Stability and motion of intrinsic localized modes in nonlinear periodic lattices

K. W. Sandusky, J. B. Page, and K. E. Schmidt
Department of Physics and Astronomy, Arizona State University, Tempe, Arizona 85287-1504
(Received 26 December 1991)

Previous theoretical studies and molecular-dynamics simulations show that a *periodic* one-dimensional lattice with nearest-neighbor quadratic and quartic interactions supports stationary localized modes. The most localized of these are an odd-parity mode with a displacement pattern $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$ and an even-parity mode $A(\ldots,0,-1,1,0\ldots)$, where A is the amplitude. These solutions are asymptotically exact for the pure even-order anharmonic lattice in the limit of increasing order. We show here that in both this asymptotic limit and for the harmonic plus quartic lattice, the odd-parity mode is unstable to infinitesimal perturbations, while the even-parity mode is stable. For the pure quartic case, the predicted growth rate for the instability is 0.15 in units of the mode frequency, in excellent agreement with the rate observed in our molecular-dynamics simulations. In contrast, we observe the even-parity mode to persist unchanged over more than 32 000 mode oscillations. Our simulations show that the instability does not destroy the odd mode, but causes it to move. We will also discuss a smoothly traveling version of these modes. As they move, these modes have a nonconstant phase difference between adjacent relative displacements, in contrast with traveling modes discussed previously by others.

I. INTRODUCTION

Previous analytical and molecular-dynamics (MD) simulations show that stationary, opticlike intrinsic localized modes exist on a one-dimensional monatomic periodic lattice with nearest-neighbor quadratic and quartic interactions.[1–4] These modes are reminiscent of defect-induced localized modes for harmonic lattices, except they occur in perfect lattices and can occur on any lattice site. Furthermore, it has been shown that these intrinsic localized modes can also move.[4,5] It has been suggested that three-dimensional versions of these modes could exist in strongly anharmonic crystals, such as solid He and ferroelectric systems.[6]

The most localized versions of the stationary modes are an even-parity mode with approximate displacements $A(\ldots,0,1,-1,0,\ldots)$ (Ref. 2) and an odd-parity mode with displacements $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$ (Ref. 1), where A is the amplitude. For positive anharmonicity, both of these modes have amplitude-dependent frequencies above the maximum harmonic phonon frequency. Moreover, they become *exact* solutions for a pure even-order anharmonic lattice in the asymptotic limit of increasing anharmonic order.[2]

In this paper we first use this asymptotic limit to show very simply that the odd-parity mode for this case is in fact unstable against certain velocity and displacement perturbations, whereas the even mode is stable against analogous perturbations. This is done in Sec. II. In Secs. III and IV, we then focus on the case of a quadratic plus quartic lattice and use perturbation theory to show that the odd-parity mode for this case remains unstable against similar perturbations. We predict the growth rates for the instability and find that they agree well with rates measured in our MD simulations. These simulations show that the unstable nature of the odd-parity localized mode does not destroy the mode; instead, it causes it to move. In contrast to the odd-parity case, no instabilities are predicted for the even-parity mode for the quadratic plus quartic lattice and none are observed in our simulations. Indeed, we find this mode to be extremely stable. Finally, for a wide range of anharmonicity, we have observed a type of smoothly moving localized mode with nonconstant phase difference between adjacent relative displacements. These modes are discussed in Sec. V, and the paper is concluded in Sec. VI.

II. ASYMPTOTIC MODE STABILITY

To bring out clearly the physics of the odd-parity-mode instability in the harmonic plus quartic lattice, we will first discuss the much simpler case of an odd-parity mode in a pure even-order anharmonic lattice in the asymptotic limit of increasing anharmonic order. For a purely anharmonic lattice of even order r, the potential energy is

$$V=\frac{k_r}{r}\sum_n (u_{n+1}-u_n)^r , \tag{1}$$

where k_r is the rth-order spring constant and u_n is the displacement of the nth particle from its equilibrium site. Figure 1 shows the particle oscillations for the odd-parity mode, obtained via MD simulations for the case $r=6$. These oscillations are seen to resemble closely those for free particles undergoing elastic collisions at the turning points. This suggests that, as the order increases, the portion of an oscillation during which the particles are subject to large accelerations decreases and the system behaves like a chain of elastically colliding point masses attached to each other by nearest-neighbor inextensible

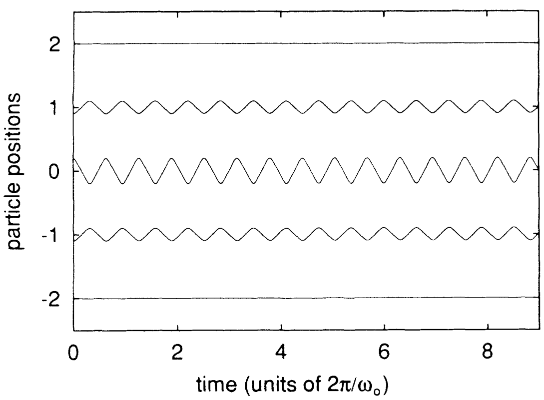

FIG. 1. Molecular-dynamics-simulation results for the displacements of an odd-parity localized mode $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$, centered at site zero in a 21-particle pure anharmonic lattice of order 6. For this simulation, k_6 and the amplitude were chosen so that $\omega=1.6\omega_0$, where $\omega_0=1.00$ $[\mathrm{eV}/(\mathrm{\AA}^2\,\mathrm{amu})]^{1/2}$ is a convenient frequency unit. The displacements for the particles not shown are negligible. The oscillations are seen to resemble closely those of free particles undergoing elastic collisions at the turning points.

strings. The effect of the string is just to produce an instantaneous velocity change whenever they are fully extended. The particles will collide when their relative displacements satisfy $u_{n+1}-u_n=-a$, where a is the lattice constant. Since the potential is symmetric in the displacements, the string length between adjacent point particles must then be $2a$, producing a reversal when $u_{n+1}-u_n=a$, as illustrated in Figs. 2 and 3 for the even- and odd-parity modes, respectively.

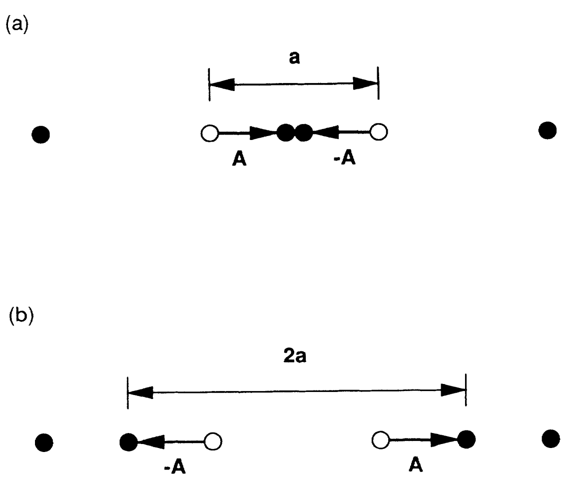

FIG. 2. (a) Collision and (b) "snap" for the even-parity mode $A(\ldots,0,1,-1,0,\ldots)$ in the hard-sphere–string model. The particles are perfectly elastic point masses with adjacent particles connected by inextensible strings of length $2a$, where a is the lattice constant. As shown in the text, this model exactly describes the mode in the asymptotic limit of increasing order in a purely even-order anharmonic lattice. The open circles show the equilibrium positions. The point masses collide halfway between their equilibrium positions; the amplitude for the mode is $A=a/2$.

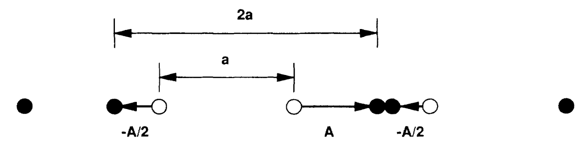

FIG. 3. Simultaneous collision and snap for the odd-parity mode $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$ in the asymptotically exact hard-sphere–string model. The amplitude for this mode is $A=2a/3$. As discussed in the text, this mode is unstable to any perturbation which destroys the simultaneity of the collision and snap.

A. Theory

To verify this "hard-sphere–string" model in the limit of large even anharmonic order, consider the potential between two adjacent particles in the limit of large r:

$$\frac{k_r b^r}{r}[(u_{n+1}-u_n)/b]^r \to \begin{cases} \infty\,, & |u_{n+1}-u_n|>b \\ 0, & |u_{n+1}-u_n|<b\,, \end{cases} \tag{2}$$

where $k_r b^r/r$ approaches a finite constant as $r\to\infty$. This is a square-well potential of width b, involving the relative displacements between two adjacent particles. This is just the type of potential described by the above hard-sphere–string model. For point masses the width of the well must be $b=a$.

The equations of motion are separable into spatial and temporal parts, so that the solutions for the stationary modes will have the form $u_n=A\xi_n f(t)$, where A is the amplitude, $\{\xi_n\}$ is the normalized displacement pattern, and $f(t)$ is a periodic function describing the time dependence of the mode oscillations.[7] Energy conservation yields

$$E=\frac{1}{2}mA^2\dot{f}^2\sum_n \xi_n^2+\frac{k_r A^r}{r}f^r\sum_n(\xi_{n+1}-\xi_n)^r\,, \tag{3}$$

where m is the particle mass. If we scale $f(t)$ such that $|f(t)|=1$ when $\dot{f}(t)=0$, the amplitude is given by

$$A=b\left[\frac{rE}{k_r b^r}\right]^{1/r}\left[\sum_n(\xi_{n+1}-\xi_n)^r\right]^{-1/r}. \tag{4}$$

To determine the period, the energy-conservation equation can be rewritten as

$$\tfrac{1}{2}mA^2\dot{f}^2\sum_n\xi_n^2=E(1-f^r)\,, \tag{5}$$

which can be integrated to yield

$$\tau=4A\left[\frac{m\sum\xi_n^2}{2E}\right]^{1/2}\int_0^1 df(1-f^r)^{-1/2}\,. \tag{6}$$

In the limit $r\to\infty$, $(rE/k_r b^r)^{1/r}\to 1$, since $rE/k_r b^r$ remains finite, so that the amplitude becomes

$$A\to a\Lambda'\,, \tag{7}$$

where Λ' is the limit of $[\sum_n(\xi_{n+1}-\xi_n)^r]^{-1/r}$ for large r and we have replaced b with its point-mass value a. For large r the integral in Eq. (6) approaches unity, and the amplitude approaches the value given by Eq. (7). Hence the period becomes

$$\tau \rightarrow 4a\Lambda' \left[\frac{m \sum_n \xi_n^2}{2E} \right]^{1/2} . \tag{8}$$

In this limit the period depends only upon lattice spacing, the normalized displacement pattern $\{\xi_n\}$, and the energy.

B. Even-parity mode

For the even mode $A(\ldots,0,1,-1,0,\ldots)$, Eq. (7) gives $A \rightarrow a/2$ and Eq. (8) gives $\tau \rightarrow 2a(m/E)^{1/2}$, which can be identically rewritten as $\tau = 2a/v$, where v is the particle speed. As illustrated in Fig. 2, this is the same amplitude obtained for this mode in the hard-sphere–string model. Also, since $2a$ is the distance traveled by one of the oscillating particles during an oscillation, the period is just what one obtains for a particle undergoing elastic collisions at its turning points. Hence the above asymptotically exact results for the amplitude and period show that the even-parity mode is correctly described by the hard-sphere–string model.

C. Odd-parity mode

For the odd mode $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$, Eq. (7) gives $A \rightarrow 2a/3$ and Eq. (8) gives $\tau \rightarrow 8a/3v$, where v is the speed of the central particle. This is the same amplitude predicted by the hard-sphere–string model, as shown in Fig. 3. Again, the period is the distance traveled by the central particle divided by its speed. Hence the exact results for both the amplitude and period show that the odd-parity mode is also correctly described by the hard-sphere–string model.

For this mode the central particle has twice the speed of the two adjacent particles. At the turning points, the central particle simultaneously interacts with both of its neighbors: It collides with one of its neighbors *at the same time* that the string attaching it to the other neighbor snaps taut.

D. Instability

In the large-order anharmonicity limit, any perturbation of the odd-parity mode which causes the collision and string snap to occur at different times will destroy the mode. For example, an even-parity *velocity* change, i.e., $(\ldots,0,-\Delta v,0,\Delta v,0,\ldots)$, will increase the speed of one of the central particle's adjacent neighbors while decreasing the speed of the other adjacent neighbor. This destroys the simultaneity of the collision and snap, obviously destroying the stationary mode. Similarly, an even-parity *displacement* perturbation, i.e., $(\ldots,-\Delta u,0,\Delta u,0,\ldots)$, will increase the amplitude of one of the central particle's adjacent neighbors while decreasing the amplitude of the other adjacent neighbor. This too will destroy the simultaneity of the snap and collision. Thus the odd-parity mode is unstable against both even-parity velocity and displacement perturbations. In contrast, this mode *is* stable against odd-parity perturbations because such perturbations change the speed and amplitude of both of the central particle's neighbors by the same amount; the collision and snap remain simultaneous.

Finally, we note that the even-parity mode involves *no* simultaneous interactions. Hence it is stable.

III. STABILITY ANALYSIS THEORY FOR THE HARMONIC PLUS QUARTIC CASE

While the asymptotic limit of high-order anharmonicity brings out very simply the qualitative difference between the odd and even modes with regards to stability, it remains to quantitatively investigate stability for finite orders. Accordingly, we now focus on a lattice with nearest-neighbor harmonic plus quartic interactions. To determine if the odd-parity mode in this lattice is also unstable, we will consider the effects of small perturbations on this mode.

The potential for a periodic lattice with harmonic and quartic nearest-neighbor interactions is

$$V = \frac{k_2}{2} \sum_n (u_{n+1} - u_n)^2 + \frac{k_4}{4} \sum_n (u_{n+1} - u_n)^4 , \tag{9}$$

where k_4 and k_2 are the quartic and harmonic spring constants, respectively. The stationary intrinsic localized modes may be obtained analytically by first substituting a solution of the form $u_n = A\xi_n \cos(\omega t)$ into the equations of motion. One then makes the "rotating-wave approximation,"[1] by identically rewriting the resulting $\cos^3(\omega t)$ factor as $\frac{3}{4}\cos(\omega t) + \frac{1}{4}\cos(3\omega t)$ and keeping just the $\cos(\omega t)$ term. The equations may then be solved to determine the frequency and displacement patterns as functions of the amplitude.[1,2]

To study the stability of the odd and even modes for the harmonic plus quartic lattice, we will assume a solution of the form $u_n = A\xi_n(t)\cos[\omega t + \phi_n(t)]$, where we are now allowing the normalized displacement pattern $\{\xi_n\}$ to vary with time and have added a time- and site-dependent phase ϕ_n to the $\cos(\omega t)$ term. In Ref. 8 it was argued that stationary intrinsic localized solutions for a one-dimensional harmonic plus quartic periodic lattice would be stable, provided $k_4 > 0$. However, the stability analysis given there neglected the possibility of a time- and site-dependent phase, which we have found to be essential.

Since our molecular-dynamics simulations show that the odd and even localized modes are generally stable over at least several periods, the phases and displacement patterns must vary slowly in time on the scale of the mode period. If we assume that the relative phase differences between adjacent particles introduced are small, we can write

$$\begin{aligned} \cos(\omega t + \phi_{n\pm1}) &= \cos(\omega t + \phi_n)\cos(\phi_{n\pm1} - \phi_n) \\ &\quad - \sin(\omega t + \phi_n)\sin(\phi_{n\pm1} - \phi_n) \\ &\approx \cos(\omega t + \phi_n) - \sin(\omega t + \phi_n)(\phi_{n\pm1} - \phi_n) . \end{aligned} \tag{10}$$

Substituting this into the equations of motion yields an equation involving first and third powers of $\cos(\omega t+\phi_n)$ and $\sin(\omega t+\phi_n)$. We next multiply by $\cos(\omega t+\phi_n)$ and integrate over a mode period, obtaining

$$\ddot{\xi}_n-\dot{\phi}_n^2\xi_n-2\omega\xi_n\dot{\phi}_n-\omega^2\xi_n=\frac{k_2}{m}(\xi_{n+1}+\xi_{n-1}-2\xi_n)+\frac{3}{4}\frac{k_4}{m}A^2[(\xi_{n+1}-\xi_n)^3+(\xi_{n-1}-\xi_n)^3]\ . \tag{11}$$

Analogously, a second equation is obtained by multiplying the equations of motion by $\sin(\omega t+\phi_n)$ and integrating:

$$\xi_n\ddot{\phi}_n+2\omega\dot{\xi}_n+2\dot{\phi}_n\dot{\xi}_n=\frac{k_2}{m}[\xi_{n+1}(\phi_{n+1}-\phi_n)+\xi_{n-1}(\phi_{n-1}-\phi_n)]+\frac{3}{4}\frac{k_4}{m}A^2[(\xi_{n+1}-\xi_n)^2\xi_{n+1}(\phi_{n+1}-\phi_n)+(\xi_{n-1}-\xi_n)^2\xi_{n-1}(\phi_{n-1}-\phi_n)]\ . \tag{12}$$

Only the linear terms in the difference $\phi_{n\pm1}-\phi_n$ have been kept in the second equation, since we have assumed that these terms are small. Since we are assuming that the normalized displacement pattern and phase vary slowly with respect to the mode period, these quantities should be unaffected by the time average.

We note that these equations are the same as those one would obtain by using the rotating-wave approximation on both the $\sin^3(\omega t+\phi_n)$ and $\cos^3(\omega t+\phi_n)$ terms and making no time averages. In obtaining Eqs. (11) and (12) using the time-averaging method, we explicitly required that the phase and normalized displacements vary slowly on the scale of the mode period. The derivation of Eqs. (11) and (12) utilizing the rotating-wave approximation would place no restrictions on the time variation of the normalized displacements and phases. However, our simulations show that these quantities do evolve slowly compared with the mode period. Hence we feel that our time-averaging approach more correctly reflects the physical situation. Moreover, we will see just below that the zeroth-order version of our Eq. (11) reproduces precisely the same stationary mode as given by the use of the rotating-wave approximation. In view of our derivation, any perturbation obtained from these equations whose time variation is greater than or comparable to the mode period should be unphysical.

Now we let $\xi_n=\xi_n^0+\delta\xi_n(t)$ and $\phi_n=\phi^0+\delta\phi_n(t)$, where the $\{\xi_n^0\}$ are the normalized displacements which describe the unperturbed stationary mode and where the time-dependent terms are infinitesimal perturbations. To zeroth order in the perturbations, Eq. (11) reduces to

$$-\omega^2\xi_n^0=\frac{k_2}{m}(\xi_{n+1}^0+\xi_{n-1}^0-2\xi_n^0)+\frac{3}{4}\frac{k_4}{m}A^2[(\xi_{n+1}^0-\xi_n^0)^3+(\xi_{n-1}^0-\xi_n^0)^3]\ , \tag{13}$$

which is just the equation that determines the frequency and normalized displacement pattern for the unperturbed modes.[1,2] The first-order equations involve first time derivatives, which can be eliminated by making the substitutions $\psi_n=\delta\dot{\phi}_n$ and $\zeta_n=\delta\dot{\xi}_n$. This doubles the number of variables, but if we assume that the perturbations have an exponential time dependence $\exp(\lambda t)$, we can reduce the problem to an eigenvalue equation involving λ. The four first-order equations for the nth particle are then

$$\lambda\zeta_n=2\omega\xi_n^0\psi_n+\omega^2\delta\xi_n+\frac{k_2}{m}(\delta\xi_{n+1}+\delta\xi_{n-1}-2\delta\xi_n)+\frac{9}{4}\frac{k_4}{m}A^2[(\xi_{n+1}^0-\xi_n^0)^2(\delta\xi_{n+1}-\delta\xi_n)+(\xi_{n-1}^0-\xi_n^0)^2(\delta\xi_{n-1}-\delta\xi_n)]\ , \tag{14}$$

$$\lambda\psi_n=-2\omega\zeta_n/\xi_n^0+\frac{k_2}{m}[\xi_{n+1}^0(\delta\phi_{n+1}-\delta\phi_n)+\xi_{n-1}^0(\delta\phi_{n-1}-\delta\phi_n)]/\xi_n^0+\frac{3}{4}\frac{k_4}{m}A^2[(\xi_{n+1}^0-\xi_n^0)^2\xi_{n+1}^0(\delta\phi_{n+1}-\delta\phi_n)+(\xi_{n-1}^0-\xi_n^0)^2\xi_{n-1}^0(\delta\phi_{n-1}-\delta\phi_n)]/\xi_n^0\ , \tag{15}$$

$$\lambda\delta\phi_n=\psi_n\ , \tag{16}$$

$$\lambda\delta\xi_n=\zeta_n\ . \tag{17}$$

To determine the eigenvalues, we have to solve a $4m\times4m$ eigenvalue problem, where m is the number of sites included in the perturbation theory. The mode will be unstable if a perturbation exists which produces an eigenvalue with a positive real part, since this means that the perturbation will grow exponentially with time.

IV. RESULTS

A. Pure quartic case

First, we will consider the simpler case of the odd-parity mode in a pure quartic lattice. In this case the stationary odd-parity-mode normalized displacement pattern is independent of the amplitude and is accurately given by $(\ldots,0,0.02,-0.52,1.0,-0.52,0.02,0,\ldots)$.[2] There are five particles with nonzero displacements, so Eqs. (14)–(17) generate a 20×20 eigenvalue problem that determines the growth rate λ. By casting Eqs. (14)–(17) into a dimensionless form and solving the eigenvalue equation numerically, we find that the odd-parity mode is unstable for all values of the amplitude and k_4. The eigenvectors show that this mode is unstable against infinitesimal even-parity perturbations in either the particle phases, i.e., $(\ldots,\delta\phi,0,-\delta\phi,\ldots)$, or in the displacements, i.e., $(\ldots,\delta\xi,0,-\delta\xi,\ldots)$. Since a change in a particle's phase produces a change in its velocity, these are just the same type of velocity and displacement perturbations which result in instability for the asymptotic pure anharmonic odd-parity mode, as discussed above in Sec. II D. Furthermore, our eigenvalue solutions predict that the growth rate for the instability is 0.151ω, where ω is the unperturbed odd-parity-mode frequency.

In order to test the predictions of the perturbation theory, we performed molecular-dynamics simulations by numerically integrating the equations of motion using the fifth-order Gear predictor-corrector method.[9] The mass was taken to be 39.95 amu, the lattice constant was 1 Å, and the harmonic spring constant, when included, was $k_2=10.0$ eV/Å^2. This value is such that the maximum harmonic frequency $\omega_{max}=2(k_2/m)^{1/2}$ has the same value as ω_0, the frequency unit used in the pure anharmonic runs (thus the time units in Figs. 1 and 5–8 are the same). The time steps were chosen such that there were at least 100 time steps per mode oscillation, for all runs. A 21-particle lattice with periodic boundary conditions was used for the odd-parity and traveling modes. The even-parity mode was run on a 20-particle lattice, with periodic boundary conditions.

Our simulations explicitly reveal the instability of the odd-parity mode for the pure quartic lattice. We can determine the growth rate for the instability in the simulations by plotting $\ln(|u_1-u_{-1}|)$ against time, where u_1 and u_{-1} are the central particle's nearest-neighbor displacements at the displacement maxima. The difference u_1-u_{-1} isolates the even-parity perturbations of the normalized displacements $\{\xi_n\}$, so the slope of the plot will give the growth rate. For a pure quartic odd-parity mode, our measured growth rate is 0.151 ± 0.001, in units of the mode frequency, which is in excellent agreement with the rate 0.151 predicted by perturbation theory. One cannot expect better agreement than this since the frequency predicted for these modes by assuming a sinusoidal time dependence differs from the measured frequency by $\sim1\%$. The value and uncertainty for the measured growth rate are determined from a linear least-squares fit to our $\ln(|u_1-u_{-1}|)$ vs time plot.

B. Quadratic plus quartic case

When harmonic interactions (k_2) are included, the perturbation theory predicts that the growth rate decreases as the anharmonicity decreases (and hence as the mode frequency decreases). By casting Eqs. (14)–(17) into a dimensionless form, we find that the predicted growth rate only depends upon the ratio of the mode frequency to the maximum harmonic frequency. The solid curve in Fig. 4 shows the predicted growth rates as a function of ω/ω_{max}. The triangles give the growth rates observed in our simulations for various values of the amplitude and the ratio k_4/k_2. As seen in this figure, the predicted and measured growth rates are in good agreement.

The pure quartic displacement pattern $A(\ldots,0,0.02,-0.52,1.0,-0.52,0.02,0,\ldots)$ was used in our perturbation calculation of the growth rates shown in Fig. 4. However, adding the harmonic interactions slightly changes the displacement patterns for the stationary mode. For our lowest-frequency point at $\omega/\omega_{max}=1.38$, we find that the corrected displacement pattern is $A(\ldots,-0.029,0.162,-0.637,1.0,-0.637,0.162,-0.029,\ldots)$, which is somewhat broader spatially than the pure quartic pattern given above. Using this displacement pattern, we find that perturbation theory predicts a growth rate of 0.0490ω, in good agreement with the growth rate $0.0489\pm0.0001\omega$ measured in our simulations. Thus this broadening is the cause of the small discrepancies between our predicted and observed growth rates in Fig. 4 for the lower ω/ω_{max} values.

Even though the odd-parity mode is unstable, it can still persist (in either the harmonic plus quartic or in the pure quartic cases) for several oscillations before being affected by a perturbation. For example, with a displacement perturbation $(\ldots,\delta a,0,-\delta a,\ldots)$, where δa is 0.01% of the unperturbed mode amplitude, the odd-parity mode shown in Fig. 5 oscillates for roughly 15 periods before the instability alters its displacements

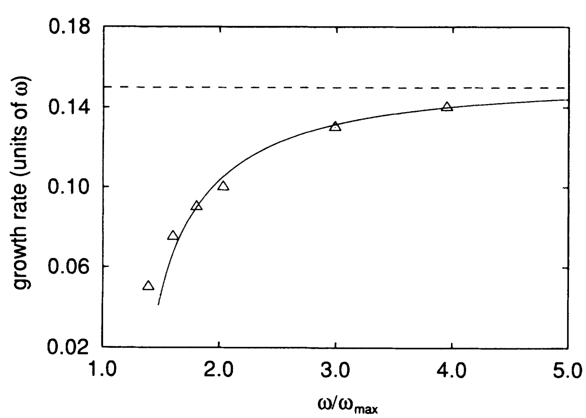

FIG. 4. Growth rate for the odd-parity intrinsic localized mode instability for a 21-particle harmonic plus quartic lattice, as a function of the ratio of the mode frequency to the maximum harmonic frequency. The solid line gives the theoretical prediction obtained using the odd-parity-mode displacement pattern $A(\ldots0,0.02,-0.52,1.0,-0.52,0.02,0,\ldots)$, and the triangles are results obtained from our molecular-dynamics simulations for various values of the amplitude and k_4/k_2. For reference, the dashed line gives the growth rate for the odd-parity mode in the pure quartic lattice. As discussed in the text, the discrepancy between the predicted and measured growth rates for the lowest-frequency point is completely removed when the spatial broadening of this mode is taken into account.

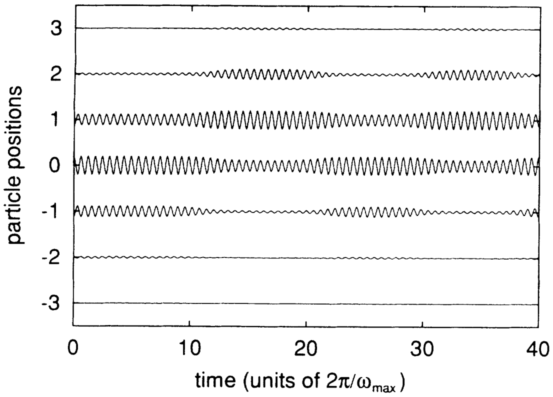

FIG. 5. Example of the instability of the odd-parity mode for a 21-particle harmonic plus quartic lattice. Here $\omega/\omega_{max}=1.63$, $J\equiv k_4A^2/k_2=1.25$, $A=0.1$ Å, and the $t=0$ unperturbed displacement pattern was $A(\ldots,0,-0.011,0.106,-0.595,1.0,-0.595,0.106,-0.011,0,\ldots)$, centered at site zero. This mode was seeded with a displacement perturbation $A(\ldots,0,-0.0001,0,0.0001,0,\ldots)$, resulting in the mode evolving into a moving mode that oscillates between sites. For clarity, the displacements have been scaled up by a factor of 2. The displacements for the particles not shown are negligible.

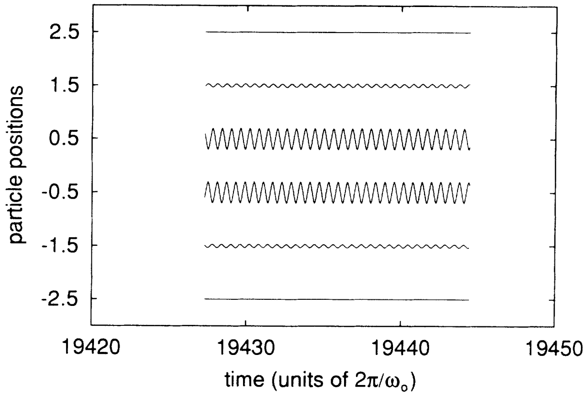

FIG. 6. Corrected even-parity mode $A(\ldots,0,-\frac{1}{6},1,-1,\frac{1}{6},0,\ldots)$ for a 20-particle pure quartic lattice, observed in our simulations after more than 32 000 oscillations. The mode is centered at sites $(-0.5,0.5)$. For this simulation, k_4 and the amplitude were chosen so that $\omega=1.7\omega_0$, where $\omega_0=1.00$ $[\mathrm{eV}/(\text{Å}^2\,\mathrm{amu})]^{1/2}$ is a convenient frequency unit. The displacements for the particles not shown are negligible. This mode is extremely stable, in agreement with the perturbation-theory analysis.

significantly. As seen in this figure, the instability does not destroy the mode, but rather causes it to begin oscillating between neighboring sites. Subject to the same perturbation, a pure quartic odd-parity mode survives for roughly 10 oscillations before beginning to oscillate between sites.

In contrast, no instabilities are predicted for the even-parity mode in either the pure quartic or harmonic plus quartic case, and we have found the even-parity mode to be extremely stable in our simulations. For instance, we have run both the pure quartic and harmonic plus quartic even-parity modes in simulations for more than 32 000 mode oscillations and have seen no changes in the mode whatsoever, as shown in Fig. 6 for the pure quartic case. Even if we include a displacement perturbation with the same relative magnitude, 0.01% A, as the perturbation used to seed the instability for the odd-parity mode shown in Fig. 5, our simulations show that the even-parity mode *still* remains unchanged after more than 32 000 mode oscillations.

V. TRAVELING LOCALIZED MODES

We have shown that the odd-parity localized mode on the harmonic plus quartic lattice is unstable against infinitesimal perturbations. Nevertheless, as illustrated in the particular case shown in Fig. 5, the instability does not destroy the mode; rather it causes it to move. Depending on the initial conditions and strength of the anharmonicity, the odd-parity mode has been observed in our simulations to manifest its instability by evolving into three different types of modes: one that oscillates between adjacent sites, as shown in Fig. 5; one that travels smoothly from site to site with constant velocity, as exemplified in Fig. 7; or one which becomes trapped at a site and evolves into an even-like mode. These modes make many oscillations in the time required to move between adjacent sites. Also, as the modes move from site to site, their displacement patterns alternate between the even- and odd-parity-mode patterns, and the mode frequency remains constant.

For example, for a relative phase perturbation

$$\delta\phi_1-\delta\phi_0=\delta\phi_0-\delta\phi_{-1}\approx-0.09\ \mathrm{rad}\ ,$$

our simulations yield smoothly traveling modes having a very well-defined velocity, for a wide range of anharmoni-

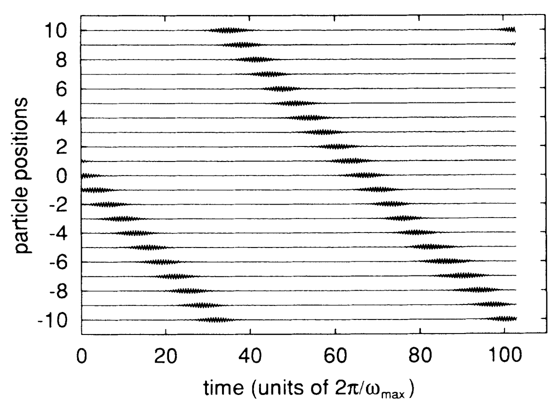

FIG. 7. Traveling localized mode in a 21-particle quartic plus harmonic lattice. For this mode $J\equiv k_4A^2/k_2=1.63$, $A=0.1$ Å, $\omega/\omega_{max}=1.67$, and the $t=0$ unperturbed displacement pattern was $A(\ldots,0,-\frac{1}{2},1,-\frac{1}{2},0,\ldots)$, centered at site zero. This mode was seeded with an initial velocity perturbation $\dot{u}_1=-\dot{u}_{-1}=0.00718$, in units of Å ω_{max}, corresponding to a relative phase perturbation of $\delta\phi_1-\delta\phi_0=\delta\phi_0-\delta\phi_{-1}=-0.086$. The velocity of this traveling mode is -0.053 in the units Å ω_{max}, well below the harmonic sound speed of 0.5. As in Fig. 5, the particle displacements have been scaled up by a factor of 2, for clarity.

city. For all of the traveling-mode simulations discussed below, the $t=0$ amplitude was set to 0.1 Å, one-tenth of the lattice spacing. To characterize the anharmonicity, we used the dimensionless parameter $J=k_4A^2/k_2$. Traveling solutions were observed over a range from $J=0.763$, which was the lowest value considered, to $J=2.46$, corresponding to a frequency range of 1.35–1.94, measured in units ω/ω_{max}. The speeds for these traveling modes, measured in units of Å ω_{max}, increased monotonically with J, from $v=0.029$ for $J=0.763$ to $v=0.067$ for $J=2.46$ All of these speeds are well below the speed of sound for the corresponding purely harmonic lattice, which in our units is 0.5. Figure 7 shows the traveling mode for the case of $J=1.63$ and an initial phase perturbation of

$$\delta\phi_1-\delta\phi_0=\delta\phi_0-\delta\phi_{-1}=-0.086 \text{ rad} .$$

The speed for this traveling mode is 0.053. When J is increased to 3.44, the frequency becomes 2.3 and the mode travels 12 sites before rapidly evolving into a mode which oscillates between two sites.

Previous analytical work on the traveling modes used the relative coordinates $d_n=u_{n+1}-u_n$ and assumed a solution with a constant phase difference between these quantities.[4,5] In particular, in Ref. 5, a solution was assumed of the form $d_n=A\xi_n(t)\cos(\omega t+\phi_n)$, with $\phi_n=nka$, meaning that there is a constant phase difference between adjacent relative displacements. The derivative $\dot{d}_n$ is then given by

$$\dot{d}_n=-\omega A\xi_n\sin(\omega t+\phi_n)+A\dot{\xi}_n\cos(\omega t+\phi_n) . \quad (18)$$

The envelope $\{\xi_n\}$ should vary slowly in time with respect to the mode period. Thus the second term in this equation should be small, provided $\sin(\omega t+nka)$ is not close to zero. In this case we can determine the phase difference from the equation

$$\phi_{n+1}-\phi_n=\tan^{-1}\left[\frac{-\dot{d}_{n+1}}{\omega d_{n+1}}\right]-\tan^{-1}\left[\frac{-\dot{d}_n}{\omega d_n}\right] . \quad (19)$$

Figure 8 shows $\phi_{-4}-\phi_{-3}$ as a function of time for the traveling mode shown in Fig. 7. The times span the interval during which the traveling mode passes the $n=-3$ particle. The phase differences in the plot were measured near the velocity extrema for the oscillation, where the $\dot{\xi}_n$ terms should be negligible. As shown in the figure, the phase difference is *not* constant as assumed in Ref. 5. Moreover, nonconstant phase differences of similar magnitude were observed between the adjacent displacements themselves, as well as between the relative displacements. Hence the phase changes need to be taken into account in analytical models describing these traveling modes. Similar results were obtained for modes with lower anharmonicity, down to $J=0.763$, the lowest value considered. This value produced a mode with $\omega/\omega_{max}=1.35$.

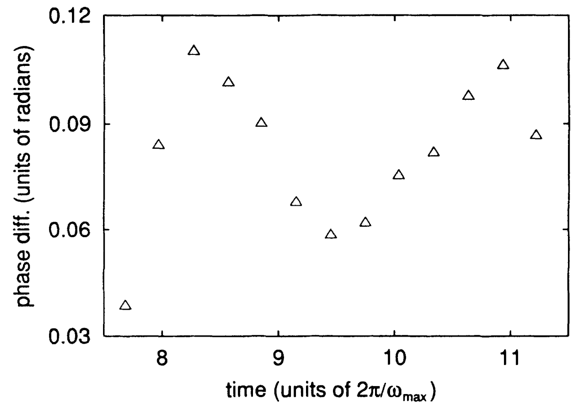

FIG. 8. Phase difference between the relative displacements $d_{-4}=u_{-4}-u_{-3}$ and $d_{-3}=u_{-3}-u_{-2}$ for the traveling mode of Fig. 7. The triangles give the relative phase as the traveling mode passes the $n=-3$ particle. This is a type of traveling localized mode where the phase is nonconstant.

VI. CONCLUSIONS

In this paper we have shown that in the limit of increasing even-order anharmonicity, the dynamics of the odd- and even-parity modes are very simply described by the asymptotically exact hard-sphere–string model, which describes the lattice as elastic point masses connected by inextensible nearest-neighbor strings. In this limit one easily sees that the even-parity mode is stable, whereas the odd-parity mode is unstable against even-parity velocity and displacement perturbations.

We then used perturbation theory to show that the odd-parity mode is also unstable in the harmonic plus quartic periodic lattice. Instability growth rates predicted by the perturbation analysis agree well with the rates measured in our molecular-dynamics simulations. Moreover, the simulations show that the even-parity mode is stable, in agreement with our perturbation-theory results.

The simulations show that the instability does not destroy the odd-parity mode, but causes it to move. Although we have considered only constant-energy systems here, we note that if there were a mechanism which could create an odd-parity mode and then feed energy into it, the amplitude would grow. In practice, there would always be a triggering mechanism for the odd-parity mode instability, i.e., fluctuations, numerical round-off errors in simulations, etc. Thus the amplitude would grow until the instability overtakes it and causes the mode to move. This appears to have occurred in the simulations of Bourbonnais and Maynard,[10] where they applied a periodic force to a single-lattice site in a periodic one-dimensional lattice having harmonic and quartic nearest-neighbor interactions and observed the subsequent production of traveling intrinsic localized modes.

The unstable odd-parity mode is observed to evolve into several different types of moving localized modes. For certain perturbations the odd-parity mode evolves into a mode which smoothly travels from site to site with a constant velocity. Preliminary results show that these traveling modes exist over a wide range of anharmonicity and can become trapped as the anharmonicity increases. These modes are a type of traveling localized mode that have a nonconstant phase difference between relative displacements.

ACKNOWLEDGMENTS

This research was supported by NSF Grants Nos. DMR-9012143 and DMR-9014729.

[1]A. J. Sievers and S. Takeno, Phys. Rev. Lett. **61**, 970 (1988).

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

[3]V. M. Burlakov, S. A. Kiselev, and V. N. Pyrkov, Solid State Commun. **74**, 327 (1990); V. M. Burlakov, S. A. Kiselev, and V. I. Rupasov, Phys. Lett. A **147**, 130 (1990).

[4]K. Yoshimura and S. Watanabe, J. Phys. Soc. Jpn. **60**, 82 (1991).

[5]S. Takeno and K. Hori, J. Phys. Soc. Jpn. **59**, 3037 (1990).

[6]S. R. Bickham and A. J. Sievers, Phys. Rev. B **43**, 2339 (1991).

[7]S. A. Kiselev, Phys. Lett. A **148**, 95 (1990).

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

[9]See, for instance, M. P. Allen and D. J. Tildesley, *Computer Simulations of Liquids* (Clarendon, Oxford, 1987).

[10]R. Bourbonnais and R. Maynard, Int. J. Mod. Phys. C **1**, 233 (1990).