an example for the perturbation analysis, where the symmetry breaking can be traced using Poincaré maps. Next we consider a lattice and derive the dependence of the bifurcation energy on the parameters of the Hamiltonian function in the limit of large system sizes. A necessary condition for the occurence of the bifurcation is the repelling of the band edge plane wave from the linear spectrum with increasing energy. We conclude that the bifurcated orbits will consequently exponentially localize in the configurational space.

## 1. Introduction

An increasing number of publications deal with the phenomenon of discrete breathers in nonlinear translationally invariant Hamiltonian lattices (for a history on the subject see [1-8], and references therein). Discrete breathers are time-periodic solutions of the equations of motion. These solutions are exponentially localized in the configurational space (see [9] and in detail [10]). One can view discrete breathers as analog of the breather solutions of the sine-Gordon (sG) partial differential equation [3]. Breathers of the sG equation are structurally unstable (nongeneric) against perturbations of the Hamiltonian density of the sG field [11,12]. In contrast discrete breathers appear to be structurally stable (generic) solutions, with the seeming necessary ingredients being the nonlinearity and the discreteness (i.e. the existence of a finite upper bound of the linear spectrum) [13]. One could think that the sG PDE is the 'bottleneck' which gives contact to the discrete breathers by simply discretising the spatial differential operator. This thought is most probably wrong, because

---

[1] E-mail: flach@idefix.mpipks-dresden.mpg.de

in order to maintain structural stability of discrete breathers one has to avoid resonances of multiples of the breather's frequency with the linear spectrum [10]. Thus discrete breathers appear to be rather unrelated to their counterpart in the sG case.

Proofs of existence of discrete breathers have been given so far for (i) arrays of weakly coupled anharmonic oscillators by use of analytical continuation of periodic orbits [14] and for (ii) chains with homogeneous interaction potentials by use of discrete map analysis of the Fourier coefficients (with respect to time) [13]. Structural stability of discrete breathers has been shown for one-dimensional lattices by use of discrete map analysis of Fourier coefficients [13].

It turns out to be rather complicated to give a proof of existence for discrete breathers for an arbitrarily chosen Hamiltonian function. Still for applications or numerical studies it is important to know whether a given system can possess discrete breathers. From the Fourier coefficient analysis in [10] we can predict, that if the frequency of the breather comes close to the linear spectrum, then the exponent of the spatial decay becomes very small. If the energy of the breather solution becomes small in the same limit, then the breather solution comes close to the solution of a band edge plane wave (here band edge plane wave stands for a plane wave with a wave vector of the band edge of the band of allowed frequencies of the linearized equations of motion). Consequently one could expect that discrete breathers appear due to tangent bifurcations of band edge plane waves if one increases the energy $E_{ZB}$ of the plane wave starting from $E_{ZB} = 0$. Indeed the birth of discrete breather solutions as bifurcating periodic orbits due to the tangent bifurcation of band edge waves has been observed numerically for one-dimensional Fermi–Pasta–Ulam (FPU) lattices [15] with the number $N$ of lattice sites ranging between $N = 40$ and $N = 100$. Note that tangent bifurcation implies that a pair of Floquet multipliers of the linear stability analysis of a periodic orbit collide at $+1$ on the unit circle.

The bifurcation problem of band edge plane waves has been a problem studied independently of the discrete breather phenomenon [16,17]. Budinsky and Bountis [16] have approached the problem using Floquet theory. They have then analyzed the eigenvalue problem for large $N$. However there were discrepancies between the results in [16] and the study by Sandusky and Page [15]. Also in both cases only Fermi–Pasta–Ulam (FPU) chains were considered. Further no analytical results about the properties of the new bifurcated orbits were given. Consequently the goal of the present paper is (i) to derive exact conditions for the tangent bifurcation of band edge plane waves for large $N$, (ii) to consider both FPU and nonlinear Klein–Gordon (KG) systems, and (iii) to show that the bifurcated orbits will break the permutational symmetry of the system and exponentially localize in the configurational space.

In Section 2 we analyze the bifurcational problem for a system of two coupled oscillators ($N = 2$). With the help of Poincaré maps we will show that the derived formula apply. In Section 3 the general lattice with $N$ degrees of freedom is introduced, and the periodic orbits of the band edge plane waves are obtained. The results of the bifurcational analysis are presented in Sections 3.1, 3.2. In Section 3.3 we show that the bifurcated orbits break the permutational symmetry. We discuss our results in Section 4.

## 2. The case of two coupled oscillators

Let us consider the following Hamilton function:

$$H = \tfrac{1}{2}\dot{X}_1^2 + \tfrac{1}{2}\dot{X}_2^2 + V(X_1) + V(X_2) + \Phi(X_1 - X_2),$$  (2.1)

which describes the dynamics of two coupled oscillators using the equations of motion

$$\ddot{X}_{1,2} = -\frac{\partial H}{\partial X_{1,2}}.$$

The potential functions from (2.1) can be expanded in the form

$$V(z) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} v_\mu z^\mu,$$ (2.2)

$$\Phi(z) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} \phi_\mu z^\mu.$$ (2.3)

Note that we have to demand $v_2 \geq 0$ and $\phi_2 > 0$ in order to ensure the potential energy in (2.1) being a positive definite quadratic form in the limit of small energies.

### 2.1. The normal mode periodic orbits

For small energies we can neglect the anharmonic terms $\mu > 2$ in (2.2), (2.3). In that case it is appropriate to transform the original variables into normal coordinates

$$Y_1 = \tfrac{1}{2}(X_1 + X_2), \quad Y_2 = \tfrac{1}{2}(X_1 - X_2).$$ (2.4)

Using the relations given above we obtain the equations of motion for the normal modes including all anharmonic terms of the potential functions (2.2), (2.3):

$$\ddot{Y}_1 = -\sum_{\mu=2}^{\infty} v_\mu \sum_{\nu=0,2,\ldots}^{(\nu \leq (\mu-1))} \binom{\mu-1}{\nu} Y_1^{\mu-1-\nu} Y_2^\nu,$$ (2.5)

$$\ddot{Y}_2 = -\sum_{\mu=2}^{\infty} v_\mu \sum_{\nu=1,3,\ldots}^{(\nu \leq (\mu-1))} \binom{\mu-1}{\nu} Y_1^{\mu-1-\nu} Y_2^\nu - \sum_{\mu=2}^{\infty} \phi_\mu (2Y_2)^{\mu-1}.$$ (2.6)

Note that the sums over $\nu$ in these equations run over even or odd values of $\nu$ respectively because cancellation of terms due to (2.4).

We can now solve (2.5), (2.6) immediately for the two periodic orbits, which correspond to the standard harmonic normal mode solutions in the limit of small energies:

$$\text{I}: \quad Y_2 = 0, \quad \ddot{Y}_1 = -\sum_{\mu=2}^{\infty} v_\mu Y_1^{\mu-1},$$ (2.7)

$$\text{II}: \quad Y_1 = 0, \quad \ddot{Y}_2 = -\sum_{\mu=2}^{\infty} \tilde{v}_\mu Y_2^{\mu-1}, \quad v_{2m+1} = 0.$$ (2.8)

Here the renormalized constants $\tilde{v}_\mu$ for case II in (2.8) are given by

$$\tilde{v}_\mu = v_\mu + 2^{\mu-1} \phi_\mu.$$ (2.9)

Note that we had to require $v_{2m+1} = 0$ in case II (2.8), since in the case of nonvanishing odd terms in the potential $V(z)$ the right hand side of (2.5) has terms containing the variable $Y_2$ only, and the solution would be characterized by nonzero $Y_1$.

The solutions of the differential equations (2.7), (2.8) are given in terms of elliptic functions. Here we will be interested in the limit of small energies (amplitudes) and apply standard perturbation theory ([18] Chapter 7). For case I (Eq. (2.7)) we obtain

$$Y_1 = \sum_{k=-\infty}^{+\infty} A_k e^{ik\omega t} , \quad A_k = A_{-k} ,$$ (2.10)

$$\omega^2 = v_2 + \left( \frac{3v_4}{2v_2} - \frac{5v_3^2}{3v_2^2} \right) E_1 ,$$ (2.11)

$$A_0 = -\frac{v_3}{v_2^2} E_1 , \quad A_1^2 = \frac{1}{2v_2} E_1 , \quad A_2 = \frac{v_3}{6v_2^2} E_1 ,$$ (2.12)

$$E_1 = \tfrac{1}{2} \dot{Y}_1^2 + V(Y_1) .$$ (2.13)

For case II (Eq. (2.8)) we obtain in a similar way

$$Y_2 = \sum_{k=-\infty}^{+\infty} A_k e^{ik\omega t} , \quad A_k = A_{-k} ,$$ (2.14)

$$\omega^2 = \tilde{v}_2 + \left( \frac{3\tilde{v}_4}{2\tilde{v}_2} - \frac{5\tilde{v}_3^2}{3\tilde{v}_2^2} \right) E_2 ,$$ (2.15)

$$A_0 = -\frac{\tilde{v}_3}{\tilde{v}_2^2} E_2 , \quad A_1^2 = -\frac{1}{2\tilde{v}_2} E_2 , \quad A_2 = \frac{\tilde{v}_3}{6\tilde{v}_2^2} E_2 ,$$ (2.16)

$$E_2 = \tfrac{1}{2} \dot{Y}_2^2 + \tilde{V}(Y_2) , \quad \tilde{V}(z) = \sum_{\mu=2}^{\infty} \frac{1}{\mu} \tilde{v}_\mu z^\mu .$$ (2.17)

All terms not present in (2.10)–(2.17) are of order $E_{1,2}^2$ or higher and can be neglected, as we will see in the following.

## 2.2. Tangent bifurcation for periodic orbit I

Let us consider a small perturbation $\delta_{1,2}$ of the periodic orbit I

$$Y_{1,2} \rightarrow Y_{1,2} + \delta_{1,2} .$$

If we linearize the resulting equations of motion for the perturbation we obtain

$$\ddot{\delta}_1 = -\sum_{\mu=2}^{\infty} (\mu - 1) v_\mu Y_1^{\mu-2} \delta_1 ,$$ (2.18)

$$\ddot{\delta}_2 = -\sum_{\mu=2}^{\infty} (\mu - 1) v_\mu Y_1^{\mu-2} \delta_2 - 2\phi_2 \delta_2 .$$ (2.19)

Note, that the variable $Y_1$ in (2.18), (2.19) is the time-periodic solution of (2.7). As we see, the perturbations do not couple with each other. Equation (2.18) describes the continuation of the periodic orbit (2.7) along itself (shift of time origin) or along the one-parameter family (change of energy $E_1$ or frequency $\omega$). The associated pair of Floquet multipliers is obviously located at $+1$ on the unit circle [18].

Eq. (2.19) then describes the nontrivial perturbations (the associated phase space is two-dimensional, and can be visualized with the help of Poincaré maps). Let us rewrite (2.19):

$$\ddot{\delta}_2 = -\left[ (v_2 + 2\phi_2) + f(t) \right] \delta_2 ,$$ (2.20)

$$f(t) = \sum_{\mu=3}^{\infty} (\mu - 1) v_\mu Y_1^{\mu-2} .$$ (2.21)

This type of equation is called Hill's equation [19], since the function $f(t)$ is periodic in time (with the period of $Y_1$):

$$f(t) = f(t + 2\pi/\omega) .$$

We are interested in tangent bifurcations which appear when

$$\frac{\sqrt{v_2 + 2\phi_2}}{\omega} \approx 1 .$$ (2.22)

The function $f(t)$ in (2.21) can be expanded in a Fourier series:

$$f(t) = \sum_{k=-\infty}^{+\infty} F_k e^{ik\omega t} , F(k) = F_{-k} .$$ (2.23)

If the function $f(t)$ becomes infinitesimally small, then according to the Floquet theory [19] parametric resonance can appear for the cases

$$\frac{\sqrt{v_2 + 2\phi_2}}{k\omega} = \frac{k'}{2} , \quad k' = 1, 2, 3, \ldots .$$ (2.24)

With (2.22) the relevant pairs $(k, k')$ become (1,2), (2,1). In the limit of small values of $E_1$ we can then retain in (2.20) the significant terms only:

$$\ddot{\delta}_2 = - \left[ \Omega^2 + 2F_1 \cos(\omega t) + 2F_2 \cos(2\omega t) \right] \delta_2 ,$$ (2.25)

$$\Omega^2 = v_2 + 2\phi_2 + F_0 .$$ (2.26)

Using relations (2.11)–(2.13) we obtain for small $E_1$

$$F_0 = \left( -2\frac{v_3^2}{v_2^2} + 3\frac{v_4}{v_2} \right) E_1 ,$$ (2.27)

$$F_1 = \sqrt{2}\frac{v_3}{\sqrt{v_2}}\sqrt{E_1} ,$$ (2.28)

$$F_2 = \left( \frac{1}{3}\frac{v_3^2}{v_2^2} + \frac{3}{2}\frac{v_4}{v_2} \right) E_1 .$$ (2.29)

A tangent bifurcation will appear if the solution for the perturbation $\delta_2(t)$ becomes periodic with the period of the function $f(t)$ (since at the bifurcation the associated pair of Floquet multipliers has to merge at $+1$ on the unit circle):

$$\delta_2(t) = \delta_2(t + 2\pi/\omega) .$$

For given potential functions (2.2), (2.3) this can happen only at certain energies $E_1^c$. Applying the method of strained parameters [18] to our problem we obtain two solutions

(i) : $\phi_2 = 0 , E_1^c$ arbitrary , (2.30)

(ii) : $E_1^c = \frac{6v_2^2}{10v_3^2 - 9v_2v_4}\phi_2 .$ (2.31)

Since we have to require positive values for $E_1$ and $\phi_2$ tangent bifurcation can take place only if

$$\frac{v_4}{v_2} \leq \frac{10}{9}\frac{v_3^2}{v_2^2} \tag{2.32}$$

is fulfilled. Remarkably this condition (2.32) is equivalent to requiring the frequency of the periodic orbit I being a decreasing function of $E_1$ (cf. (2.11)). Note that we have to exclude the nongeneric case of $v_3 = v_4 = 0$ (however we have no restrictions on $\phi_{3,4,...}$ since the anharmonic interaction terms simply do not contribute to the linearized equations (2.18), (2.19)). The two solutions (2.30), (2.31) define two lines in the space $\{E_1, \phi_2\}$. The area between the two lines corresponds to the parameter cases when the periodic orbit is hyperbolic due to tangent bifurcation. Note that the requirement of small energies implies also small values of $\phi_2$. For large values of $E_1$ and $\phi_2$ higher order corrections will appear.

### 2.3. Tangent bifurcation for periodic orbit II

In analogy to the previous chapter we derive the linearized equations for the perturbation of the periodic orbit II:

$$\ddot{\delta}_1 = -\sum_{\mu=2}^{\infty}(\mu - 1)v_{\mu}Y_2^{\mu-2}\delta_1, \tag{2.33}$$

$$\ddot{\delta}_2 = -\sum_{\mu=2}^{\infty}(\mu - 1)\tilde{v}_{\mu}Y_2^{\mu-2}\delta_2. \tag{2.34}$$

Note that we had to require $v_{2m+1} = 0$. Again the perturbations do not couple with each other. Eq. (2.34) describes continuation of the periodic orbit II.

Eq. (2.33) gives the nontrivial perturbations. It is again a Hill's equation. In the limit of small energies $E_2$ we obtain in analogy to (2.20)-(2.29)

$$\ddot{\delta}_1 = -[\Omega_2 + 2F_2\cos(2\omega t)]\delta_1, \tag{2.35}$$

$$\Omega^2 = v_2 + F_0, \tag{2.36}$$

$$F_0 = 3\frac{v_4}{v_2}E_2, \tag{2.37}$$

$$F_2 = \frac{3}{2}\frac{v_4}{v_2}E_2. \tag{2.38}$$

Requiring periodicity $\delta_1(t) = \delta_1(t + 2\pi/\omega)$ and applying the method of strained parameters we find the two solutions for a tangent bifurcation

$$(\text{i}): \quad E_2^c = \frac{6v_2^2}{80\phi_3^2 - 36v_2\phi_4}\phi_2, \tag{2.39}$$

$$(\text{ii}): \quad E_2^c = \frac{6v_2^2}{9v_2v_4 + 80\phi_3^2 - 36v_2\phi_4}\phi_2. \tag{2.40}$$

Again these two solutions define two lines in the space $\{E_2, \phi_2\}$. The area between the lines corresponds to the parameter cases when the periodic orbit II is hyperbolic due to tangent bifurcation.

## 2.4. Symmetry breaking

The scenario of the tangent bifurcations of periodic orbits I and II from the last two chapters can be studied numerically by use of Poincaré maps. For that we always fix the total energy of the system, and plot the pair $\{X_1, \dot{X}_1\}$ if the conditions $X_2 = 0$, $\dot{X}_2 > 0$ are fulfilled. First we use this circumstance for checking the validity of our results. We find excellent agreement. More precisely we test our analytical calculations by evaluating numerically the Hill's eigenvalue problem (2.19) and (2.33) for the two orbits. We find the tangent bifurcation, i.e. the merging of the two Floquet multipliers at $+1$ exactly for the predicted parameter combinations.

An example for the bifurcation of periodic orbit I is shown in Fig. 1 for the parameter cases $v_2 = 1$, $v_3 = 3$, $v_4 = 1$, $\phi_2 = 0.01$, $\phi_3 = 1$, $\phi_4 = 1$. According to (2.31) the bifurcation energy is given by $E_1^c = 7.407 \times 10^{-4}$. In Fig. 1a we show the Poincaré map of the surrounding of the periodic orbit I for $E_1 = 7 \times 10^{-4}$ and in Fig. 1b for $E_1 = 7.7 \times 10^{-4}$ (note that we did not show Poincaré maps too close to the bifurcation point only because of the computational time which increases to infinity at the bifurcation point because the winding number comes very close to unity). Clearly in Fig. 1a the orbit I is still of elliptic character, whereas in Fig. 1b the bifurcation already occurred, giving rise to the birth of two new periodic orbits labelled by $A$ and $B$ in the plot respectively. These bifurcated orbits are separated by a separatrix which contains the old periodic orbit I.
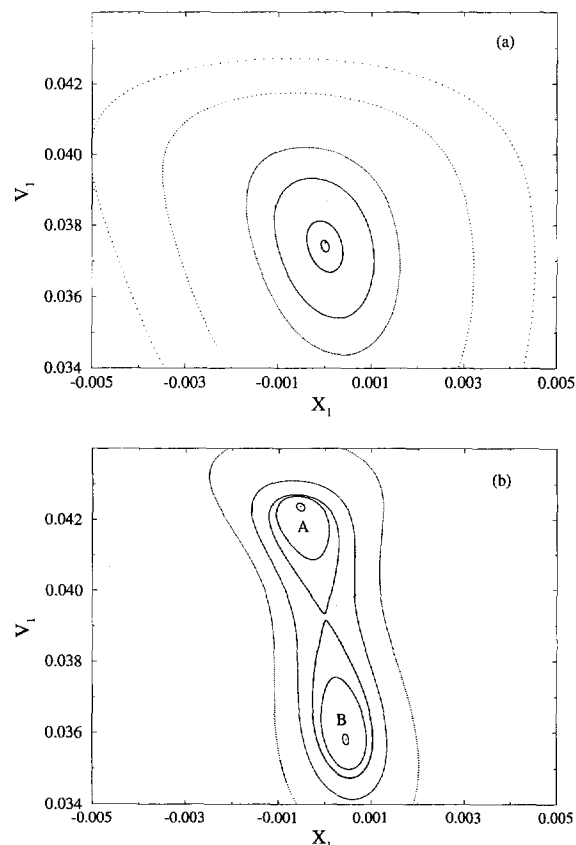


Fig. 1. Poincaré plot for the system of two coupled oscillators. The condition is $X_2 = 0$, $\dot{X}_2 > 0$. The parameters are given in the text. Only a part of the available phase space is shown, which includes the relevant periodic orbit I. (a) The energy is below the bifurcation; (b) The energy is above the bifurcation. A and B labels the two new periodic orbits, which appeared due to the bifurcation of the periodic orbit I.
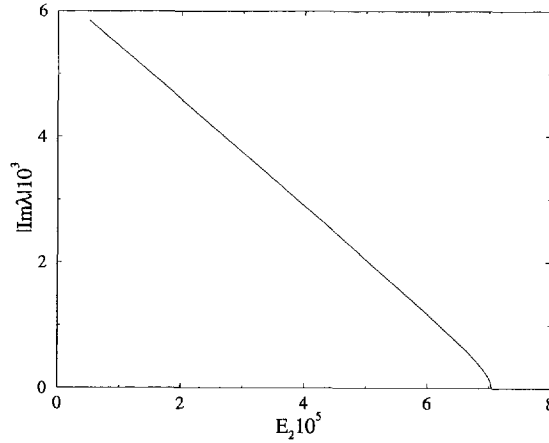
Fig. 2. The imaginary part of the Floquet multiplier (absolute value) of the Hill's equation as a function of the energy $E_2$ for periodic orbit II and parameters as given in the text. At energies larger than the bifurcation energy the imaginary part vanishes.

The bifurcation of periodic orbit II is demonstrated in Fig. 2 for the parameter cases $v_2 = 1$, $v_3 = 0$, $v_4 = 1$, $\phi_2 = 0.001$, $\phi_3 = 1$, $\phi_4 = 0.1$. According to (2.39), (2.40) the bifurcation occurs for $E_2^c = 7.0258 \times 10^{-5}$. We plot the imaginary part of the Floquet multiplier evaluated from Eq. (2.33) as a function of the energy $E_2$. The obtained value for the bifurcation energy is $E_2^c = 7.042 \times 10^{-5}$, which gives a deviation of 0.2% of the value from our perturbation approach.

The considered system of two coupled oscillators exhibits permutational symmetry $H(X_1, X_2) = H(X_2, X_1)$ if we require $\phi_{2m+1} = 0$. Still the tangent bifurcation of orbits I and II occur. If we define the permutational operator $\widehat{P}$ as

$$\widehat{P}g(X_1, X_2, \dot{X}_1, \dot{X}_2) = g(X_2, X_1, \dot{X}_2, \dot{X}_1)$$

then the normal coordinates are transformed as

$$\widehat{P}Y_1 = Y_1, \quad \widehat{P}Y_2 = -Y_2. \tag{2.41}$$

Let us consider the bifurcation of orbit I. This orbit corresponds to a closed loop in the phase space of the system. Its position is restricted to the subspace $\{Y_2 = \dot{Y}_2 = 0\}$. The trajectory of orbit I evolves along the loop parametrically with time. If a tangent bifurcation occurs, then the bifurcated orbits will correspond to slightly deformed loops of the original one. These deformed loops will move out of the subspace $\{Y_2 = \dot{Y}_2 = 0\}$ as we have shown. Let us assume that the deformed loops are invariant under permutation. Applying $\widehat{P}$ to such a loop is equivalent to a reflection at the subspace $\{Y_2 = 0, \dot{Y}_2 = 0\}$. It is clear that it is impossible to construct such a deformed loop without crossing the subspace $\{Y_2 = 0, \dot{Y}_2 = 0\}$. But it is forbidden to cross this subspace, since any point from it belongs to a periodic orbit I (parametrized by its energy). Thus we conclude that the deformed loops can not be invariant under permutation. So the bifurcated orbits break permutational symmetry. Then there have to exist at least two bifurcated orbits, which are transformed into each other by applying $\widehat{P}$. Indeed in Fig. 1b we observe two bifurcated orbits. We have tested the permutation of these orbits numerically, and found that both orbits break the permutational symmetry and are transformed into each other by applying $\widehat{P}$. Moreover, all quasiperiodic motions surrounding any one of the bifurcated orbits and bounded by the separatrix also have broken permutational symmetry. The whole corresponding phase space regions are connected to each other by $\widehat{P}$.

It is straightforward to show that also the tangent bifurcation of orbit II creates bifurcated orbits which break the permutational symmetry. The scenario of both bifurcations are identical. This symmetry breaking of the dynamics of two coupled oscillators has been observed also numerically by Vakakis and Rand [20].

Let us summarize what we have shown so far. We studied the problem of two coupled oscillators and derived the dependence of the energy of tangent bifurcation of normal modes on the model parameters for small energies. We have shown analytically and demonstrated numerically that the new bifurcated orbits will break the permutational symmetry of the system (if it existed).

## 3. The case of the lattice

Let us now turn to the main subject – the bifurcational problem of periodic orbits of a lattice. We will consider a one-dimensional lattice with nearest neighbour interaction and one degree of freedom per unit cell. We will then show that the derived results apply also to lattices with larger interaction ranges. The problem of lattices with higher dimension will be discussed.

The Hamilton function of the lattice is given by

$$H = \sum_{l=1}^{N} \left[ \tfrac{1}{2} \dot{X}_l^2 + V(X_l) + \Phi(X_l - X_{l-1}) \right] . \tag{3.1}$$

The potential functions $V(z)$ and $\Phi(z)$ are again represented in the form (2.2), (2.3). We assume periodic boundary conditions

$$X_l = X_{l+N} , \quad \dot{X}_l = \dot{X}_{l+N} .$$

Then system (3.1) exhibits permutational symmetry. The permutational operator $\widehat{P}$ is defined by

$$\widehat{P} g(X_1, X_2, ..., X_N, \dot{X}_1, \dot{X}_2, ..., \dot{X}_N) = g(X_2, X_3, ..., X_N, X_1, \dot{X}_2, \dot{X}_3, ..., \dot{X}_N, \dot{X}_1) . \tag{3.2}$$

Clearly $\widehat{P}^N = \widehat{1}$ and $\widehat{P} H = H$.

Let us introduce normal coordinates

$$Q_q = \frac{1}{N} \sum_{l=1}^{N} e^{iql} X_l . \tag{3.3}$$

The wave number $q$ can take any of the values

$$q = \frac{2\pi}{N} n , \quad n = 0, 1, 2, ..., (N - 1) .$$

The inverse transform of (3.3) is given by

$$X_l = \sum_{q} e^{-iql} Q_q . \tag{3.4}$$

The equations of motion for the normal coordinates $Q_q$ read

$$\ddot{Q}_q = \frac{1}{N} \sum_{l=1}^{N} e^{iql} \ddot{X}_l = -\frac{1}{N} \sum_{l=1}^{N} e^{iql} \frac{\partial H}{\partial X_l} . \tag{3.5}$$

Using (3.1) and (2.2), (2.3) we obtain the following lengthy expression:

$$\ddot{Q}_q = -\omega_q^2 Q_q - \sum_{\mu=3}^{\infty} v_\mu \sum_{q_1,q_2,\dots,q_{\mu-2}} \left[\prod_{\nu=1}^{\mu-2} Q_{q_\nu}\right] Q_{q-\sum_{\nu=1}^{\mu-2} q_\nu}$$

$$-\sum_{l=1}^{N} e^{iql} \sum_{\mu=3}^{\infty} \phi_\mu \left[\left\{\sum_{q'}(1-e^{iq'})\,e^{-iq'l}\,Q_{q'}\right\}^{\mu-1} - \left\{\sum_{q''}(e^{-iq'}-1)\,e^{-iq''l}\,Q_{q''}\right\}^{\mu-1}\right]. \tag{3.6}$$

Here $\omega_q$ abbreviates the eigenfrequencies of the linearized (in $Q_q$) equations of motion and is given by the dispersion relation

$$\omega_q^2 = v_2 + 4\phi_2\sin^2\left(\frac{q}{2}\right). \tag{3.7}$$

Let us give the solutions for two periodic orbits of the considered lattice, which correspond to the band edge plane waves ($q = 0$ and $q_{N/2} = \pi$) in the limit of small energies:

$$\text{I}: \quad Q_{q\neq 0}=0, \quad \ddot{Q}_{q=0} = -\sum_{\mu=2}^{\infty} v_\mu Q_{q=0}^{\mu-1}, \tag{3.8}$$

$$\text{II}: \quad Q_{q\neq\pi}=0, \quad \ddot{Q}_{q_{N/2}} = -\sum_{\mu=2,4,6,\dots}^{\infty} \bar{v}_\mu Q_{q_{N/2}}^{\mu-1}. \tag{3.9}$$

The parameter $\bar{v}_\mu$ is given by

$$\bar{v}_\mu = v_\mu + 2^\mu \phi_\mu$$

(note the difference to (2.9)). In case II we have to demand (as in the previous chapters for the two oscillators)

$$\text{II}: \quad v_{2m+1} = 0$$

in order to be able to continue the upper band edge plane wave to finite energies in the given form. The terms $\phi_{2m+1}$ can be in general nonzero, but they simply do not contribute to (3.9) because of the odd symmetry of the upper band edge plane wave [15].

### 3.1. Tangent bifurcation of orbit I

Let us consider a small perturbation $\{\delta_q\}$ of the periodic orbit I

$$Q_q \rightarrow Q_q + \delta_q.$$

Linearizing the equations of motion for the perturbation we obtain

$$\ddot{\delta}_q = -\omega_q^2 \delta_q - \sum_{\mu=3}^{\infty}(\mu-1)v_\mu Q_{q=0}^{\mu-2}\delta_q. \tag{3.10}$$

The analogy to the problem of two coupled oscillators is striking (cf. (2.7), (2.18), (2.19)). For $q = 0$ Eq. (3.10) describes the continuation of the periodic orbit itself. All other perturbations do not couple with each other, so that we can consider (3.10) for each value of $q$ separately. If we increase the energy

$$E_I = \tfrac{1}{2}\dot{Q}_{q=0}^2 + V(Q_{q=0}) \tag{3.11}$$

(note that the periodic orbit solution has to be inserted in (3.11)) then the first tangent bifurcation will occur if $q_1 = 2\pi/N$ is chosen in Eq. (3.10). For large values of $N$ we have

$$\omega_{q_1}^2 = v_2 + 4\phi_2 \frac{\pi^2}{N^2}$$

and consequently obtain (using (2.10)-(2.13) and (2.20)-(2.29)) the following bifurcation energy $E_I^c$:

$$(\text{i}) : \quad \phi_2 = 0, \quad E_I^c \text{ arbitrary}, \tag{3.12}$$

$$(\text{ii}) : \quad E_I^c = \frac{1}{N^2} \frac{12\pi^2 v_2^2 \phi_2}{10v_3^2 - 9v_2 v_4}. \tag{3.13}$$

Since we have to require positive values for $E_I^c$ and $\phi_2$ tangent bifurcation can take place only if

$$\frac{v_4}{v_2} \leq \frac{10}{9} \frac{v_3^2}{v_2^2} \tag{3.14}$$

in full accordance to Eq. (2.32). Note that this condition is only necessary, since we have also to require $v_2 \neq 0$ (in the case $v_2 = 0$ the dependence of the periodic orbit solution on $E_I^c$ becomes different; since this is a nongeneric case, we ignore it). Condition (3.14) is equivalent to the condition, that the frequency of the lower band edge plane wave decreases with increasing energy, In other words, the necessary condition for a tangent bifurcation of the lower band edge plane wave is the repelling of its frequency from the linear spectrum (3.7) with increasing energy.

The energy $E_I$ is on the scale of total energy per particle (cf. (3.1), (3.3), (3.11)). Consequently the energy threshold of the tangent bifurcation decreases as $N^{-2}$ on the scale of energy per particle. In the limit $N \to \infty$ the threshold goes to zero.

It is important to note, that if all variables $X_l$ are real, the normal coordinates as defined are complex. However since the equation (3.10) is linear in $\delta_q$ and since the mode $Q_{q=0}$ is real, we can consider the perturbational problem always separately for the real and imaginary parts of a perturbation $\delta_q$.

## 3.2. Tangent bifurcation for orbit II

We again derive the linearized equations for the perturbation $\delta_q$:

$$\ddot{\delta}_{q_{a,b}} = -\omega_{q_{a,b}}^2 \delta_{q_{a,b}} \sum_{\mu=4,6,\dots}^{\infty} (\mu-1) \bar{v}_{\mu,q_{a,b}} Q_{q_{N/2}}^{\mu-2} \delta_{q_{a,b}} - i \sum_{\mu=3,5,\dots}^{\infty} (\mu-1) \bar{\phi}_{\mu,q_{b,a}} Q_{q_{N/2}}^{\mu-2} \delta_{q_{b,a}}. \tag{3.15}$$

Here we have used the following notations:

$$\bar{v}_{\mu,q_{a,b}} = v_\mu + \sin^2 \left( \frac{q_{a,b}}{2} \right) 2^\mu \phi_\mu, \tag{3.16}$$

$$\bar{\phi}_{\mu,q_{a,b}} = -\sin(q_{a,b}) 2^\mu \phi_\mu. \tag{3.17}$$

The two wave numbers $q_{a,b}$ are related to each other by

$$q_b = q_a \pm \pi \mod 2\pi. \tag{3.18}$$

In contrast to the previous cases we have a coupling between a pair of normal coordinates (3.18) in (3.15). Notice that the coupling term is given by the second sum on the right hand side of (3.15) and is zero if

$\phi_{2m+1} = 0$. Also this coupling term is proportional to $i$, which causes a mixing of real and imaginary parts of the perturbations.

Interestingly for the pair $q_a = \pi, q_b = 0$ we obtain again no coupling, because (3.17) vanishes for both wavenumbers. Consequently for $q = \pi$ (3.15) describes the continuation of the periodic orbit II.

### 3.2.1. The case $\phi_{2m+1} = 0$

If we assume $\phi_{2m+1} = 0$ then the equations for the perturbations $\delta_{q_{a,b}}$ decouple. In analogy to the case of orbit I we have the first tangent bifurcation of orbit II if we consider the perturbation $q = \pi(1 - 2/N)$. Consequently we obtain for the bifurcation energy $E_{II}^c$

$$(\mathrm{i}) : \quad \phi_2 = 0, \quad E_{II}^c \text{ arbitrary}, \tag{3.19}$$

$$(\mathrm{ii}) : \quad E_{II}^c = \frac{1}{N^2} \frac{v_2 + 4\phi_2}{3(v_4 + 16\phi_4)} 4\pi^2 \phi_2 . \tag{3.20}$$

Again we observe that a bifurcation will take place only if $\bar{v}_\mu$ is positive, i.e. only if the frequency of the periodic orbit II is repelled from the linear spectrum with increasing energy.

We can compare these findings with the calculation of Budinsky and Bountis [16], who have calculated the bifurcation energy for $v_{\mu=0}$, $\phi_2 = \phi_4 = 1$, $\phi_\mu = 0$ otherwise. They obtain $E^c = 3.226/N^2$ (Eq. (2.22) from [16]). Our result gives $E^c = \pi^2/(3N^2) \approx 3.29/N^2$. Budinsky and Bountis have roughly estimated the eigenvalue spectrum of the corresponding Hill's matrix in the original coordinates. We think that this circumstance is the reason for the small deviation of their approximate result from our exact one.

Note that Budinsky and Bountis are looking for the first bifurcation to occur, either tangent or period doubling. It can happen that a period doubling bifurcation occurs prior the tangent one. In that case only the result for the period doubling bifurcation would be given in their paper. In the quoted comparison indeed the tangent bifurcation takes place first, thus the apparent coincidence in the results. However for other cases period doubling bifurcations can occur first. Then our results can not be compared to the ones of Budinsky and Bountis (cf. also the discussion section).

### 3.2.2. The case $\phi_{2m+1} \neq 0$

Now the coupling between two perturbations has to be taken into account. We use the fact that $Q_{q_{N/2}}$ is real and the equations for the complex perturbations are linear. By taking the complex conjugate of any of the two equations defined by (3.15) and considering say only the real part of $\delta_{q_a}$ and the imaginary part of $\delta_{q_b}$ we find in the limit of small energies $E_{II}$

$$\ddot{\delta}_{q_{a,b}} = -(\omega_{q_a}^2 + 3\bar{v}_{4,q_{a,b}} Q_{q_{N/2}}^2)\delta_{q_{a,b}} - \bar{\phi}_{3,q_{b,a}} Q_{q_{N/2}} \delta_{q_{b,a}} . \tag{3.21}$$

Note that we have changed the relation between $q_a$ and $q_b$ to

$$q_b = |q_a - \pi|, \quad q_a \bmod \pi/2 .$$

The lowest tangent bifurcation energy of orbit II appears for

$$q_a = \pi(1 - \frac{2}{N}), \quad q_b = \frac{2\pi}{N} .$$

Then it follows

$$\bar{\phi}_{3,q_a} = \bar{\phi}_{3,q_b} = -16\phi_3 \frac{\pi}{N} .$$

One could expect that in the limit of large $N$ the coupling between $q_a$ and $q_b$ vanishes. That is indeed so if we require $v_2 \neq 0$ (linear spectrum is optical-like) but turns out to be wrong for the case $v_2 = 0$ (linear spectrum is acoustic-like). The details of these subtleties are given in Appendix A. Here we proceed to the final result for the tangent bifurcation energy $E_{II}^c$:

$$(i) : \quad E_{II}^c = \frac{1}{2\phi_3^2} (v_2 + 4\phi_2)(\phi_2 + \tfrac{3}{16}v_2)\phi_2 , \tag{3.22}$$

$$(ii) : E_{II}^c = \begin{cases} \dfrac{4\pi^2}{N^2} \dfrac{v_2 + 4\phi_2}{3(v_4 + 16\phi_4)}\phi_2 , & v_2 \neq 0 \\[3mm] \dfrac{16\pi^2}{N^2} \dfrac{\phi_2^3}{3\phi_2(v_4 + 16\phi_4) - 64\phi_3^2} , & v_2 = 0 \end{cases} \tag{3.23}$$

As we can see solution (i) (3.22) is always positive (since $\phi_2 > 0$ and $v_2 \geq 0$) but is not dependent on $N$. Since we applied perturbation theory, (3.22) is correct only in the limit of small energies. For larger energies corrections apply. Solution (ii) (3.23) is the one which gives arbitrarily small bifurcation energies for sufficiently large $N$. Since $\phi_3$ does not enter the energy dependence of periodic orbit II, we then again obtain as the necessary condition for the existence of the bifurcation, that the frequency of the upper band edge plane wave has to be repelled from the linear spectrum with increasing energy. However for the case $v_2 = 0$ a more restrictive condition is obtained by demanding

$$3\phi_2(v_4 + 16\phi_4) \geq 64\phi_3^2 . \tag{3.24}$$

Sandusky and Page [15] have considered the case $\phi_2 \neq 0$, $\phi_3 \neq 0, \phi_4 \neq 0$, $\phi_\mu = 0$ otherwise. However in contrast to Budinsky and Bountis no clear finite size studies are done in [15]. Instead these authors use dimensionless parameters, which however contain the amplitude (energy). Still we can consider Eq. (24) from [15] and by performing the limit of small amplitudes we recover our necessary condition (3.24). Figs. 8 and 9 from [15] are showing a crossover from the parameter region where (3.24) holds into the region where it is not valid. From our analysis it follows that this corresponds to a change from (3.23) to (3.22) and consequently to a change from infinitesimally small energy (amplitude) thresholds to finite thresholds. Indeed finite amplitude thresholds for the instability have been observed in [15] after leaving the parameter region where (3.24) is valid.

It is interesting to note that condition (3.24) has been obtained with the help of multiple scale expansions already in 1972 by Tsurui [21] (Eq. (4.8), $\omega_c^2 = 4$) and more recently by Flytzanis, Pnevmatikos and Remoissenet [22] (Eq. (5.15)) for systems with $v_\mu = 0$.

### 3.3. Symmetry breaking

Using (3.2), (3.3) it follows

$$\hat{P}^n Q_q = e^{iqn} Q_q , \quad q = \frac{2\pi}{N}m , \quad m = 0, 1, 2, ..., (N-1) . \tag{3.25}$$

First we notice that the permutational operator does not mix the space of the normal coordinates. In other words, every subspace $\{\dot{Q}_q, Q_q\}$ is invariant under (3.2). However since the phase space is higher dimensional compared to the case of two coupled oscillators, the new bifurcated orbits can not be confined to some subspace (in order to use the argumentation of the two coupled oscillators case).

Let us consider the bifurcation of orbit I. We will project a new bifurcated orbit loop into the subspace $\{Q_0, \dot{Q}_0, Q_1, \dot{Q}_1\}$. We can use a reference picture in a three-dimensional space, where the $Z$-axis contains both
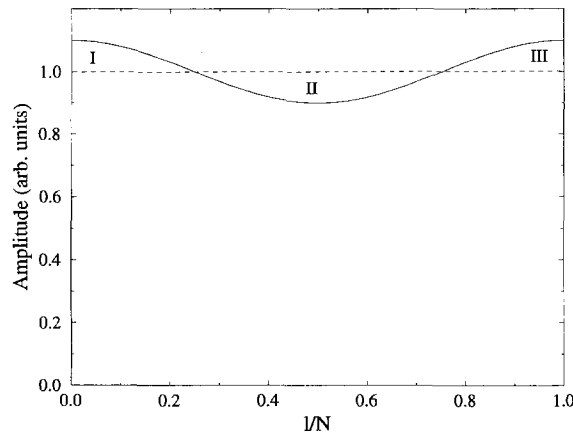
Fig. 3. Schematic representation of the relevant perturbation of a periodic orbit I due to the symmetry breaking. The x-axis represents the normalized spatial variable $l/N$, and the y-axis the amplitude of the solution in arbitrary units. The dashed line indicates the amplitude distribution of the original periodic orbit I.

variables $Q_0$ and $\dot{Q}_0$. Now the projected loop can cross the $Z$-axis (in contrast to the case of two coupled oscillators), because at the moment of the crossing the original loop can still not intersect with the subspace $\{Q_0, \dot{Q}_0\}$. However we notice that every loop (also the projected one) have a certain direction of rotation of the trajectory. If the loop is invariant under $\hat{P}$, so is its projection. The direction of rotation can either be conserved or change sign under permutation. So if we choose $n = N/2$, $n$ even, in (3.25) then the direction of rotation is conserved. Then we observe, that the constructed operation $\hat{P}^{N/2}$ leaves the periodic orbit I, but switches the sign of the coordinates of the relevant perturbation $Q_1$. Applying the permutation to the projected loop is equivalent to reflecting the loop at the subspace $\{Q_0, \dot{Q}_0\}$ (the $Z$-axis in the reference picture). Clearly this reflection switches the direction of rotation. Consequently our initial assumption was wrong, and the bifurcated orbits indeed break permutational symmetry. It is straightforward to show that also the new bifurcated orbits in the case of a tangent bifurcation of orbit II break permutational symmetry.

Then in general the new bifurcated orbits will be not invariant under $\hat{P}$, and thus the bifurcated orbits will correspond to band edge modes. which are spatially modulated by the relevant perturbation. This perturbation can be represented as a wave with a wavelength equal to the length of the system (see Fig. 3). Note that the modulation refers to the additive perturbation, so the bifurcated orbits do not vanish in real space for certain coordinates $X_l$. They are thus formally similar to standing waves, but also inherently different. Applying a permutational operation, we will simply shift the modulated object through the lattice. Consequently we arrive at the result, that after the tangent bifurcation of a band edge plane wave (orbit I or II) takes place, at least $N$ new periodic orbits bifurcate from the original one.

It is much harder to argue about the exponential character of spatial localization of the bifurcated orbits. For any large but finite $N$ the qualitative form of the bifurcated orbit as shown in Fig. 3 is correct if the amplitude of the perturbation is small compared to the amplitude of the bifurcating orbit (I or II) at the bifurcation. The frequency of the orbits I (II) and of the newly bifurcated ones are outside the linear spectrum. Let us consider the analytical continuation of a newly bifurcated orbit. Its frequency will follow (with deviations of higher order) the one of the original periodic orbit (I or II), i.e. $\Delta(\omega^2) \sim E/N$. So we can assume that the frequency is further repelled from the linear spectrum. The amplitude of the original periodic orbit grows like $(E/N)^{1/2}$. The amplitude of the relevant perturbation however grows much faster. That is due to the fact, that at the bifurcation at least $N$ new periodic orbits occur. So in terms of catastrophe theory we would be confronted

with an $A_N$ singularity [23]. The amplitudes of the relevant perturbations will grow as $(E/N - E^c)^\alpha$, where $\alpha \leq 1/2$. Thus the amplitude of the relevant perturbation (describing the deviation of the new periodic orbits from the original one) will grow much faster than the amplitude of the original orbit as a function of energy. Consequently we can expect, that the overall amplitudes in region II in Fig. 3. will be drastically lowered, whereas in regions I and III they will grow with energy. This gives us a tendency towards localization, but not more than that. If it indeed localizes more with increasing energy then the spatial decay will be exponential in region II, because the frequency of the bifurcated orbit is outside the linear spectrum. Clearly it is necessary to explicitly take into account all nonlinearities in order to give a more precise answer on the question of localization.

## 4. Discussion of the results

We have studied the tangent bifurcation properties of band edge plane waves in the limit of large system size. We have restricted the consideration to one-dimensional lattices with nearest neighbour interaction and one degree of freedom per unit cell. Clearly the results can be generalized.

First we consider the case of higher dimensional lattices. Breathers have been numerically observed in [8,24,25] and analytically obtained in [14] for selected systems. Again the used approach can be applied. It is essential to know the properties of the linear spectrum. Then one has to evaluate the system size dependence of the relevant perturbations (the ones with the eigenvalues closest to the band edge frequency) and to repeat the calculations. Without performing this calculation (which is anyway easy to do using the results of this work) we mention that the system size $N$ of the one-dimensional lattice (i.e. the number of degrees of freedom) has to be changed to $N^{1/d}$ in the expressions for the bifurcation energy derived in this paper, where $d$ is the dimensionality of the lattice. So except for some changes in the formula no qualitative differences appear. Still there is a problem – as one can see, the total bifurcation energy is independent of $N$ for $d = 2$ and even increasing with $N^{1/3}$ for $d = 3$. Using [14] we know that in weakly coupled anharmonic oscillator arrays discrete breathers exist at arbitrary small energy for zero coupling, and thus at small energy for weak coupling. Consequently the bifurcation of the band edge plane wave for $d = 2, 3$ might be not directly related to these solutions.

We can only suspect, that other channels of breather birth through bifurcations exist. In any of the considered systems standing waves occur in the linearized case which correspond to resonant tori (two identical frequencies). These standing waves already in the linear case break the permutational symmetry. The interesting cases correspond to wavenumbers closest to the band edge plane wave. The standing wave would then have two distinct knots along either spatial direction, since the original waves had a wavelength equal to the system size. These resonant tori will most probably transform into chains of regular islands separated by a separatrix, once the nonlinearities are included. The newly bifurcated orbits can shift their frequencies out of the linear spectrum with increase of energy. Since they were close to the band edge plane wave it is likely, that the energy dependence of the frequencies of these new orbits is similar to the one of the band edge plane wave. If this scenario is true, then one could still predict the existence of breathers in higher dimensional lattices by analyzing the energy dependence of the band edge plane wave frequency. A logical question would be, whether the same effect of breather birth through resonant tori (rather then through tangent bifurcation of a band edge plane wave) takes place in the $d = 1$ systems, which were considered in the present paper. At the present the answer is, that it might well be. Still there exist breathers at infinitely small energies which are bifurcating from the band edge plane wave, as shown in this work, and as also observed in numerical studies [15]. One could argue that for the $N = 40$ example in Fig. 8 of [15] the disappearance of the discrete breather at the

frequency of the band edge plane wave (of same energy) could be nearly reproduced by the breather merging with a standing wave which has a difference of about $1/1600$ in frequency compared to the band edge one. But the main problem with the standing wave is, that the bifurcating objects will have the symmetry of two breathers. At the present we do not see another channel for a single breather birth via bifurcation rather than the band edge plane wave bifurcation discussed in the present paper.

Secondly we consider the problem of larger interaction range. Again changes in the linear spectrum have to be considered, and for the upper band edge plane wave (orbit II) also some changes in the derivation have to be expected. For the case of weak next-to-nearest neighbour interaction (compared to the nearest neighbour one) a smooth change of the derived results will apply. Especially we observe, that the tendency is to increase the distances between the eigenvalues of the linearized spectrum (at fixed $N$) and thus to increase the bifurcation energy. Thus increasing the interaction range corresponds to a gradual suppression of bifurcation and localization. That seems to be plausible, since in certain limits of mean-field type interaction no localization should occur.

The analysis of systems with several degrees of freedom per unit cell seems to be more complicated, although the presented approach can be used. It becomes a matter of right dealing with polarization vectors etc. Here we can only expect that tangent bifurcations of band edge modes will appear if the necessary condition of the mode frequency repelling from the linear spectrum (band) occur.

In this work we have studied only tangent bifurcations of band edge plane waves. These cases have to be clearly separated from e.g. period doubling bifurcations (cf. [15]). Especially the subtle connection between tangent bifurcation of band edge plane waves and the appearance of new periodic orbits which break permutational symmetry and exponentially localize in the configurational space is not easily transferred to the case of period doubling bifurcations. Since period doubling bifurcations will occur only for the upper band edge plane wave, the bifurcated orbits will have frequencies located inside the linear spectrum. Thus we doubt that any tendency for exponential localization can occur in these cases.

Let us estimate the bifurcation energy of a period doubling bifurcation of periodic orbit II. The relevant perturbation is given by $q = \pi/6$ for the one-dimensional case (the upper band edge of the linear spectrum is given by $2\sqrt{\phi_2}$, the relevant frequency of the perturbation has to be close to $\sqrt{\phi_2}$). If $N/6$ is an integer, then we have to expect a period doubling bifurcation at zero energies, since the normal modes resonate already in the linear problem. If $N/6$ is noninteger, then the distance of the closest eigenvalue of the linear spectrum to the value $\phi_2$ is of the order $1/N$. Note that this is different from the tangent bifurcation cases considered above, where the distance of the closest eigenvalue to the squared band edge was always of the order $1/N^2$. Thus we conclude that for the generic cases period doubling bifurcations occur at energies $E^c \sim 1/N$ (cf. Budinsky and Bountis [16], Eq. (3.8)) whereas the tangent bifurcation occurs at energies $E^c \sim 1/N^2$. So generically tangent bifurcations appear at lower energies than period doubling bifurcations. Then we can conclude, that with increase of energy first exponentially localized orbits (discrete breathers) are generated through tangent bifurcations.

If we consider a nonlinear Klein–Gordon lattice (optical-like linear spectrum, $v_2 \neq 0$) then for small bandwidth ($\phi_2 \ll v_2$) no period-doubling bifurcations occur at small energies. Since generically any nonlinearity will repel the frequency of one of the two band edge plane waves with increase of energy, tangent bifurcation always occurs. This result is in agreement with MacKay and Aubry [14], who have shown that discrete breathers exist for these lattices for any nonlinearity, provided the bandwidth is small.

Let us give an example where no discrete breathers are expected. The one-dimensional Toda chain is characterized by [26] $v_\mu = 0$, $\phi_2 = 1$, $\phi_3 = -1/2$, $\phi_4 = 1/6$. Clearly (3.24) is not satisfied (note that in that case the frequency of the upper band edge plane wave *is* repelled from the linear spectrum with increase of energy, so the repelling condition is a necessary condition, but not a sufficient one). Thus in the limit of

large system size no tangent bifurcation occurs at small energies, and no discrete breathers should occur. This circumstance should make clear, that discussions about 'nonexistence of breathers in systems with realistic potentials' are simply based on the fact, that a potential called realistic can be chosen in a way that (3.24) does not allow for tangent bifurcation of an upper acoustic band edge phonon.

A few words should be added in order to explain the subtleties of the result of the previous paragraph. If we consider a system with an acoustic-type linear spectrum (like that of the Toda chain) then we deal with Eqs. (3.22) and (3.23). The first tangent bifurcation occurs at the value of energy which corresponds to the smallest nonnegative outcome of any of both equations. If (3.24) is fulfilled, then (3.23) gives positive energies, which become arbitrarily small as the size of the system is increased to infinity. Consequently the new bifurcating orbits have zero amplitudes and energy densities outside their modulation center and eventually evolve into discrete breathers with increase in energy. If however (3.24) does not hold (e.g. as in the case of the Toda chain) then (3.23) gives negative bifurcation energies. So we have to use (3.22), which gives finite energy values even for infinite system size. Despite the fact that (3.22) is only a result of perturbation theory, and corrections apply for finite but not too small energies, we can conclude for sure that the tangent bifurcation energy in this case stays finite with increase of the size of the system. So the new bifurcated orbits will have finite nonzero amplitudes and energy densities outside their modulation center even if being infinitely close to the bifurcation. Those objects can not be called discrete breathers, because their amplitudes can not decay exponentially in space, and because their total energy on an infinite lattice will be infinite. Rather they correspond to discrete breathers 'sitting' on a nondecaying carrier wave. We suspect that precisely those solutions were observed in Figs. 8,9 in [15] but were not identified as being different from discrete breathers with exponential spatial decay. So the result of the previous paragraph is that there exist no discrete breathers in a Toda chain. But the next result and prediction is that there exist discrete breathers on carrier waves in the Toda chain (this last statement should be still considered to have some uncertainty, because of the mentioned use of perturbation theory for deriving (3.22)).

Nonlinearity shifts frequencies of periodic orbits with change of energy. For an optical band no matter whether the shift results in an increase or decrease of the frequency, tangent bifurcation will take place nearly always – either for the upper or for the lower band edge phonon. In the case of an acoustic band we need increase of frequencies in order to obtain tangent bifurcation, and even this condition is only a necessary one (cf. the two previous paragraphs). Thus acoustic band related breathers will occur rarely compared to the optical band related ones. This circumstance is in accordance with numerical findings [27,28] where periodic modulation of masses (diatomic chain instead of monoatomic chain) allows for tangent bifurcation of band edge plane waves of the optical band (which is absent in the monoatomic case, as were the breathers for the chosen parameters).

From our results we can follow, that breathers will be likely to occur in lattices with optical bands in the linear spectrum, which are narrow and well separated from the rest of the spectrum (we have recently learned about a numerical study of Bonart, Meyer and Schröder [29], where similar guides have been successfully applied in order to obtain discrete breathers on surfaces of 3d crystals). Of course the nonlinearity has to be strong enough – that can be accomplished either by not too low temperatures (especially for systems with structural phase transitions) or by local excitation of the lattice using e.g. laser pulses, so that sufficiently large amplitudes occur, which should then provide for strong enough nonlinearities in the forces. Breathers will certainly influence the thermal conductivity acting as strong scatterers of small-amplitude phonons [30] and may also influence other transport properties of other degrees of freedom (e.g. electrons) if the coupling is strong enough.

Finally we want to note, that for systems with acoustic-like linear spectra (say $v_\mu = 0$) and $\phi_{2m+1} \neq 0$ numerical simulations of discrete breathers in one-dimensional chains always lead to the presence of static

displacements (dc terms) in the solution $X_l(t)$ which seemingly decay linearly in space, due to the periodic boundary conditions [15,5,31]. In the limit of large system sizes the slope goes as $1/N$ and thus vanishes in the limit $N \rightarrow \infty$. This result can be immediately obtained using the fact that the decay rate of the dc term is zero for an infinite lattice with an acoustic linear spectrum [10]. Thus discrete breathers in the mentioned lattice types are similar to a kink+localized vibration for the one-dimensional case, and to a kink bubble+localized vibration in higher dimensional lattices. This statement stems from the observation, that far away from the center of the breather the static displacements can be described as a strain field caused by a point-like source (in full analogy to the corresponding Maxwell equation for the electric field) [32]. Then the strain field will be radial and isotropic, and its decay can be calculated using Gauss's theorem. The resulting decay is $\sim 1/r^{d-1}$, where $d$ is the dimension of the system. So for three-dimensional lattices we obtain $1/r^2$ decay, for two-dimensional systems $1/r$ decay and for one-dimensional systems non-decaying strains. Consequently even in three-dimensional lattices these discrete breathers (which bifurcated from an acoustic band in the presence of $\phi_{2m+1} \neq 0$) are composed out of a dynamical (time-periodic) solution decaying exponentially fast, and a strain field decaying as $1/r^2$. If we choose $v_2 \neq 0$ (i.e. if we consider a breather which bifurcated from an optical band) then the spatial decay of the dc terms becomes exponential. Similar to that we find that the tangent bifurcation energy of the upper band edge plane wave behaves also differently for the two cases (3.23). Performing first the limit $N \rightarrow \infty$ we thus find that the two different classes of lattices (acoustic-like or optic-like linear spectra) have no simple contact. This is connected to the circumstance, that the case of acoustic-like linear spectra implies the existence of an additional integral of motion - the total mechanical momentum. In the case of systems with more than one degrees of freedom per unit cell it can happen, that tangent bifurcation appears for an optical band edge plane wave. However the nonlinearities can couple the band variables of the optical band with the acoustic band variables. Then the existence of a local strain due to the discrete breather will still cause a nonexponential decay of the strain as described above. Thus we agree with the conclusion in [27] (where a nondecaying strain was found in a one-dimensional diatomic lattice - with the breather bifurcating from the optical band) that the existence of breathers in crystals should be in general accompanied with anomalies in the thermal expansion.

There exist approximate methods of testing whether a lattice allows for the existence of breathers [6,8,33]. These methods use the hypothetical existence of breathers and construct then energy dependencies of their frequencies. If the breather frequencies are attracted by the linear spectrum, then the conclusion was that breathers most probably do not exist. These predictions were usually successful. However this method of argumentation is not well-defined, since it uses objects which are not defined (as long as we do not know whether breathers exist, we can not calculate any property of a breather). In the present work instead a well-defined and clear criterion is given - whether or not the frequency of a band edge plane wave is repelled from the linear spectrum with increase in energy. There should be even experimental methods of testing this property of a lattice, if the first corrections to the linear spectrum due to nonlinearity can not be well estimated theoretically.

## 5. Summary

We have shown, that band edge plane waves of nonlinear Hamiltonian lattices undergo tangent bifurcations. A necessary condition for that is the repelling of the frequency of the plane wave from the linear spectrum with increase of energy. If this condition is fulfilled, then the bifurcation energy (in units of one-particle energy) scales as $N^{-2/d}$ where $d$ is the dimensionality of the lattice. The new bifurcated periodic orbits break the permutational symmetry of the lattice (if periodic boundary conditions are used). The shape of the new

bifurcated orbits corresponds to a localized vibration. It is argued that the spatial decay of the amplitudes becomes exponential with further increase of energy. Thus we confirm the numerical findings of [15], who have shown that the new bifurcated orbits are related to discrete breathers in finite chains. In accord with the strong evidence that discrete breathers are generic solutions of nonlinear lattices we find that tangent bifurcation of band edge plane waves is generic too.

## Acknowledgements

## Appendix A. Perturbation theory for bifurcation of orbit II in the lattice

Here we want to sketch the derivation of the critical lines of tangent bifurcation for periodic orbit II (upper band edge plane wave) for $\phi_{2m+1} \neq 0$. We start from the set of two equations (3.21) and rewrite them in the following way:

$$\ddot{x} = - \left[ \Omega_x^2 + 2F_2^x \cos(2\omega t) \right] x - 2A\alpha \cos(\omega t) y, \tag{A.1}$$

$$\ddot{y} = - \left[ \Omega_y^2 + 2F_2^y \cos(2\omega t) \right] y - 2A\alpha \cos(\omega t) x. \tag{A.2}$$

Here we used the different notations

$$x = \delta_{q_a}, \quad y = \delta_{q_b}, \quad \omega_{x,y}^2 = \omega_{q_{a,b}}^2, \quad \alpha = \bar{\phi}_{3,q_{a,b}}.$$

The other parameters are defined in the limit of small energies of the band edge plane wave as

$$\Omega_{x,y}^2 = \omega_{x,y}^2 + F_0^{x,y}, \tag{A.3}$$

$$F_0^{x,y} = 3\frac{\bar{v}_{4,q_{a,b}}}{\bar{v}_2} E, \tag{A.4}$$

$$F_2^{x,y} = \tfrac{1}{2} F_0^{x,y}, \tag{A.5}$$

$$A = a_1 E^{1/2}, \quad a_1^2 = \frac{1}{2\bar{v}_2}, \tag{A.6}$$

$$\omega_x^2 = v_2 + 4\phi_2 - \frac{4\pi^2}{N^2}\phi_2, \tag{A.7}$$

$$\omega_y^2 = v_2 + \frac{4\pi^2}{N^2}\phi_2. \tag{A.8}$$

We expand the solutions of the differential equations (A.1), (A.2) into series of powers of $E^{1/2}$:

$$x(t) = x_0(t) + E^{1/2} x_1(t) + E x_2(t) + ..., \tag{A.9}$$

$$y(t) = y_0(t) + E^{1/2} y_1(t) + E y_2(t) + ..., \tag{A.10}$$

$$\Omega_x^2 = \omega^2 + g_1 E^{1/2} + g_2 E + .... \tag{A.11}$$

Note that we did not expand $\Omega_y$, since in the given problem this frequency is far away from the frequency of the periodic orbit $\omega$.

Inserting (A.9)–(A.11) into (A.1), (A.2) and sorting with respect to powers of $E^{1/2}$ we obtain in lowest order

$$\ddot{x}_0 = -\omega^2 x_0, \qquad \ddot{y}_0 = -\omega_y^2 y_0. \tag{A.12}$$

Since we are looking for solutions periodic with $2\pi/\omega$ it follows

$$x_0 = a\cos(\omega t) + b\sin(\omega t), \qquad y_0 = 0. \tag{A.13}$$

In order $E^{1/2}$ we get

$$\ddot{x}_1 = \omega^2 x_1 - g_1 x_0, \qquad \ddot{y}_1 = -\omega_y^2 y_1 - 2\alpha a_1 \cos(\omega t) x_0. \tag{A.14}$$

The solution reads

$$g_1 = 0, \qquad x_1 = 0, \tag{A.15}$$

$$y_1 = \kappa + c\cos(2\omega t) + d\sin(2\omega t), \tag{A.16}$$

$$\kappa = -\frac{\alpha a_1}{\omega_y^2} a, \qquad \frac{c}{a} = \frac{d}{b} = \frac{\alpha a_1}{4\omega^2 - \omega_y^2}. \tag{A.17}$$

Note that the solution $x_1 = 0$ is not strictly required at this level. However we would have to do so at the next level, so we remove it already here. The constant $\kappa$ is inverse proportional to $\omega_y^2$. This circumstance will lead to the difference in the final results for the optical like spectrum ($\omega_y^2$ finite) and the acoustic like spectrum ($\omega_y^2 \sim 1/N^2$).

In order $E$ we obtain

$$\ddot{x}_2 = -\omega^2 x_2 - g_2 x_0 - f_{2,x}\cos(2\omega t)x_0 - 2\alpha a_1 \cos(\omega t)y_1, \tag{A.18}$$

$$\ddot{y}_2 = -\omega_2^2 y_2. \tag{A.19}$$

Eq. (A.19) simply requires $y_2 = 0$. Removing the secular terms from Eq. (A.18) it follows

$$(\mathrm{i}): \quad E^c = \frac{4\pi^2}{N^2}\phi_2 \frac{4\omega^2 - \omega_y^2}{a_1^2 \alpha^2}, \tag{A.20}$$

$$(\mathrm{ii}): \quad E^c = \frac{4\pi^2}{N^2}\phi_2 \frac{1}{2f_{2,x} - \left(\frac{2a_1^2}{\omega_y^2} - \frac{a-1^2}{4\omega^2-\omega_y^2}\right)\alpha^2}. \tag{A.21}$$

Note that $\alpha^2 \sim 1/N^2$. Thus we obtain that the $N$-dependence is removed from Eq. (A.20). Now we see the cause for the mentioned difference between the optical and acoustic spectra. If $\omega_y^2$ stays finite for large $N$, then the whole second term in the denominator of the right hand side of Eq. (A.21) scales to zero. In the case of the acoustic spectrum $\omega_y^2 \sim 1/N^2$, and the same term in (A.21) gives a finite contribution in the limit of large $N$.

# References

[1] S. Takeno, K. Kisoda and A.J. Sievers, Prog. Theor. Phys. Suppl. 94 (1988) 242.

[2] J.B. Page, Phys. Rev. B 41 (1990) 7835.

[3] D.K. Campbell and M. Peyrard, in: CHAOS – Soviet American Perspectives on Nonlinear Science, ed. D.K. Campbell (American Institute of Physics, New York, 1990).

[4] S. Takeno, J. Phys. Soc. Jpn. 61 (1992) 2821.

[5] S.R. Bickham, S.A. Kisilev and A.J. Sievers, Phys. Rev. B 47 (1993) 14206.

[6] S. Flach, C.R. Willis and E. Olbrich, Phys. Rev. E 49 (1994) 836.

[7] S. Flach and C.R. Willis, Phys. Rev. Lett. 72 (1994) 1777.

[8] S. Flach, K. Kladko and C.R. Willis, Phys. Rev. E 50 (1994) 2293.

[9] S. Takeno and K. Hori, J. Phys. Soc. Jpn. 60 (1991) 947.

[10] S. Flach, Phys. Rev. E 50 (1994) 3134.

[11] J. Denzler, Commun. Math. Phys. 158 (1993) 397.

[12] B. Birnir, Comm. Pure Appl. Math. XLVII (1994) 103.

[13] S. Flach, Phys. Rev. E 51 (1995) 1503.

[14] R.S. MacKay and S. Aubry, Nonlinearity 7 (1994) 1623.

[15] K.W. Sandusky and J.B. Page, Phys. Rev. B 50 (1994) 866.

[16] N. Budinsky and T. Bountis, Physica D 8 (1983) 445.

[17] Y.A. Kosevich, Phys. Rev. Lett. 71 (1993) 2058.

[18] A.H. Nayfeh, Introduction to Perturbation Techniques (Wiley, New York, 1993).

[19] W. Magnus and S. Winkler, Hill's Equation (Dover, New York, 1979).

[20] A.F. Vakakis and R.H. Rand, Int. J. Nonlin. Mech. 27 (1992) 861.

[21] A. Tsurui, Prog. Theor. Phys. 48 (1972) 1196.

[22] N. Flytzanis, St. Pnevmatikos and M. Remoissenet, J. Phys. C: Solid State Phys. 18 (1985) 4603.

[23] R. Gilmore, Catastrophe Theory for Scientists and Engineers (Wiley, New York, 1981).

[24] V.M. Burlakov, S.A. Kisilev and V.N. Pyrkov, Phys. Rev. B 42 (1990) 4921.

[25] F. Fischer, Ann. Phys. (Germany) 2 (1993) 296.

[26] M. Toda, Theory of Nonlinear Lattices (Springer, Berlin, 1989).

[27] S.A. Kisilev, S.R. Bickham and A.J. Sievers, Phys. Rev. B 48 (1993) 13508.

[28] M. Aoki, S. Takeno and A.J. Sievers, J. Phys. Soc. Jpn. 62 (1993) 4295.

[29] D. Bonart, A.P. Mayer and U. Schröder, Phys. Rev. Lett., in press (1995).

[30] S. Flach and C.R. Willis, in: Nonlinear Excitations in Biomolecules, ed. M. Peyrard, Les Editions de Physique (Springer, Les Ulis, 1995) pp. 165–174.

[31] G. Huang, Z. Shi and Z. Xu, Phys. Rev. B 47 (1993) 14561.

[32] L.D. Landau and E.M. Lifshitz, Elastizitätstheorie, Lehrbuch der Theoretischen Physik VII (Akademie-Verlag, Berlin, 1991).

[33] S. Flach, Phys. Rev. E 51 (1995) 3579.