Multiparticle breathers for a chain with double-quadratic on-site potential

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We investigate the existence and properties of multiparticle breathers for a one-dimensional model with harmonic nearest neighbor interactions where a group of r particles ($r=1,2,3,\ldots$) perform interwell oscillations between both wells of a double-quadratic on-site potiential. We find two types of such breathers. For the first type the breather frequency Ω is within the single-particle oscillator spectrum, and the "residence" time of each breather particle in the left and right well is about the same. For the second breather Ω is below that spectrum, and the ratio τ_L/τ_R of the residence time in the left and right wells is different from zero, and takes approximately rational values like $\frac{1}{4},\frac{1}{3},\frac{2}{3},\frac{3}{4}$, etc. This second type of breather occurs for two and more breather particles only. [S1063-651X(99)07411-5]

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I. INTRODUCTION

Very often, the classical dynamics of macroscopic systems like crystalline and amorphous materials can be understood by a knowledge of their elementary excitations. The most prominent example are the *harmonic* lattice vibrations. For a periodic lattice these are *extended* plane waves. Introducing disorder, as present in glassy systems, part of these harmonic excitations may become localized, a phenomenon called Anderson localization. It is interesting that such localized vibrations can also occur in periodic lattices *without* disorder, due to *anharmonicity*. In recent years a lot of activity has been devoted to studying the existence and properties of such nonlinear localized excitations (NLE's), also called "discrete breathers" or just "breathers" in the following. Rather different approaches (numerical, rotating wave approximation, local ansatz, etc.) have given strong evidence of the existence of NLE's, mainly in one-dimensional systems but also in two-dimensional systems. For more details, the reader is referred to the reviews by Flach and Willis [1] and Sievers and Page [2].

A physical understanding of why discrete breathers may occur comes from the exact existence proof by MacKay and Aubry [3] (see also Ref. [1]). Since we will come back to this point below, let us briefly describe the main idea. Considering a classical N-particle Hamiltonian for particles with mass m of the form

$$H(p_1,\ldots,p_N;u_1,\ldots,u_N) = \sum_{n=1}^{N}\left[\frac{1}{2m}p_n^2+V_0(u_n)\right]+C\,V_1(u_1,\ldots,u_N) \tag{1}$$

for the displacements u_n from the lattice site n of a d-dimensional lattice and their conjugate momenta p_n, these authors started from the so-called anti-integrable limit $C=0$, where the interaction potential V_1 is turned off. In that limit the dynamics is determined exclusively by the on-site potential V_0, leading to independent periodic orbits for the N particles. For the generic case of an anharmonic potential V_0 the corresponding frequencies Ω_n may be different for all particles. Now take the case where all particles are at rest, i.e., $\Omega_n=0$, $n\neq m$ but the mth particle is oscillating with $\Omega_m=\Omega>0$. Turning on the interaction one can prove that (under rather general conditions) the orbits for small but nonzero C continuously develop from this special situation for $C=0$. This means that all the particles perform periodic oscillations with frequency Ω and amplitudes decaying exponentially with distance from particle number m. Hence the existence of *periodic breathers* is proven, provided C is small enough.

If the on-site potential has a multiwell structure, two different types of NLE's may exist: first, where all particles are oscillating within one of the wells for all times, and, second, where one particle or a group of particles are oscillating between, e.g. two wells, and the others stay in their well forever. This second type of breather was recently observed [4] for a one-dimensional version of Hamiltonian (1) with $V_0(u)$ a symmetric, double-quadratic (DQ) potential:

$$V_0(u)=\tfrac{1}{2}(u-\sigma(u))^2, \tag{2a}$$

where

$$\sigma(u)=\operatorname{sgn} u \tag{2b}$$

and

$$V_1(u_1,\ldots,u_N)=\tfrac{1}{2}\sum_n (u_{n+1}-u_n)^2 \tag{2c}$$

are harmonic, nearest neighbor interactions. This molecular dynamics simulation at finite constant energy, which corresponds to a finite temperature, has shown that groups of about 3–5 particles perform such periodic interwell oscillations at intermediate temperatures [4]. However, their lifetime is finite, due to nonzero temperature.

It is the main motivation of this paper to study the existence and properties of such interwell breathers made up of r particles ($r=1,2,3,\ldots$) for potentials (2) and for zero temperature. The reader should note that NLE's of the first kind do not exist for this model due to the complete harmonicity of V_0 [cf. Eqs. (2a) and (2b)] *within* each well. The particles "feel" the anharmonicity only when crossing the local barrier of $V_0(u)$ at $u=0$. Despite the rather simplified choice

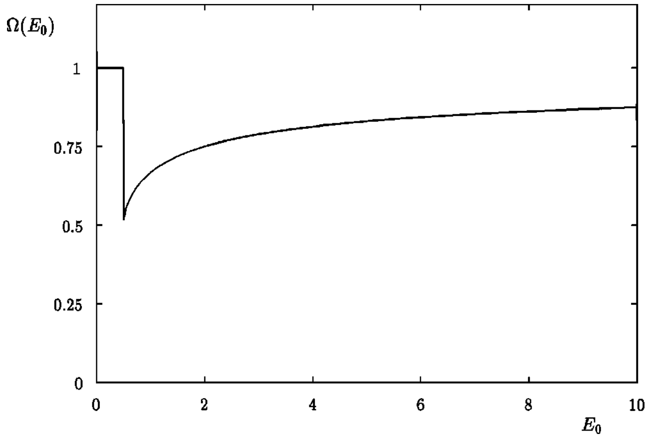

FIG. 1. Dispersion relation for the uncoupled oscillator.

for $V_0(u)$, we expect that the existence and characteristic features of its interwell NLE can be carried over to more general on-site potentials with a multiwell structure.

The outline of our paper is as follows. In Sec. II we will present the formal solution for an r-particle breather. In Sec. III the discussion of the self-consitency condition singles out the physical breathers, the properties of which will be investigated separately for $r=1$ and $r\geqslant 2$. Section IV contains a summary and some conclusions.

II. NONLINEAR EXCITATIONS: FORMAL SOLUTION

Before we come to the solution of the full equation of motion in order to search for breathers, we briefly discuss the antiintegrable limit $C=0$. Since the one-particle energy $E_0=(1/2m)p_n^2+V_0(u_n)$ is a conserved quantity, it is an easy task to calculate the frequency Ω of the periodic motion as a function of E_0. One obtains

$$\Omega(E_0)=\begin{cases}1, & E_0<\frac{1}{2}\\ \left[1+\frac{2}{\pi}\arcsin\left(\frac{1}{\sqrt{2E_0}}\right)\right]^{-1}, & E_0>\frac{1}{2},\end{cases} \tag{3}$$

which is illustrated in Fig. 1. Note that we use dimensionless units throughout this paper. For instance the frequency Ω is measured in units of $\sqrt{C_0/m}$ and the energy in units of C_0. Here C_0 is the coupling constant of the on-site potential, which in Eq. (2a) has been set to 1. For E_0 smaller than the barrier height $V_0(0)=\frac{1}{2}$ the frequency is constant, and equal to 1, due to the harmonic intrawell motion. At $V_0(0)$ the frequency makes a jump to the value $\frac{1}{2}$ and increases monotonously with E_0 toward its asymptotic value $\Omega(\infty)=1$. Application of the argumentation of MacKay and Aubry [3] would imply the existence of breathers for frequencies $\Omega\in[\frac{1}{2},1]$.

Now we turn to the full equation of motion. For potential (2) and choosing $m=1$, this reads:

$$\ddot{u}_n(t)+(1+2C)u_n(t)-C[u_{n-1}(t)+u_{n+1}(t)]=\sigma_n(t), \tag{4a}$$

where $u_n(t)$ has to fulfill the self-consistency condition (SCC)

$$\sigma_n(t)=\operatorname{sgn} u_n(t). \tag{4b}$$

Let us assume for a moment that all of the particles remain within their well (left or right) forever, i.e., it is $\sigma_n(t)\equiv\sigma_n$ for all t, where $\sigma_n=\pm 1$ can be chosen arbitrarily. Let $u_n(\sigma)$ be the stationary solution of Eq. (4) for given $\sigma=(\sigma_1,\dots,\sigma_N)$. It has been shown [5] that a one-to-one correspondence exists between all stationary, metastable configurations $u(\sigma)=(u_1(\sigma),\dots,u_N(\sigma))$ and all Ising spin configurations σ, provided the modulos of

$$\eta=\frac{1}{2C}(1+2C-\sqrt{1+4C}) \tag{5}$$

are smaller than $\frac{1}{3}$ [5]. The metastability holds provided $C>-\frac{1}{4}$. With the ansatz

$$u_n(t)=u_n(\sigma)+\varepsilon_n(t),\quad |\varepsilon_n(t)|\ll 1,$$

from Eq. (4a) we obtain

$$\ddot{\varepsilon}_n(t)+(1+2C)\varepsilon_n(t)-C[\varepsilon_{n-1}(t)+\varepsilon_{n+1}(t)]=0. \tag{6}$$

Its solutions are plane waves $\varepsilon_n(t)=\varepsilon_0\exp[i(\omega(q)t-qn)]$ with phonon frequencies

$$\omega(q)=[1+2C-2C\cos q]^{1/2},\quad q\in[-\pi,\pi], \tag{7}$$

which are within the phonon band $[\omega_{\rm low}(C),\omega_{\rm up}(C)]$. The lower and upper phonon band edge are given by

$$\omega_{\rm low}(C)=\begin{cases}1, & C\geqslant 0\\ \sqrt{1+4C}, & -\frac{1}{4}<C\leqslant 0,\end{cases}$$

$$\omega_{\rm up}(C)=\begin{cases}\sqrt{1+4C}, & C\geqslant 0\\ 1, & -\frac{1}{4}<C\leqslant 0.\end{cases} \tag{8}$$

Since we are looking for periodic breathers with an exponentially decaying amplitude it is obvious (see also Ref. [1]) that the breather frequency Ω and all its higher harmonics $k\Omega, k\geqslant 2$ must be outside the phonon band. For a given C, this condition restricts Ω to the finite number of nonresonant bands $\{\Omega\}_k=(\omega_{\rm up}/(k+1),(\omega_{\rm low}/k)), k=1,2,\dots,k_{\rm max}(C)$ shown in Fig. 2. It is easy to prove that

$$k_{\rm max}(C)=\left[\frac{\omega_{\rm low}(C)}{\omega_{\rm up}(C)-\omega_{\rm low}(C)}\right],$$

where $[x]$ denotes the largest integer less than or equal to x. Frequencies Ω above the phonon band trivially fulfill the nonresonant conditions for all harmonics. This part is not depicted in Fig. 2. But in our investigations we have not found breathers with $\Omega>\omega_{\rm up}(C)$. We will come back to this point in Sec. IV.

In addition to this, two further observations can be made from Fig. 2. First, the nonresonant band $\{\Omega\}_1$ is only a subset of the single-oscillator spectrum $[\frac{1}{2},1]$ for $C\neq 0$. Second,

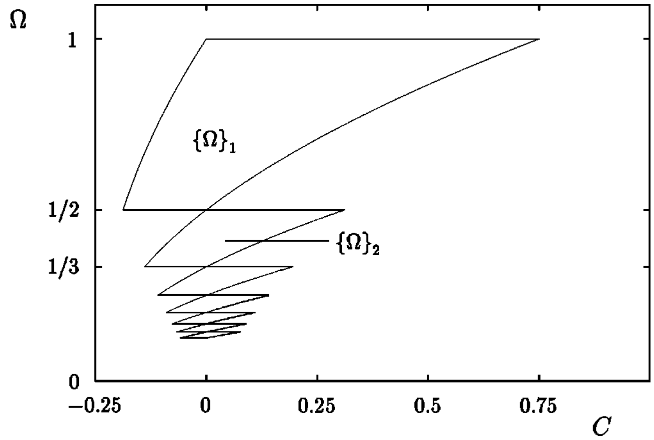

FIG. 2. Nonresonant frequency bands (bounded areas).

if breathers will exist with $\Omega \in \{\Omega\}_k$, $k \geqslant 2$, they cannot be obtained from the single-oscillator behavior for $C=0$ by continuation.

Now we turn to the investigation of breathers. Due to the simple form of $V_0(u)$ the type of breather can be specified by the pseudospin functions $\sigma_n(t)$. Let us assume that particles $n=0,1,2,\ldots,r-1$ perform periodic interwell oscillations, whereas all the others remain in their ground state well [6], i.e.,

$$\sigma_n(t) \equiv -1, \quad n \neq 0,1,\ldots,r-1 \tag{9a}$$

for all t. The behavior of $\sigma_n(t)$ for $n=0,1,\ldots,r-1$ during a period $-T/2 \leqslant t \leqslant T/2$ can be rather complicated, e.g., more than one transition $-1 \rightarrow +1 \rightarrow -1$ may occur. To make progress we will consider breathers characterized by

$$\sigma_n(t) = \begin{cases} \operatorname{sgn} \ \tau_n, & |t| \leqslant \frac{1}{2}|\tau_n| \\ -\operatorname{sgn} \ \tau_n, & \frac{1}{2}|\tau_n| \leqslant |t| \leqslant \frac{1}{2}T, \end{cases} \quad n=0,1,\ldots.r \tag{9b}$$

where $|\tau_n| < T$. If $\tau_n > 0$, the ''breather particle'' $n(n=0,1,\ldots,r-1)$ is in its ground state well $(\sigma_n = -1)$ for $t \notin [-\tau_n/2, \tau_n/2]$, and resides in the right well of $V_0(u)$ $(\sigma_n = +1)$ for $t \in [-\tau_n/2, \tau_n/2]$. The reverse holds it $\tau_n < 0$. The r-particle breather is then characterized by its frequency Ω, and the interwell transition times $\tau_0, \tau_1, \ldots, \tau_{r-1}$.

The restriction to periodic breathers $u_n(t)$, which also implies the periodicity of $\sigma_n(t)$, allows one to represent both by Fourier series. If in addition we also require time inversion symmetric breathers, i.e., $u_n(-t) = u_n(t)$, we have

$$u_n(t) = -1 + \sum_{k=0}^{\infty} A_n^{(k)} \cos k\Omega t \tag{10a}$$

and

$$\sigma_n(t) = -1 + \sum_{k=0}^{\infty} \sigma_n^{(k)} \cos k\Omega t. \tag{10b}$$

Our choice [Eq. (9)] yields, for the coefficients $\sigma_n^{(k)}$,

$$\sigma_n^{(k)} = 0, \quad n \neq 0,1,\ldots,r-1, \tag{11a}$$

$$\sigma_n^{(k)} = \begin{cases} -1 + (2|\alpha_n| - 1)\operatorname{sgn} \alpha_n, & k=0 \\ 4(\sin k\pi\alpha_n)/(\pi k), & k \geqslant 1, \end{cases} \quad n=0,1,\ldots,r-1. \tag{11b}$$

For convenience we have introduced the dimensionless times

$$\alpha_n = \tau_n / T \tag{12}$$

Substituting Eqs. (10) into Eq. (4a) leads to

$$\kappa_k(\Omega) A_n^{(k)} + A_{n-1}^{(k)} + A_{n+1}^{(k)} = -\frac{1}{C}\sigma_n^{(k)} \tag{13}$$

with

$$\kappa_k(\Omega) = \frac{1}{C}[(k\Omega)^2 - (1+2C)]. \tag{14}$$

This equation can be solved for $n \leqslant -1$ and $n \geqslant r$ due to Eq. (11a), which gives, for the amplitudes,

$$A_n^{(k)} = \begin{cases} A_0^{(k)} \eta_k^{|n|}, & n \leqslant -1 \\ A_{r-1}^{(k)} \eta_k^{n-(r-1)}, & n \geqslant r, \end{cases} \tag{15}$$

with

$$\eta_k(\Omega) = -\tfrac{1}{2}[\kappa_k(\Omega) - \operatorname{sgn} \kappa_k(\Omega)\sqrt{(\kappa_k(\Omega))^2 - 4}]. \tag{16}$$

It is easy to see that $|\kappa_k(\Omega)| > 2$ for $k\Omega$ outside the phonon band. Then Eq. (16) yields $|\eta_k(\Omega)| < 1$, consistent with our requirement of exponentially decaying breather amplitude. We note that η_0 coincides with η from Eq. (5).

For $0 \leqslant n \leqslant r-1$ a finite set of inhomogeneous linear equations for $A_n^{(k)}$ results,

$$\sum_{n'=0}^{r-1} M_{nn'} A_{n'}^{(k)} = -\frac{1}{C}\sigma_n^{(k)}, \tag{17}$$

with the tridiagonal r-dimensional matrix

$$\mathbf{M} = (M_{nn'}) = \begin{bmatrix} \kappa_k + \eta_k & 1 & 0 & \cdots & 0 \\ 1 & \kappa_k & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & 1 & \kappa_k & 1 \\ 0 & \cdots & 0 & 1 & \kappa_k + \eta_k \end{bmatrix}. \tag{18}$$

Then the remaining amplitudes follow from

$$A_n^{(k)} = -\frac{1}{C}\sum_{n'=0}^{r-1} (\mathbf{M}^{-1})_{nn'} \sigma_{n'}^{(k)}, \tag{19}$$

with $\sigma_n^{(k)}$ from Eq. (11b). The inverse of $\mathbf{M}$ can be calculated analytically:

$$(\mathbf{M}^{-1})_{nn'} = -\frac{\operatorname{sgn}\kappa_k(\Omega)}{\sqrt{\kappa_k^2(\Omega)-4}}\,\eta_k^{|n-n'|} \equiv \frac{(\operatorname{sgn}\kappa_k)|\eta_k|}{1-\eta_k^2}\,\eta_k^{|n-n'|}. \tag{20}$$

Equations (10)–(20) yield the formal r-particle breather solution $u_n(t)$, which still has to fulfill the SCC (4b).

III. PHYSICAL BREATHER SOLUTIONS

In this section we will determine conditions for the breather frequency Ω and the dimensionless transition times $a_0, \alpha_1, \ldots, \alpha_{r-1}$, such that the SCC [Eq. (4b)] is fulfilled.

A. One-particle breathers

For $r=1$, Eqs. (10)–(20) yield the explicit but formal breather solution

$$u_n(t) = -1 + A_n^{(0)}(\alpha) + \sum_{k=1}^{\infty} A_n^{(k)}(\Omega,\alpha)\cos k\Omega t, \tag{21a}$$

with

$$A_n^{(0)}(\alpha) = \frac{2\alpha}{\sqrt{1+4C}}\,\eta_0^{|n|}, \tag{21b}$$

$$A_n^{(k)}(\Omega,\alpha) = -\frac{4}{\pi}\,\frac{\sin k\pi\alpha}{k}\,\frac{\operatorname{sgn}\ \kappa_k(\Omega)}{C\sqrt{\kappa_k^2(\Omega)-4}}\,(\eta_k(\Omega))^{|n|},\quad k\geqslant 1, \tag{21c}$$

where we have set $\alpha_0 = \alpha > 0$. The reader should note that η_0 does not depend on Ω. Inspection of Eq. (21) shows that, for $k \geqslant 1$,

$$|\kappa_k(\Omega)| \to 2 \Rightarrow A_n^{(k)}(\Omega,\alpha) \to \frac{4}{\pi}\,\frac{\sin k\pi\alpha}{k}\,\frac{1}{2C\sqrt{|\kappa_k(\Omega)|-2}} \tag{22}$$

and

$$k\to\infty \Rightarrow A_n^{(k)}(\Omega,\alpha) \sim \frac{1}{k^3}k^{-2|n|}. \tag{23}$$

The asymptotic behavior [Eq. (23)] of $A_n^{(k)}(\Omega,\alpha)$ guarantees the absolute convergence of the infinite series in Eq. (21a). For $n=0$ it follows that $u_0(t)$ and its first derivative $\dot{u}_0(t)$ is continuous for all t, whereas $\ddot{u}_0(t)$ discontinuously changes at $t=\pm\tau/2$. With increasing $|n|$ the solutions become smoother. Equation (22) just describes what happens when the kth harmonics approaches the phonon band from below or above. Since $\kappa_k(\Omega) \to -2(+2)$ for kΩ $\to \omega_{\rm low}(C)(\omega_{\rm up}(C))$ the corresponding amplitude $A_n^{(k)}(\Omega,\alpha)$ diverges. In addition $|\eta_k(\Omega)|$ converges to one such that the amplitudes decay very slowly with $|n|$. Result (22) demonstrates that for $k\Omega$ outside the phonon band but near to the band edges it is the kth harmonic which governs $u_n(t)$ (see also Ref. [7]). In that case it is rather easy to fix α. A *necessary* condition that the SCC holds is

$$u_0(\pm\tau/2) \equiv u_0(\pm\alpha T/2) \equiv u_0(\pm\pi\alpha/\Omega) = 0. \tag{24}$$

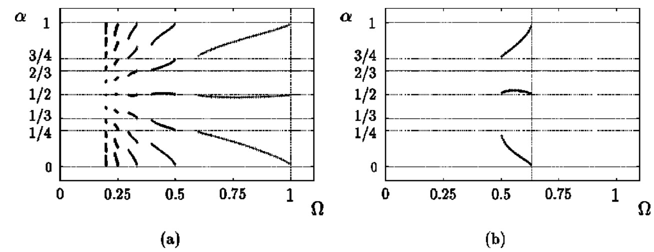

FIG. 3. Parameter α as a function of the breather frequency Ω for (a) $C>0$ and (b) $C<0$. The vertical lines mark the lower phonon band edge.

Let $\Omega \in \{\Omega\}_k = ([\omega_{\rm up}/(k+1)],(\omega_{\rm low}/k))$ for fixed k. For Ω near to the edges of the nonresonant band $\{\Omega\}_k$, which implies that $(k+1)\Omega$ and $k\Omega$ is a bit above and a bit below the phonon band, respectively, it follows from Eqs. (21) and (22) that $u_0(t)$ can be well approximated by

$$u_0(t) \cong -1 + \frac{2\alpha}{\sqrt{1+4C}} + \frac{2}{\pi C}\left[\frac{\sin k\pi\alpha}{\sqrt{|\kappa_k(\Omega)|-2}}\cos k\Omega t + \frac{\sin(k+1)\pi\alpha}{\sqrt{|\kappa_{k+1}(\Omega)|-2}}\cos(k+1)\Omega t\right], \tag{25}$$

such that Eq. (24) leads to

$$\frac{\sin 2\pi k\alpha}{\sqrt{|\kappa_k(\Omega)|-2}} + \frac{\sin 2\pi(k+1)\alpha}{\sqrt{|\kappa_{k+1}(\Omega)|-2}} \cong \frac{\pi C}{2}\left(1 - \frac{2\alpha}{\sqrt{1+4C}}\right). \tag{26}$$

The right-hand side of Eq. (26) is finite for all α and Ω. In order that this is also true for its left-hand side, we must choose

$$\alpha(\Omega) \cong \alpha_\nu^{(k)} = \begin{cases} \dfrac{\nu+1}{2(k+1)}, & \Omega \to \dfrac{\omega_{\rm up}}{k+1} \\[2ex] \dfrac{\nu}{2k}, & \Omega \to \dfrac{\omega_{\rm low}}{k}, \end{cases} \tag{27}$$

where $\nu = 0,1,2,\ldots,2k$. To determine $\alpha(\Omega)$ for all $\Omega \leqslant \omega_{\rm low}(C)$, we have calculated $u_0(t)$ from Eqs. (21) numerically. For this we have introduced a cutoff $k_0=50$ in Eq. (21a). A change from $k_0=50$ to $k_0=100$ has not changed the result for $u_0(t)$ more than 10^{-8}. The numerical calculation of $u_0(\pm\tau/2)$ then yields [with Eq. (24)] $\alpha(\Omega)$, which is shown in Fig. 3. We see that within each nonresonant band $\{\Omega\}_k$ the *necessary* condition (24) leads to$(2k+1)$ solutions $\alpha_\nu^{(k)}(\Omega)$ for $\alpha(\Omega)$ which converge to the limiting values (27) at the edges. However, we have found that the SCC (4b) can only be fulfilled for $\alpha(\Omega) \equiv \alpha_{\nu=1}^{(k=1)}(\Omega) \approx \frac{1}{2}$.

Writing

$$\alpha(\Omega) \equiv \tfrac{1}{2} + \delta(\Omega), \tag{28a}$$

an approximate, analytical expression can be derived for $\delta(\Omega)$ [7]:

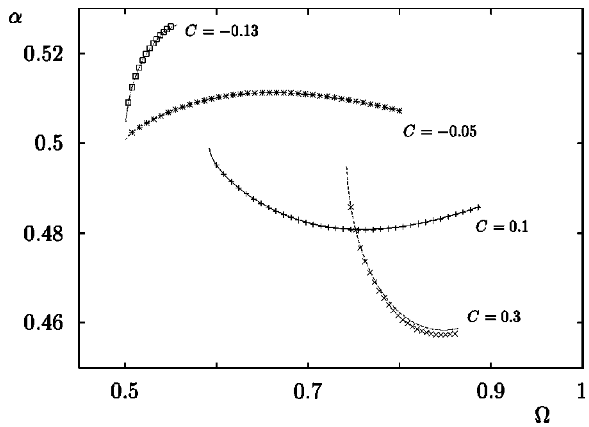

FIG. 4. Analytical approximation of $\alpha\approx\frac{1}{2}+\delta(\Omega)$ (lines) in comparison to numerical results (symbols) for different values of C.

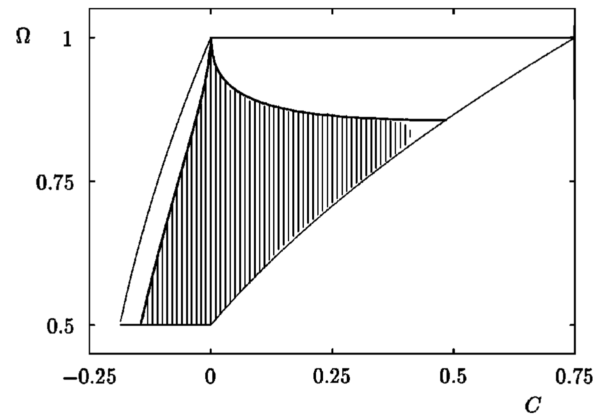

FIG. 5. Phase diagram for single-particle breathers. Thick solid lines indicate the analytical approximations to the limiting frequencies $\Omega_{\min}(C)$ and $\Omega_{\max}(C)$ (cf. text).

$$\delta(\Omega)=\frac{1}{2}\,\frac{\sqrt{1+4C}-1}{1-2\sqrt{1+4C}\left[s_1(\Omega)+\sum_{k=2}^{\infty}(-1)^k s_k(\Omega)\right]},\tag{28b}$$

with

$$s_k(\Omega)=\frac{1}{|C|}(\kappa_k^2(\Omega)-4)^{-1/2}.\tag{28c}$$

Comparison of the numerical exact result for $\alpha(\Omega)$ with the analytical result (28) is made in Fig. 4 for different values of the coupling constant C. Note that the edges of $\{\Omega\}_1$ depend on C. The agreement between both results is remarkably good. The deviation is less than 1%. Therefore we can consider result (28) as almost exact.

The final step now is to check whether the SCC is fulfilled for all C with $-\frac{3}{16}\leqslant C\leqslant\frac{3}{4}$, for which $\{\Omega\}_1$ exists (cf. Fig. 2). Both limits for C follow from the condition $\omega_{\mathrm{up}}(C)/2=\omega_{\mathrm{low}}(C)$ for $C<0$ and $C>0$. The answer is no. The numerical investigation of the SCC yields that one-particle breather exist only for

$$C_{\min}=-0.1368(1)\leqslant C\leqslant 0.4126(1)=C_{\max},$$

and that their frequencies are restricted to

$$\Omega_{\min}(C)\leqslant\Omega\leqslant\Omega_{\max}(C).$$

This region in the $\Omega-C$ plane, where physical one-particle breathers exist (which is only a subset of $\{\Omega\}_1$) is presented in Fig. 5. The solid lines (boundary lines of the hatched region) in that figure represent approximate, analytical results for the phase boundaries $\Omega_{\min}(C)$ and $\Omega_{\max}(C)$. Since these expressions are not quite simple [8], we do not represent them here explicitly, but just mention that $\Omega_{\min}(C)$ follows from the condition that for $\Omega\in\{\Omega\}_1$ it must be $\Omega>\omega_{\mathrm{up}}(C)/2$. For Ω near to $\omega_{\mathrm{up}}(C)$ it is the second harmonic in Eq. (21a) which is dominant. Taking for $u_0(t)$ only the terms with $k=0$ and 2 into account, $\Omega_{\min}(C)$ follows from the SCC (4) for this approximate result for $u_0(t)$. $\Omega_{\max}(C)$ follows similarly from the SCC for $u_{\pm1}(t)$which is $u_{\pm1}(t)<0$ for all t.

Again, the agreement between the numerical exact and the analytical phase boundaries is remarkably good. For $|C|\ll1$, the allowed breather frequencies are between $\frac{1}{2}$ and 1 which is the range of the single-oscillator frequencies. The range of allowed frequencies shrinks with increasing $|C|$.

The results we have found demonstrates that only one-particle breathers exist which can continuously be derived from the single oscillator excitation for $C=0$. This also is consistent with the fact that breather solutions for $C\neq0$ only exist for $\alpha\approx\frac{1}{2}$, because for the single oscillator the time τ where the particle is in the right well is just half of the period T, i.e., it is $\alpha=\frac{1}{2}$. That no breathers exist for $\Omega\in\{\Omega\}_1$ and $\alpha(\Omega)=\alpha_0^1(\Omega)$ or $\alpha(\Omega)=\alpha_2^1(\Omega)$ can at least be understood for Ω at the edges which implies, e.g., $\alpha_0^1(\Omega)\approx0$ and $\alpha_1^1(\Omega)\approx1$, respectively. $\alpha_0^1(\Omega)\approx0$ means that particle zero is in the right well for a very short time $\alpha_0^1(\Omega)T/2$, only. Therefore, $u_0(t)$ and $\ddot{u}_0(t)$ can be made arbitrary small for $-\alpha_0^1(\Omega)T/2\leqslant t\leqslant\alpha_0^1T/2$ by decreasing $\alpha_0^1(\Omega)$. On the other hand, the breather amplitude is decaying with $|n|$. Therefore $u_1(t)$ and $u_{-1}(t)$ must also be small. Consequently, the left-hand side of the equation of motion (4a) for $u_0(t)$ can be made arbitrarily small, which is in contradiction with the fact that its right-hand side $\sigma_0(t)$ is equal to 1 in that time interval. For $\alpha(\Omega)=\alpha_2^1(\Omega)\approx1$ the proof is quite similar. One has just to notice that particle zero is in the left well for a short time only. The nonexistence of breathers with $\Omega\in\{\Omega\}_k$ for $k\geqslant2$ can also easily be understood at least at the edges of $\{\Omega\}_k$. At these edges it is the kth harmonic with $k\geqslant2$ which dominates the solution $u_0(t)$. Since their time dependence is given by $\cos(2\pi kt/T)$ there will be $k\geqslant2$ oscillations within the period $[-T/2,T/2]$ which leads to a violation of the SCC. Figure 6 illustrates this situation for $\Omega\in\{\Omega\}_2$ and $C=0.1$. In Fig. 6(a) and 6(b), the SCC is violated within the time interval $0\leqslant|t|\leqslant\tau/2$ and $\tau/2\leqslant|t|\leqslant T/2$, respectively.

Finally, it is instructive to investigate the energy $E(\Omega,C)$ of the one-particle breather with frequency Ω for given coupling constant C. It is easy to prove that its Ω dependence is given by

$$E(\Omega,C)=\Omega^2\tilde{E}_{\mathrm{kin}}(C)+\tilde{E}_{\mathrm{pot}}(C),\tag{29}$$

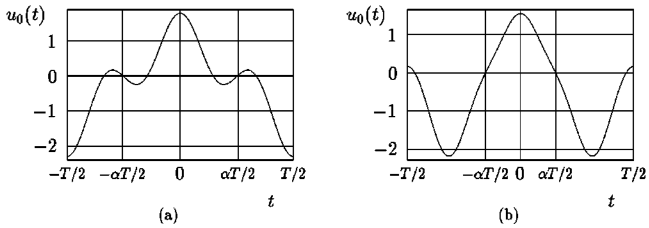

FIG. 6. Two formal solutions for $u_0(t)$ as a function of time for Ω in the second nonresonant frequency band for (a) $\alpha=0.51046$ and (b) $\alpha=0.310319$.

where $\tilde{E}_{\mathrm{kin}}(C)$ and $\tilde{E}_{\mathrm{pot}}(C)$ follow from Eqs. (1), (2), and (21) by taking into account that $u_n(t)=\tilde{u}_n(t/T)$ with $\tilde{u}_n(x+1)=\tilde{u}_n(x)$. The one-particle breather we consider corresponds to a periodic motion between the two metastable configurations characterized by σ, with $\sigma_n=-1$ for all n and σ' with $\sigma_n=-1$ for all $n\neq 0$ and $\sigma_0=+1$, i.e., both pseudospin configurations differ from each other by a single spin flip at $n=0$. The barrier height E_b, which has to be surmounted when passing from the metastable configuration $\{u_n(\sigma)\}$ to $\{u_n(\sigma')\}$, can be calculated similarly as was done for a double spin flip in Ref. [5], just by adding a force term $F\delta_{n,0}$ on the right-hand side of Eq. (4a), where in addition $\ddot{u}_n(t)$ must be set to zero. Then we obtain the stationary configurations $\{u_n(F)\}$, from which E_b follows. The result is

$$E_b(C)=\frac{1}{2}\,\frac{1+\eta_0(C)}{1-\eta_0(C)}, \tag{30}$$

where $\eta_0(C)\equiv\eta(C)$ from Eq. (5). Since $E(\Omega,C)>E(\Omega_{\mathrm{min}}(C),C)\equiv E_{\mathrm{min}}(C)$, we compare the minimum breather energy E_{min} with E_b, which is done in Fig. 7. Except for $C=0$, the case of the single oscillator, it is $E_{\mathrm{min}}(C)>E_b(C)$, i.e., the dynamical barrier E_{min} is always larger than the static one, as one would expect. Their deviation is largest for $C\to C_{\mathrm{min}}$ and $C\to C_{\mathrm{max}}$.

Let us finally comment on one-particle breathers with Ω above the phonon band. In contrast to a ϕ^4 potential we have not found such breathers. We have not been able to rigorously disprove their existence, but we are convinced that their nonexistence is related to the fact that the single-oscillator frequencies for $C=0$ are either below or within the phonon band, depending on the sign of C.

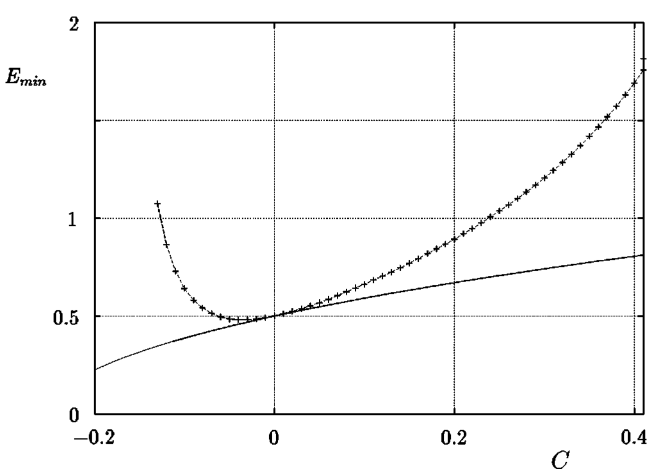

FIG. 7. Minimum energy of the single-particle breather in dependence on C (symbols). The solid line represents the static barrier E_b (cf. text), and the dashed line is a guide for the eye.

B. Multiparticle breathers

Having studied the existence and properties of one-particle breathers, we will now investigate breathers where r adjacent particles ($r\geqslant 2$) perform coherent interwell oscillations. As already mentioned in Sec. II multiparticle breathers can have a rather complex time dependence, particularly due to their ''internal dynamics.'' For instance, the particles may oscillate in phase, antiphase, or may even have arbitrary phase relations. Here we will restrict ourselves to in-phase and antiphase breathers, which are specified by the pseudospin oscillations for $n=0,1,\ldots,r-1$,

$$+++\cdots+\leftrightarrow---\cdots-$$

and

$$+-+\cdots-\leftrightarrow-+-\cdots+,$$

respectively. Of course, the times $\pm\tau_n/2\equiv\pm\alpha_n T/2$ where the nth breather particles crosses $u_n=0$, still depend on n.

The r-particle breathers have been obtained by numerical calculation of $u_n(t)$ from Eqs. (10a), (15), and (19) taking Eqs. (11), (12), (14), (16), and (20) into account. The necessary condition

$$u_n(\pm\alpha_n T/2)=0, \quad n=0,1,\ldots,r-1 \tag{31}$$

yields, for $\alpha_n(\Omega)$, a qualitatively similar result as for $r=1$, shown in Fig. 3. Let us first discuss the in-phase breathers. The detailed discussion of the SCC reveals that in-phase breathers can only exist for $\Omega\in\{\Omega\}_1$ and $\alpha_n\approx\frac{1}{2}, n=0,1,\ldots,r-1$, as we have found for $r=1$. The $\Omega-C$ phase diagram for the existence of multiparticle breathers is shown in Fig. 8 for $r=2$, 3, and 5. The solid lines which are the approximate border lines for the region where r-particle breathers exist can analogously be obtained as the corresponding lines $\Omega_{\mathrm{min}}(C)$ and $\Omega_{\mathrm{max}}(C)$ for $r=1$ [8]. From Fig. 8 we see that the region of existence does not depend sensitively on r, but slightly shrinks with increasing r.

The result for *antiphase* breathers with $\alpha_n\approx\frac{1}{2}$, $n=0,1,\ldots,r-1$ does not differ much from the results for the in-phase breathers. The phase diagram shown in Fig 9 for $r=2$, 3, and 5 exhibits qualitatively the same structure as that in Fig. 8. We note that again no such multiparticle breathers with $\alpha_n\approx\frac{1}{2}$ exist for $\Omega\in\{\Omega\}_k$ with $k\geqslant 2$. However, the situation changes significantly if we search for antiphase breathers with α_n quite different from $\frac{1}{2}$. For $r=2$ and $\Omega\in\{\Omega\}_k$, with $k=2$ and 3, we represent the allowed values $\alpha_0(\Omega)$ versus $\alpha_1(\Omega)$ in Fig. 10. Two features are remarkable: (i) $\alpha_n(C)$ are close to rational numbers, e.g., $\frac{1}{4},\frac{1}{3},\frac{2}{3}$, and $\frac{3}{4}$, which shows that $\alpha_n(\Omega)$ is close the limiting value $\alpha_\nu^{(k)}$ [cf. Eq. (27)] and (ii) $\alpha_0(\Omega)+\alpha_1(\Omega)$ is about 0 or 1. The $\Omega-C$ phase diagram represented for $r=2$ and restricted to $\{\Omega\}_2$ and $\{\Omega\}_3$ in Fig. 11 is qualitatively different from the corresponding diagrams (Figures 5, 8, and 9) for breathers with $\alpha(\Omega)\approx\frac{1}{2}$. In contrast to the latter, there are no

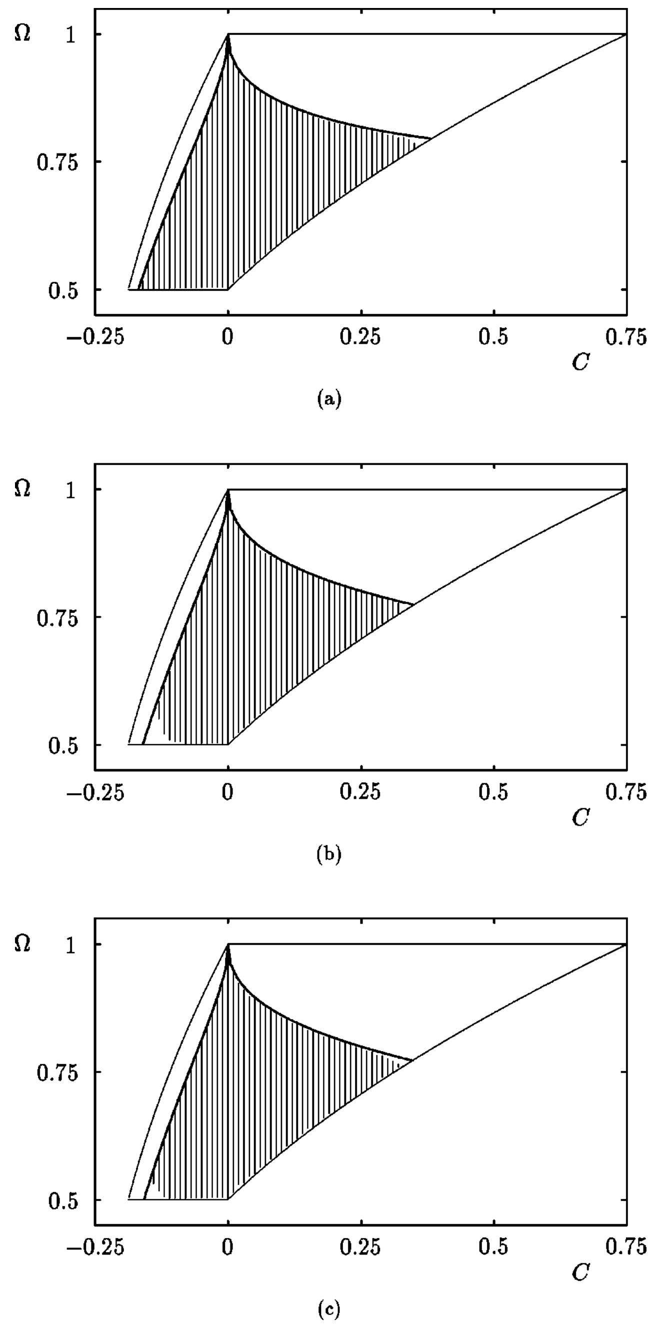

FIG. 8. Phase diagrams for in-phase multiparticle breathers. (a) $n_0=2$, (b) $n_0=3$, and (c) $n_0=5$. The hatched region represents the numerical result, and the thick solid lines are analytical approximations for $\Omega_{\min}(C)$ and $\Omega_{\max}(C)$.

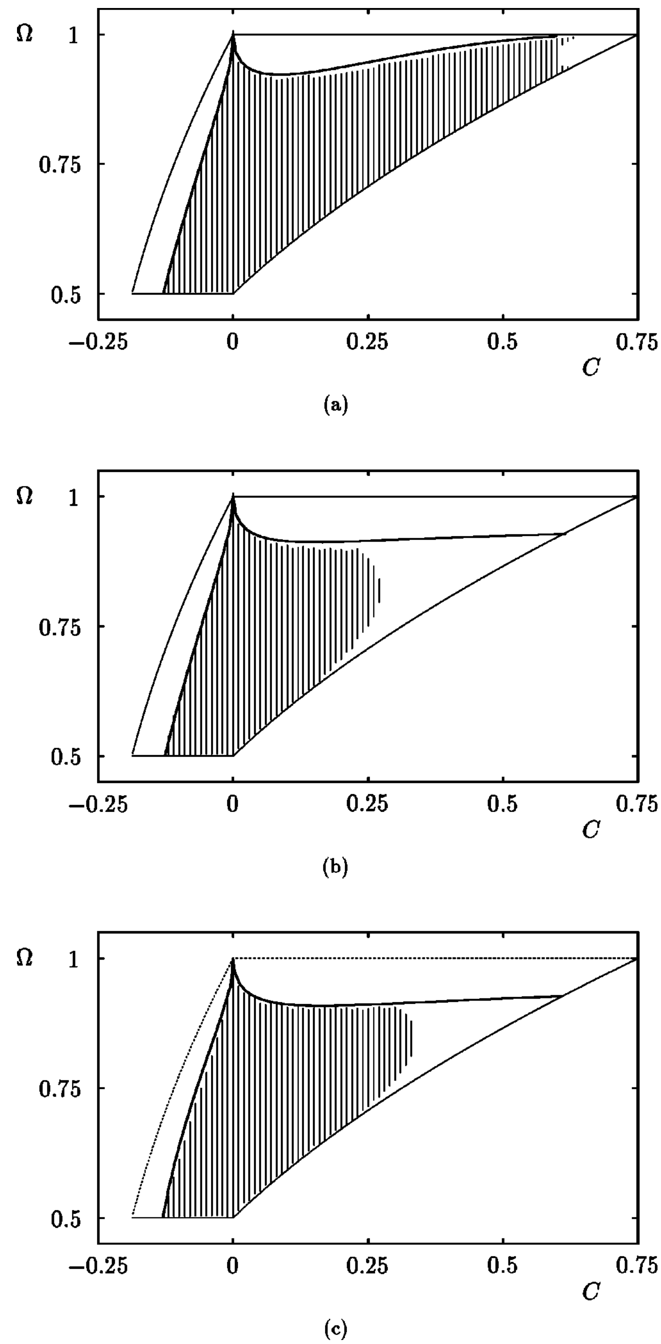

FIG. 9. Similar to Fig. 8, but phase diagrams for antiphase multiparticle breathers. (a) $n_0=2$, (b) $n_0=3$, and (c) $n_0=5$ (cf. text).

antiphase breathers with α_n quite different from $\frac{1}{2}$ for $C\to 0$. This result is obvious since $C\to 0$ converges to the single-particle oscillator for which it must be $\alpha=\frac{1}{2}$. Hence it is interesting that we have found breather solutions for $r>1$ with α different from about $\frac{1}{2}$ and $\Omega\in\{\Omega\}_k, k\geqslant 2$, which cannot continuously be obtained from those of the single-particle oscillators for $C=0$. However, a generalization of MacKay and Aubry's approach to independent two-particle, three-particle, etc. oscillators coupled to each other via the nearest neighbor interaction may serve as a basis to generate these multiparticle breathers after the coupling of these two-particle, three-particle, etc. particle oscillators to the remaining part of the chain has been turned on continuously.

IV. SUMMARY AND CONCLUSIONS

For a one-dimensional model with double-quadratic onsite and harmonic nearest neighbor interactions, we have investigated the existence and properties of *periodic* multiparticle breathers where r adjacent particles ($r\geqslant 1$) perform anharmonic oscillations between both local wells of the onsite potential. Although simple, this model has the advantage that the breather solutions can be found in a closed analytical form. This form parametrically depends on $\Omega=2\pi/T$, the breather frequency and $\tau_n, n=0,1,\ldots,r-1$ where $\pm\frac{1}{2}\tau_n$

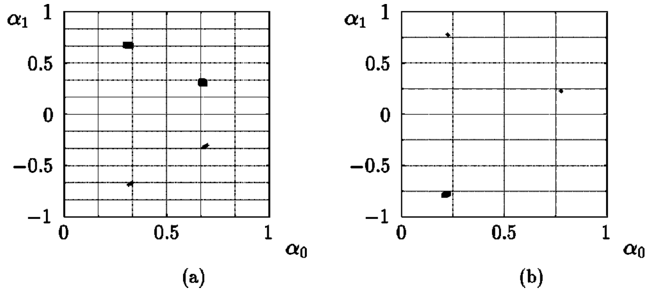

FIG. 10. Parameters α_1 vs α_0 for a two-particle breather with Ω in the (a) second and (b) third nonresonant frequency bands. Small points indicate negative C, larger points mark $C>0$. Vertical and horizontal lines are a guide for the eye.

$\equiv\alpha_n T$ fixes the time at which the nth breather particle crosses the local barrier of the on-site potential. In order that this analytical form describes a physical solution it must fulfill a self consistency condition (SCC). This SCC, which was investigated both analytically and numerically, fixes α_n and therefore τ_n for fixed Ω and finally yields for given coupling constant C the frequency range $\Omega_{\min}(C)\leqslant\Omega\leqslant\Omega_{\max}(C)$ for which breathers exist. C itself is restricted to $C_{\min}\leqslant C \leqslant C_{\max}$.

We have not found breathers with Ω *above* the phonon band, as they exist for a ϕ^4 model, but only below. The reason for this is that the double-quadratic on-site potential has a so-called *softening* character which means that its anharmonic oscillations have lower frequencies than its linear counterpart, the phonons. For such potentials it is generic that breathers above the phonon band do not exist [9].

Below the phonon band we have found two types of r-particle breathers, $r=1,2,\ldots$. One, for which its frequency is within the spectrum of the single-particle oscillator for $C=0$ and where the length of stay of each of the breather particles in the left and right well is about the same, i.e., $\alpha_n\approx\frac{1}{2}$ for $n=0,1,\ldots,r-1$, and another type for which Ω is below the single oscillator spectrum and α_n is different from about $\frac{1}{2}$. In contrast to the first type, the latter cannot continuously be obtained from the independent single-particle oscillator by keeping Ω fixed, i.e., from the antiintegrable limit [3]. Since this case occurs for $r\geqslant 2$ only, one probably has to start with the anharmonic oscillation of an independent r-particle cluster, or it may be possible to obtain them from an analytical continuation from $C=0$ by fixing, e.g., the energy or action. One may ask why the second type of breather occurs for two and more particles only. The answer can be seen from Fig. 12 which shows $u_n(t)$, $n=-1$, 0, 1, and 2, for a two-particle breather in antiphase and $\alpha\neq\frac{1}{2}$. For instance, the breather particle $n=1$ performs an oscillation during its time $(-\tau_1/2\leqslant t\leqslant\tau_1/2)$ in the right well without leaving it, which could violate the SCC. Breather particle $n=0$ does the same in the left well for $-T+\tau_0/2 \leqslant t\leqslant-\tau_0/2$. We have found that these kinds of intrawell oscillations are characteristic of breathers of the second kind. Such modulations may also occur for the formal solution (21) for $r=1$, but there they always violate the SCC. That this is not the case for $r>1$ is related to a subtle energy exchange among the breather particles which is not possible for $r=1$, i.e., a breather particle may oscillate for a while within one of the wells and may gain energy from its adjacent breather particle in order to be able to cross the local barrier. In the course of this process this latter particle loses energy and starts to perform intrawell oscillations, etc.

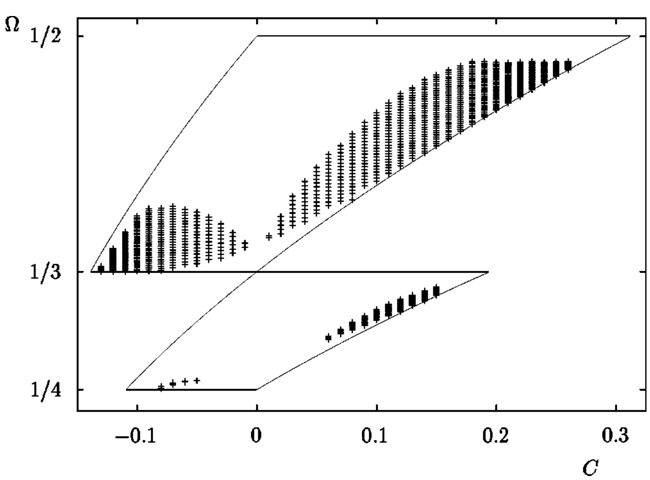

FIG. 11. Phase diagram for very slow two-particle breathers (shaded area). Solid lines indicate the bounds of the nonresonant frequency bands for $k=2$ and 3.

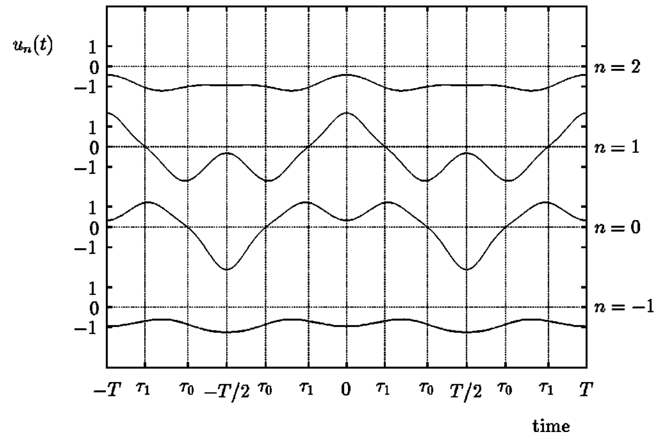

FIG. 12. Solutions $u_n(t)$ for a very slow two-particle breather and $n=-1,0,1$, and 2.

The question which naturally arises is the following: How generic are the results for the DQ potential? Since the single-particle oscillator spectrum for, e.g., a ϕ^4 model is also partly below the phonon band we expect similar type of behavior as for the DQ potential. Particularly for a symmetric *double-well* potential there should be multi-breathers for which one, two and more particles may cooperatively oscillate between both wells. It would be interesting to check this numerically.

Our results also establish an explanation for the dynamically cooperative clusters of about 3–5 particles which were observed in a molecular dynamics (MD) simulation of the DQ potential model for finite intermediate temperatures [4]. In this respect we mention that a MD simulation of a one-dimensional ϕ^4 model has also shown the existence of coherent interwell [10] as well as intrawell oscillations [11]. Unfortunately it has not been studied in detail how the size of the clusters change with temperature. Particularly interesting is the question of whether the number of particles which perform coherent interwell oscillations increases with increasing temperature, or whether there exists only a certain temperature range where interwell oscillations with about a fixed number of particles exist. For the latter case one may ask what determines the size of dynamically cooperative clusters. In this respect let us mention that neutron- and light-scattering experiments on strongly supercooled liquids yield spectra which exhibit a so-called boson peak about one decade in frequency below the ordinary phonon peak. Since this boson peak does not possess a significant dispersion, it must originate from local vibrations. Whether their existence is mainly due to the disorder or may also be influenced by anharmonicity, as recently speculated, [12] is not clear.

To summarize, we may say that besides breatherlike motions *within* a local potential well there should exist multi-breathers where a cluster of r particles performs coherent *inter-well oscillations*. This type of breather should be generic because any N-particle potential in any dimension is expected to have $\exp(\alpha N)$ (α is a constant of order 1) local minima [13], [14]. For finite temperatures they should be damped leading to a finite lifetime.

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