Recurrence times in cubic and quartic Fermi-Pasta-Ulam chains: A shifted-frequency perturbation treatment

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A shifted-frequency perturbation scheme is used to derive algebraic expressions for recurrence periods in the harmonic-mode energies of cubic and quartic Fermi-Pasta-Ulam (FPU) chains. Perturbation-theory solutions for the FPU period have been obtained for arbitrary particle numbers N. Although the convergence properties of the solutions for arbitrary N are not known, explicit evaluations of the solutions at specific values of N have been found to be in good agreement with numerical simulations and soliton theories. The perturbation-theory solutions also provide reliable results in the regime where continuum soliton theories do not apply. A beat mechanism for the superperiod phenomena in cubic FPU chains is also proposed, based on the perturbation-theory solutions. The superperiods predicted by this mechanism are generic in cubic chains but do not appear in quartic chains. This result is in agreement with our numerical simulations. An exceptional superperiod that does occur in quartic chains with $N=7$, is accounted for by a resonance mechanism unique to this chain.

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I. INTRODUCTION

The Fermi-Pasta-Ulam (FPU) chain [1]—a one-dimensional array of equimass particles coupled by linear and nonlinear nearest-neighbor interparticle forces—was originally introduced to shed light on fundamental problems such as thermal conductivity, equipartition of energy, and ergodicity in solids [2,3]. It was hoped that the presence of the nonlinear interactions, which allow energy exchange between the modes of vibration, would be sufficient to bring about an approach to equilibrium with equipartition of energy. Instead, Fermi, Pasta, and Ulam found that energy was only exchanged between a few of the lowest-frequency modes, and this energy exchange was periodic. They initially excited the chain with all the energy in the lowest-frequency mode and observed a characteristic time scale (the FPU period) over which the energy periodically returned to the initially excited mode. The FPU period was found to be long in comparison to the period of the modes but short in comparison to the Poincaré recurrence time for the system [4].

In more extensive numerical simulations over much longer time intervals, Tuck and Menzel [4] found that the FPU recurrences were modulated by an envelope (the superperiod) with a longer period than the FPU period. More energy was restored to the initially excited mode after a superperiod recurrence than after a single FPU recurrence. In a subsequent study, Drago and Ridella [5] confirmed Tuck and Menzel's results for FPU chains with cubic nonlinear potentials, but showed that the observed superperiod was a numerical artifact when the nonlinear potential was quartic.

In a recent attempt to provide a clear explanation and understanding of the numerically observed long-time recurrences in FPU chains, we presented the results of a shifted-frequency perturbation analysis to fourth order for the time evolution of the modes [6]. The usefulness of the shifted-frequency perturbation scheme in providing an explanation of periodic behavior in FPU chains has been known for a number of years [7–11]. In our treatment we were able to generalize the results of previous workers by directly applying a knowledge of the mode selection rules [12,13] to carry out a general perturbation treatment that includes all mode interactions and that is valid for chains of all lengths. We thus confirmed that the FPU period is due to a (near) resonance between the shifted-frequency expansions for the lowest excited modes. Furthermore, we were able to provide the initial explanation for the superperiod in these chains. The superperiod in cubic chains is due to a beatlike interference effect between the resonance associated with the FPU period and another secondary resonance. Similar beatlike interference effects may occur in quartic chains, but our perturbation studies suggest that the amplitude of the modulation envelope is very small, making numerical observation of this phenomena difficult.

In this paper we present the detailed calculations supporting our explanation for the long-period recurrences in FPU chains. We have also carried out more extensive numerical simulations in double precision over a large range of particle numbers (up to $N=31$) and nonlinear coupling parameters to compare with our theoretical predictions. To ensure that the numerical measurements that we report here are reliable, we have reproduced our results by carrying out a number of simulations of selected chains for the same conditions but varying step sizes (in the range $\frac{1}{64}$ to $\frac{1}{4096}$) and different (quadruple) precision.

In Sec. II we present the Hamiltonian, the normal-mode coordinates, and the mode-coupling constants for FPU chains. In Sec. III we carry out the shifted-frequency perturbation analysis to third order for the

quartic FPU chain. The shifted-frequency perturbation analysis for the cubic chain is carried out to fourth order in Sec. IV. In Sec. V we identify the mechanism for the FPU period in each of these chains. The scaling properties of the FPU recurrence time are also investigated, and the results of the perturbation scheme are compared with results from both soliton theories and from numerical simulations. In Sec. VI we investigate the possibility of superperiods in FPU chains within the framework of the shifted-frequency perturbation scheme. In addition to a simple resonance mechanism, which can arise in exceptional cases, we identify a beatlike interference mechanism that is generic for cubic chains. The superperiods predicted by these mechanisms are also compared with numerical simulations. In Sec. VII we comment on the convergence properties of shifted-frequency perturbation schemes for FPU chains. Finally, in Sec. VIII, we have included a brief summary of our results.

II. THE FERMI-PASTA-ULAM CHAIN

The Hamiltonian for FPU chains with fixed ends and N moving particles is given by

$$H=\tfrac{1}{2}\sum_{n=0}^{N}[\dot{x}_n^2+(x_{n+1}-x_n)^2]+\frac{\epsilon}{p}\sum_{n=0}^{N}(x_{n+1}-x_n)^p, \quad (1)$$

where x_i is the displacement of the ith particle from its equilibrium position and ϵ is the nonlinear-coupling parameter. The two cases corresponding to $p=3$ and 4, are referred to as the cubic (FPU) chain and the quartic (FPU) chain, respectively. The harmonic chain ($\epsilon=0$) with these boundary conditions can be described by N normal modes. The particle displacements are described by a sum over the amplitudes a_k of these modes

$$x_n=\left[\frac{2}{N+1}\right]^{1/2}\sum_{k=1}^{N}a_k\sin\left[\frac{n\pi k}{N+1}\right]. \quad (2)$$

The frequencies of the linear modes satisfy the dispersion relation

$$\omega_k=2\sin[\pi k/2(N+1)]. \quad (3)$$

The energy contained in mode k in a harmonic chain is $E_k=(\dot{a}_k^2+\omega_k^2a_k^2)/2$. Nonlinear chains can also be completely described in terms of these harmonic modes. The presence of nonlinearities causes coupling to occur between the modes. The Hamiltonian for the FPU chain in terms of the harmonic modes can be written in the form

$$H=\tfrac{1}{2}\sum_{k=1}^{N}(\dot{a}_k^2+\omega_k^2)+\frac{\epsilon}{p}\sum_{k_1=1}^{N}\sum_{k_2=1}^{N}\cdots\sum_{k_p=1}^{N}A_{k_1k_2\cdots k_p}a_{k_1}a_{k_2}\cdots a_{k_p}, \quad (4)$$

where the coupling constants are defined by

$$A_{k_1k_2\cdots k_p}=[2(N+1)]^{1-p/2}\omega_{k_1}\omega_{k_2}\cdots\omega_{k_p}\times\sum_{\text{comb.}}B(k_1+k_2+\cdots+k_p), \quad (5)$$

and the summation in Eq. 5 is over all combinations of signs for the last $p-1$ indices. The function $B(s)$ is defined by

$$B(s)=\begin{cases}+1 & \text{if } s=0,\pm4(N+1),\pm8(N+1),\ldots\\ -1 & \text{if } s=\pm2(N+1),\pm6(N+1),\ldots\\ 0 & \text{otherwise .}\end{cases}$$

III. PERTURBATION THEORY FOR QUARTIC FPU CHAINS

In this section solutions for the quartic FPU chain [$p=4$ in Eq. (1)] are developed by applying a shifted frequency perturbation scheme. This scheme gives a series solution expanded in orders of the nonlinearity ϵ.

We restrict our analysis to the initial condition $a_1(0)=1$ and $a_i(0)=\dot{a}_j(0)=0$ for $i>1$ and all j. By a change of variables in Eq. (1), it can be seen that all initial conditions with the same functional form and with the same value of $E\epsilon$ are equivalent. E is the total energy contained in the chain. The initial condition above thus represents all initial conditions for which the energy is initially contained in the amplitude of the lowest-frequency mode. The perturbation method presented here could, however, be applied to any initial condition.

The equation of motion for mode i of a quartic FPU chain is

$$\ddot{a}_i=-\omega_i^2a_i-\epsilon\sum_{j=1}^{N}\sum_{k=1}^{N}\sum_{l=1}^{N}A_{ijkl}a_ja_ka_l, \quad (6)$$

from Eq. (4). To facilitate the perturbation calculation, we first use the properties of the mode-selection rules [12,13] to reduce the number of terms in the equation of motion. For the initial condition considered here, only modes with odd-mode numbers participate in the evolution of the chain. That is, $a_i(t)=0$ for all t when i is even. This allows the indices i, j, k, and l in the equation of motion above to be restricted to odd values. Furthermore, many of the coupling constants are zero: A_{111i} are zero except when $i=3$; A_{iii1} are zero except when $i=[2(N+1)-1]/3$; A_{11ij} (with $i>j$) are zero except when $j=i-2$. Using these results the equation of motion for the initial mode, mode 1, simplifies to

$$\ddot{a}_1+\omega_1^2a_1=-\epsilon\left[A_{1111}a_1^3+3A_{1113}a_1^2a_3+3\sum_{i=3}^{N}A_{11ii}a_1a_i^2+A_{1III}a_I^3+6\sum_{i=5}^{N}A_{11ii-2}a_1a_ia_{i-2}+3\sum_{i=3}^{N}\sum_{j\neq i,1}A_{1iij}a_i^2a_j+6\sum_{i=7}^{N}\sum_{j=5}^{i-2}\sum_{k=3}^{j-2}A_{1ijk}a_ia_ja_k\right], \quad (7)$$

where $I=[2(N+1)-1]/3$.

The equations of motion of the noninitial modes [$i\neq 1$ in Eq. (6)] simplify to

$$\ddot{a}_i+\omega_i^2 a_i=-\epsilon\left[A_{iiii}a_i^3+3A_{iiiJ}a_i^2a_J+A_{iKKK}a_K^3+3\sum_{j=1}^{N}{}'A_{iijj}a_ia_j^2+6\sum_{j=1}^{N}{}'\sum_{k<j}{}'A_{iijk}a_ia_ja_k\right.$$
$$\left.+3\sum_{j=1}^{N}{}'\sum_{k\ (\neq j)}{}'A_{ijjk}a_j^2a_k+6\sum_{j=1}^{N}{}'\sum_{\substack{k,j\\k<j}}{}'\sum_{\substack{l,k\\l<k}}{}'A_{ijkl}a_ja_ka_l\right]. \tag{8}$$

The primes in Eq. (8) indicate that the summations do not include the index i. J can take any of the values $3i$, $2(N+1)-3i$, and $3i-2(N+1)$, and K can take any of the values $i/3$, $[2(N+1)-i]/3$, and $[2(N+1)+i]/3$, provided that they are odd integers in the range $(1,N)$.

It is assumed that the amplitude of each mode can be written as an expansion in powers of ϵ (see additional remarks in Sec. VII) as

$$a_i=a_{i,0}+\epsilon a_{i,1}+\epsilon^2 a_{i,2}+\cdots, \tag{9}$$

with initial conditions

$$a_{1,0}(0)=1,\quad \dot{a}_{1,0}(0)=0,\quad a_{1,k}(0)=\dot{a}_{1,k}(0)=0, \tag{10}$$

for $k>1$ and

$$a_{i,j}(0)=\dot{a}_{i,j}(0)=0, \tag{11}$$

for $i>1$ and all j. In addition, a set of N frequencies, referred to as the shifted, or nonlinear, frequencies are defined by

$$\Omega_i^2=\omega_i^2+\epsilon\mu_{i,1}+\epsilon^2\mu_{i,2}+\cdots. \tag{12}$$

The $\mu_{i,j}$ are called the frequency corrections.

The mode-amplitude expansions [Eq. (9)] are substituted into the modal equations of motion [Eqs. (7) and (8)]. In the standard shifted-frequency perturbation scheme [7–11], the frequency expansion [Eq. (12)] are substituted into the linear terms (left-hand side) of the equations of motion. In a more refined scheme, the frequency expansion could also be introduced into the nonlinear parts of the equations of motion. However, this would greatly increase the number of terms necessary for a solution in the perturbation scheme, but would only introduce minor corrections in the regime where perturbation schemes apply.

After these substitutions, equal powers of ϵ are equated in each equation of motion. This gives N equations of motion at each order that are independent of ϵ. The general form of these equations is

$$\ddot{a}_{i,n}+\Omega_i^2 a_{i,n}=\left[\sum_{p=1}^{n}\mu_{i,p}a_{i,n-p}\right]-F_{n-1}, \tag{13}$$

where F_{n-1} is a forcing term comprising all the $(n-1)$th order terms inside the brackets on the right-hand side of the Eqs. (7) and (8). An exact algebraic solution can be obtained for each of these forced-harmonic-oscillator equations.

At zero order in ϵ, the forcing term F_{-1} is zero for all modes. The resulting equations of motion for the N modes describe unforced harmonic oscillators with frequencies Ω_i. The solutions are $a_{1,0}=\cos\Omega_1 t$ and $a_{i,0}=0$ for $i\neq 1$.

The forcing terms that appear in the first-order equations of motion must be entirely made up of the only nonzero amplitude component at zero order, $a_{1,0}$. Hence, the equation of motion for mode 1 at this order is

$$\ddot{a}_{1,1}+\Omega_1^2 a_{1,1}=\mu_{1,1}a_{1,0}-A_{1111}a_{1,0}^3. \tag{14}$$

The general solution to this equation includes a secular term proportional to $(\mu_{1,1}-3A_{1111}/4)t\sin\Omega_1 t$. This unbounded term may be removed from the solution by setting $\mu_{1,1}=3A_{1111}/4$. The perturbation scheme is constructed so that whenever an unbounded term appears, a previously undefined frequency correction may be given a unique value to ensure that all the terms included in the perturbation expansion are bounded in time. The solution of Eq. (14) is

$$a_{1,1}=A_{1,1}(\cos 3\Omega_1 t-\cos\Omega_1 t), \tag{15}$$

with $A_{1,1}=A_{1111}/32\Omega_1^2$.

The only noninitial modes with a nonzero forcing term at first order are those for which $K=1$ [see Eq. (8)]. The definition of K shows that this is only true for mode 3, irrespective of the value of N. The equation of motion for mode 3 at this order is

$$\ddot{a}_{3,1}+\Omega_3^2 a_{3,1}=-\epsilon A_{3111}a_{1,0}^3. \tag{16}$$

The solution of this equation, for the initial conditions being considered here, is

$$a_{3,1}=A_{3,1}\cos\Omega_3 t+A_{3,2}\cos\Omega_1 t+A_{3,3}\cos 3\Omega_1 t, \tag{17}$$

with

$$A_{3,2}=-\frac{3A_{3111}}{4(\Omega_3^2-\Omega_1^2)},$$
$$A_{3,3}=-\frac{A_{3111}}{4(\Omega_3^2-9\Omega_1^2)}, \tag{18}$$

and

$$A_{3,1}=-A_{3,2}-A_{3,3}.$$

All the other modes are described by unforced harmonic oscillators with zero energy at this order, so $a_{i,1}=0$ for all $i>3$. Note that this result is independent of the value of N. No frequency corrections other than $\mu_{1,1}$ are defined at this order.

At second order in ϵ, all nonzero forcing terms must be constructed from the three nonzero amplitude components already defined, $a_{1,0}$, $a_{1,1}$, and $a_{3,1}$. The secular term that arises in the solution to the equation of motion for $a_{1,2}$ is removed by defining

$$\mu_{1,2}=-\tfrac{3}{4}A_{1111}A_{1,1}+\tfrac{3}{4}A_{1113}(3A_{3,2}+A_{3,3}). \tag{19}$$

The solution that describes the evolution of $a_{1,2}$ is then

$$\begin{aligned}a_{1,2}=&B_{1,1}\cos\Omega_1 t+B_{1,2}\cos 3\Omega_1 t+B_{1,3}\cos 5\Omega_1 t\\&+B_{1,4}\cos\Omega_3 t+B_{1,5}\cos(\Omega_3-2\Omega_1)t\\&+B_{1,6}\cos(\Omega_3+2\Omega_1)t.\end{aligned} \tag{20}$$

The definitions of the amplitude coefficients $B_{1,1}-B_{1,6}$ are contained in Appendix A.

The forcing term in the equation of motion for $a_{3,2}$ has contributions that are proportional to A_{3111} and A_{3311}. The term that is proportional to A_{3331}, which is nonzero if $N=4$, need not be considered at this order, because $a_{3,0}=0$. The value of the frequency correction $\mu_{3,1}$ is set to $3A_{3311}/2$ to remove the unbounded term in the solution to the equation of motion. The solution for $a_{3,2}$ is similar in form to the second-order solution for mode 1

$$\begin{aligned}a_{3,2}=&B_{3,1}\cos\Omega_3 t+B_{3,2}\cos\Omega_1 t+B_{3,3}\cos 3\Omega_1 t\\&+B_{3,4}\cos 5\Omega_1 t+B_{3,5}\cos(\Omega_3-2\Omega_1)t\\&+B_{3,6}\cos(\Omega_3+2\Omega_1)t.\end{aligned} \tag{21}$$

The coefficients $B_{3,1}-B_{3,6}$ are also defined in Appendix A. It is apparent from these definitions that the amount of information necessary to define the solutions for these expansions increases rapidly as the order of the calculation increases.

Mode 5 is the only other mode that has a nonzero forcing term in its equation of motion at this order. The equation of motion is

$$\ddot{a}_{5,2}+\Omega_5^2 a_{5,2}=-3A_{5311}a_{3,1}a_{1,0}^2. \tag{22}$$

No unbounded terms appear in the solution of this equation, so no frequency corrections are defined. The solution to this equation has a very similar form to the solutions for $a_{1,2}$ and $a_{3,2}$ given above.

By using the properties of the coupling constants and the limited number of nonzero-amplitude components available at this order, it may be shown that no other modes have nonzero amplitudes at second order. That is, $a_{i,2}=0$ for all $i>5$. Once again, this result is general for all N. No mode interactions have been neglected to get these results.

The highest order for which we have explicitly constructed solutions in the quartic chain is third order. At this order, modes 1, 3, and 5 all have nonzero forcing terms in their equations motion. Three frequency corrections are defined,

$$\begin{aligned}\mu_{1,3}=&\tfrac{3}{4}A_{1111}(3B_{1,1}+B_{1,2})\\&+\tfrac{3}{4}A_{1133}(2A_{3,1}^2+A_{3,2}^2+2A_{3,3}^2+2A_{3,2}A_{3,3}),\end{aligned} \tag{23}$$

$$\begin{aligned}\mu_{3,2}=&\frac{3}{4A_{3,1}}[A_{3111}(2B_{1,4}+B_{1,5}+B_{1,6})\\&+A_{3311}(B_{3,5}+B_{3,6}-4A_{3,1}A_{1,1})\\&+A_{3115}(2B_{5,5}+B_{5,6}+B_{5,7})],\end{aligned} \tag{24}$$

$$\mu_{5,1}=\frac{3A_{5511}}{2}. \tag{25}$$

The complete solution for $a_{1,3}$ is listed in Appendix A. This solution only contains components whose frequencies are linear combinations of Ω_1 and Ω_3. No frequencies from other modes appear because the forcing terms associated with these frequencies have zero amplitude in the equation of motion. The solutions for $a_{3,3}$ and $a_{5,3}$ are similar to the solution for $a_{1,3}$ except that they include components involving the nonlinear frequency of mode 5.

Mode 7 also has a nonzero solution at third order. This arises from the forcing terms that are proportional to A_{7331} and A_{7511}. Once again, no other modes have nonzero amplitudes at this order, regardless of the value of N.

It is important to emphasize that the generality of these expansions for all N is a result of careful manipulation of the coupling constants, and is not a feature that is necessarily inherent to this perturbation scheme. As the scheme is taken to higher orders, exceptions to the generality of the results appear. One such exception actually appears in the third-order equations. If $N=4$, the expression given above for $\mu_{3,2}$ is incomplete. In this exceptional case, $A_{3331}\neq 0$; however, terms proportional to A_{3331} were omitted from the forcing term in the equation of motion for $a_{3,3}$ in the analysis for general N. Apart from this case, the expressions given above apply to chains with any number of particles. Note also that for chains with very small numbers of particles, some of the terms in the general expressions define modes that are not present in the chain (such as the information for mode 5 and 7 when $N=3$). The correct expansions in these cases are found by simply neglecting all terms in the expansion that apply to modes whose mode numbers are larger than N.

The solutions to the components of the amplitude expansions are defined in terms of the nonlinear frequencies. To gain practical information from these expansions, the nonlinear frequencies as a function of ϵ and N need to be calculated. One disadvantage of this scheme is that only a small number of the frequency corrections were defined in the solutions above. At the orders calculated, the frequency correction $\mu_{2k+1,n}$ was defined at $(k+n)$th order in the equations of motion. This means that the calculation above gave no information on the value of the nonlinear frequencies of modes with mode numbers higher than 5.

The first-order correction in the nonlinear frequency of every mode can be derived without explicitly solving the equations of motion. To demonstrate this, assume that mode i ($i\neq 1$) has its first nonzero amplitude components at nth order. The equation of motion for that mode at nth order is

$$\ddot{a}_{i,n}+\Omega_i^2 a_{i,n}=F_{n-1}, \tag{26}$$

as can be seen from Eq. (13). There are no terms in the forcing term of this equation that include the nonlinear frequency of mode i, Ω_i. The solution of Eq. (26) is

$$a_{i,n}=C_1\sin\Omega_i t+C_2\cos\Omega_i t+\sum_p T_{i,p}\cos\Omega_p t, \tag{27}$$

where $C_1=0$ and $C_2=-\Sigma_p T_{i,p}$, and the Ω_p are linear combinations of the nonlinear frequencies of the other modes. The $(n+1)$th order equation of motion for mode i is

$$\ddot{a}_{i,n+1}+\Omega_i^2 a_{i,n+1}=\mu_{i,1}a_{i,n}-2A_{ii11}a_{1,0}^2 a_{i,n}-\cdots, \tag{28}$$

where only the terms containing the component $\cos\Omega_i t$ have been retained. The solution of this equation includes an unbounded component proportional to $C_2(\mu_{i,1}-3A_{ii11}/2)$. Because C_2 is nonzero, the first-order frequency correction must be equal to $3A_{ii11}/2$ for all $i\neq 1$. It is not possible to extend this method to higher-order corrections without a detailed knowledge of the constant C_2, and this requires a complete solution of the nth-order equations of motion.

IV. PERTURBATION THEORY FOR CUBIC FPU CHAINS

We have also derived a series solution for the cubic FPU chain [$p=3$ in Eq. (1)] by using a shifted-frequency perturbation scheme. The same initial condition was used as for the quartic chain; all the initial energy was contained in the amplitude of mode 1. Once again, we have restricted our analysis to the initial condition $a_1(0)=1$, and $a_i(0)=\dot{a}_j(0)=0$ for $i>1$ and all j. By a change of variables in Eq. (1), it can be seen that all initial conditions with the same functional form and with the same value of $E\epsilon^2$ are equivalent.

The mode-coupling rules for the cubic chain show all modes of the chain become excited with this initial condition [13]. The equations of motion were solved up to fourth order in ϵ, yielding solutions for general values of N. At second order, only modes 1, 2, and 3 have nonzero amplitudes. The solutions for these modes are

$$\begin{aligned}
a_1&=\cos\Omega_1 t\\
&\quad+\epsilon^2[B_{1,1}\cos\Omega_1 t+B_{1,2}\cos 3\Omega_1 t\\
&\qquad+B_{1,2}\cos(\Omega_2-\Omega_1)t+B_{1,4}\cos(\Omega_2+\Omega_1)t],\\
a_2&=\epsilon(A_{2,1}\cos\Omega_2 t+A_{2,2}+A_{2,3}\cos 2\Omega_1 t),\\
a_3&=\epsilon^2[B_{3,1}\cos\Omega_3 t+B_{3,2}\cos\Omega_1 t+B_{3,3}\cos 3\Omega_1 t\\
&\qquad+B_{3,4}\cos(\Omega_2-\Omega_1)t+B_{3,5}\cos(\Omega_2+\Omega_1)t].
\end{aligned} \tag{29}$$

The coefficients used in these expressions are defined in Appendix B. The amplitude components are zero at second order for mode 2. Higher-order terms will be introduced separately as they become necessary.

In this calculation, at mth order, all modes with mode numbers greater than $m+1$ have zero amplitude, no matter what value N has. The mth-order frequency correction for mode k is defined when the $(m+k-1)$th-order equations of motion are solved. This meant that no frequency corrections were defined for modes with mode numbers larger than 4. It was not possible to derive the first-order frequency correction for all modes in the same way as was done above for the quartic chain. The nonzero-frequency corrections that use the variables defined in Appendix B are

$$\begin{aligned}
\mu_{1,2}&=6A_{112}(A_{2,2}+\tfrac{1}{2}A_{2,3}),\\
\mu_{2,2}&=\frac{6}{A_{2,2}}[A_{211}(B_{1,3}+B_{1,4})+\tfrac{1}{2}A_{231}(B_{3,4}+B_{3,5})].
\end{aligned} \tag{30}$$

The frequency corrections $\mu_{1,4}$ and $\mu_{3,2}$ were also defined in our perturbation calculation. These corrections, which depend on the amplitude coefficients from the third- and fourth-order equations of motion, are not listed here. A number of the frequency corrections were found to have zero value: $\mu_{1,1}$, $\mu_{1,3}$, $\mu_{2,1}$, $\mu_{2,3}$, $\mu_{3,1}$, and $\mu_{4,1}$. All other frequency corrections remained undefined. By truncating the frequency expansions at the highest order for which a correction is defined, the nonlinear frequencies are defined by a set of nonlinear algebraic equations. These equations cannot be solved analytically, but by fixing the value of N this set of equations may readily be solved numerically to find the nonlinear frequencies as a function of ϵ.

V. THE FPU RECURRENCE

We now use our perturbation-series solution for the energy in mode 1, $E_1=(\dot{a}_1^2+\omega_1^2 a_1^2)/2$, to obtain insight into the long-time recurrence phenomena. First we deal with the cubic FPU chain. At second order, a $\cos(2\Omega_1-\Omega_2)$ component appears in the mode-1 energy. The period corresponding to this component, $[T=2\pi/(2\Omega_1-\Omega_2)]$, is long because the shifted frequencies of modes 1 and 2 are approximately resonant. This can be seen by immediate inspection of the (nearby) linear frequencies; $2\omega_1-\omega_2\simeq 0$. There are no other terms at or below second order with periods significantly longer than the period of the fundamental mode (the energy of mode 1 has no first-order components). In addition, the amplitude coefficient associated with the $\cos(2\Omega_1-\Omega_2)$ component, $B_{1,3}$ (see Appendix B), contains the resonant combination of the nonlinear frequencies in its denominator. The amplitude of this component is therefore significantly larger than the components that do not contain resonant denominators. This is an important feature of these chains; the dominant components are typically those containing resonant denominators. As found in previous calculations [3,11,10], it is this component that describes the FPU recurrence in the cubic chain. Our perturbation analysis has revealed that the resonance between modes 1 and 2 is a generic feature (irrespective of length) of cubic chains. This is consistent with numerical studies that show the FPU period in weakly nonlinear chains with different N, when initially excited in the lowest-frequency mode.

In the limit $\epsilon\to 0$, the nonlinear frequencies approach

the linear frequencies. Discarding terms higher than third order in the Taylor series of the linear frequencies shows that in this limit

$$T_{\mathrm{FPU}}=0.81(N+1)^3. \tag{31}$$

For finite values of ϵ, the nonlinear frequencies must be calculated, and the recurrence time is then given by

$$T_{\mathrm{FPU}}=\frac{2\pi}{2\Omega_1-\Omega_2}\ . \tag{32}$$

Our calculations, which were performed using all the frequency corrections defined by solving the equations of motion up to fourth order, indicate that the recurrence time decreases monotonically as ϵ is increased from zero. The predictions of Eq. (32) for the FPU period are compared with some numerical measurements in Fig. 1.

We have used the results of our perturbation analysis to examine the scaling of the FPU period as a function of N. If we assume that a general power-law scaling of the form suggested by Zabusky [14], i.e.,

$$T_{\mathrm{FPU}}\sim\alpha N^{\delta}\ , \tag{33}$$

where α is independent of N, then a plot of

$$\delta=\frac{\log[T_{\mathrm{FPU}}(N)/T_{\mathrm{FPU}}(N+1)]}{\log[N/(N+1)]} \tag{34}$$

vs N should produce a straight line. In Fig. 2 we have used our theoretical expression for T_{FPU} to plot δ vs N, for N in the range (5,20). Curves have been produced for

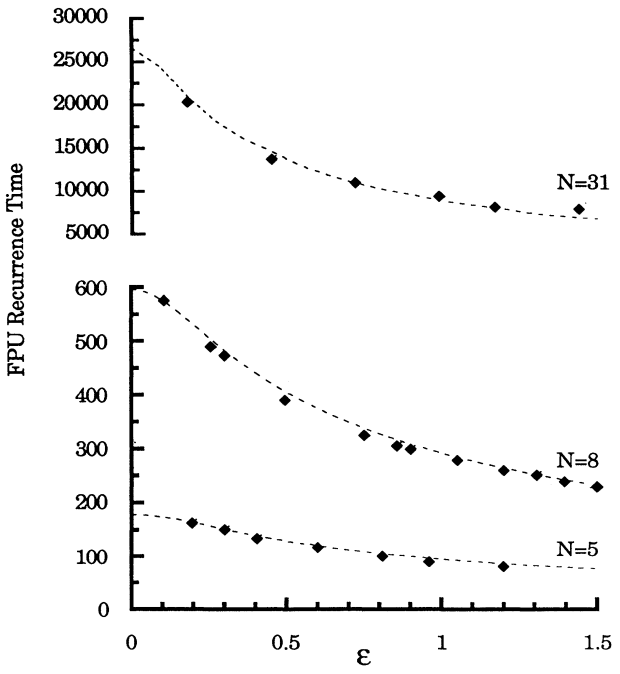

FIG. 1. The FPU recurrence time in cubic chains as a function of ϵ; the dashed lines are theoretical results from Eq. (32); measurements from numerical simulations are represented by ♦.

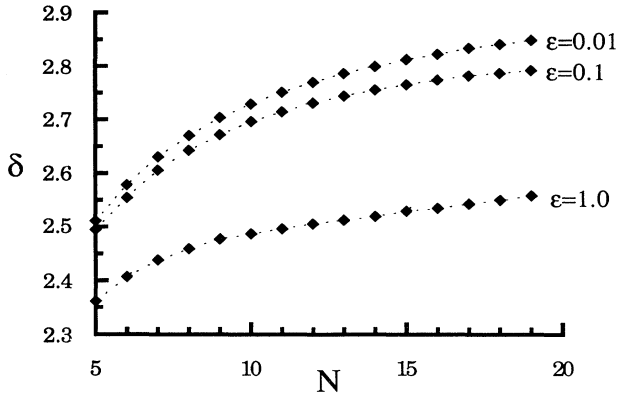

FIG. 2. The scaling exponent δ [from Eq. (34)] vs N for the cubic chain. Results for three values of the nonlinear coupling are shown.

three different values of the nonlinear coupling. We make the following observations based on this figure: (i) the power law, Eq. (33), appears to hold only in the limit of large N, and (ii) the asymptotic value of the exponent δ appears to be a function of ϵ.

In the continuum limit, the cubic FPU lattice can be described by the Korteweg–de Vries (KdV) equation. A significant amount of work has previously been carried out towards interpreting the long-period recurrences of FPU chains by examining the soliton solutions of the KdV equation [14–16]. According to the soliton mechanism,

$$T_{\mathrm{FPU}}\sim bN^{5/2}\ , \tag{35}$$

where b is independent of N. Our (ϵ-dependent) scaling results therefore suggest that the shifted-frequency perturbation scheme is valid over a larger range of nonlinear coupling parameters than the soliton mechanism.

The FPU recurrence can be interpreted in the same way in quartic FPU chains. In this case a $\cos(3\Omega_1-\Omega_3)$ component appears at second order in the mode-1 energy. The period correspond to this component, $[T=2\pi/(2\Omega_1-\Omega_2)]$, is again long, as can be seen from the approximate resonance condition; $3\omega_1-\omega_3\simeq 0$. The resonance condition also appears as a denominator in the amplitude of this component. Furthermore, this is the only component up to this order with a period significantly longer than the period of the fundamental mode. The FPU recurrence time in a quartic chain is thus

$$T_{\mathrm{FPU}}=\frac{2\pi}{3\Omega_1-\Omega_3}\ . \tag{36}$$

The predictions of Eq. (36) for the FPU period are compared with some numerical measurements in Fig. 3. Our perturbation analysis has revealed that the resonance between modes 1 and 3 is a generic feature (irrespective of length) of quartic chains. Hence the FPU period defined by Eq. (36) is valid for any value of N. In the limit $\epsilon\rightarrow 0$, the FPU recurrence time in the quartic chain approaches

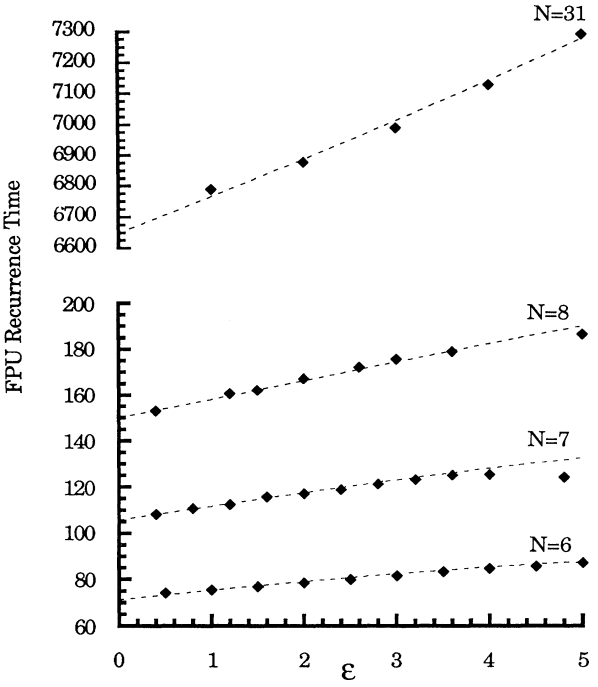

FIG. 3. The FPU recurrence time in quartic chains as a function of ϵ; the dashed lines are theoretical results from Eq. (36); measurements from numerical simulations are represented by ♦.

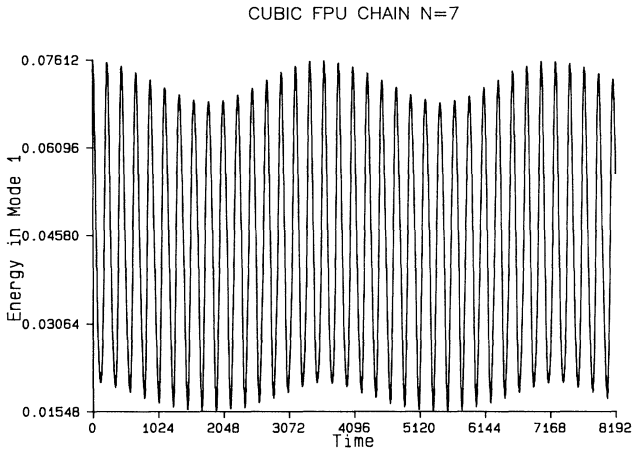

FIG. 4. The energy in mode 1 as a function of time for the cubic FPU chain with $N=7$ and $\epsilon=0.8$. The fast oscillations are the FPU recurrences. Two full superperiods are shown.

$0.20(N+1)^3$. For small but finite nonlinearities, $\Omega_i \simeq \omega_i + \epsilon\mu_{i,1}/2$, and the FPU period can be expressed in the approximate form

$$T_{\mathrm{FPU}} = \frac{3.242(N+1)^4}{16(N+1)-9\epsilon} . \tag{37}$$

The linear frequencies were replaced by a truncated Taylor series in the above expression.

One useful feature of the shifted-frequency perturbation scheme is that once the order of the components in the solutions is known, information about the recurrence periods can be deduced solely from the linear frequencies of the modes.

VI. THE SUPERPERIOD RECURRENCE

The shifted-frequency perturbation scheme also allows the superperiod recurrences of FPU chains to be predicted theoretically. Once again, we shall deal first with the cubic FPU chain. The time evolution of the energy in mode 1 obtained from a numerical simulation of a cubic chain is shown in Fig. 4. Typical FPU and superperiod recurrences can be seen in this figure. The perturbation scheme suggests that the superperiod recurrence does not arise from a simple resonance between two linear modes. Simple resonances (other than the one which leads to the FPU recurrence) do exist in cubic chains, but the periods and amplitudes associated with these resonances in the perturbation expansions are less than for the FPU recurrence. Sun [11], in his investigation of a seven-particle cubic chain, found no correlation between the periods defined by all linear combinations of up to six linear frequencies and the superperiod recurrence times of the chain. An example of a resonance of this type is the resonance between modes 1 and 3. It is easy to verify that in the linear limit $|3\omega_1-\omega_3| < |2\omega_1-\omega_2|$. This relation also holds at finite values of ϵ when the nonlinear frequencies are used.

The long-period component in the energy of mode 1 associated with the resonance between modes 1 and 3 first appears at fourth order in ϵ (the mode-1 energy has no components at third order), with period $T_2 = 2\pi/(3\Omega_1-\Omega_3)$. The period of this component is shorter than the FPU period, and the perturbation expansion predicts that the amplitude of this component is less than the leading-order component of the FPU recurrence. However, when these two components are superimposed, beatlike interference effects produce a periodic envelope that modulates the FPU recurrence.

To understand the interference phenomena produced by these two resonances, we write the oscillating contribution to the energy in mode 1 in the form

$$E_1^{\mathrm{osc}}(t) = A_{\mathrm{FPU}} \exp[i(2\Omega_1-\Omega_2)t] + A_2 \exp[i(3\Omega_1-\Omega_3)t]. \tag{38}$$

Without loss of generality we can write this in the form

$$E_1^{\mathrm{osc}}(t) = A_{\mathrm{FPU}} \exp[i(2\Omega_1-\Omega_2)t] + A_2 \exp[i(n+\gamma)(2\Omega_1-\Omega_2)t], \tag{39}$$

where n is an integer and $|\gamma| < \frac{1}{2}$. At each recurrence of the FPU period, the oscillating energy in mode 1 is therefore given by

$$E_1^{\mathrm{osc}}(t) = A_{\mathrm{FPU}} + A_2 \exp[i\gamma(2\Omega_1-\Omega_2)t]. \tag{40}$$

Thus the FPU recurrence is modulated by a periodic envelope with period

$$T_{\text{sup}} = \frac{2\pi}{\gamma(2\Omega_1 - \Omega_2)} . \tag{41}$$

The periodicity of the envelope provides a consistent explanation for the superperiod in cubic chains. As with the expressions given for the FPU recurrence time, this formula holds for general N. The predictions of Eq. (41) for the superperiod are compared with some numerical measurements in Fig. 5. These predictions are not as accurate as our previous predictions of the FPU period. This is because Ω_1 and Ω_2 are known to higher order than the new frequency Ω_3, which appears in the definition of γ.

In the quartic chain, the component causing the FPU recurrence was due to the resonance between modes 1 and 3, and appeared first at second order in the energy of mode 1. The secondary resonance in this chain is between modes 1 and 5 (recall that only the odd modes are excited). Examination of the series solution for the amplitude of mode 1 to third order shows that no component associated with this secondary resonance can appear at third order in the mode-1 energy. Furthermore, for small nonlinear coupling the ratio between the resonant denominators associated with the secondary resonance and the resonance causing the FPU recurrence is considerably smaller in the quartic chain than in the cubic chain. It follows from these two factors that the amplitude of the long-period term due to the resonance between modes 1 and 5, $\cos(5\Omega_1 - \Omega_5)t$, is very small compared to the FPU recurrence. As a consequence, the modulation of the FPU recurrence caused by interference with this long period term is also very small. That is, the superperiod recurrence, although it is present in quartic chains, has an extremely small amplitude. We have numerically simulated a large number of chains with $N < 20$ and small nonlinearities but have only observed a clear superperiod in the case $N = 7$.

We have observed superperiod recurrences in the quartic FPU chain with $N = 7$ over a range of small nonlinearities. Superperiod recurrences that were observed previously in quartic chains were subsequently shown to be numerical artifacts [5]. The time evolution of the energy in mode 1 obtained from a numerical simulation of the quartic chain with $N = 7$ is shown in Fig. 6. Typical FPU and superperiod recurrences can be seen in this figure. In this figure we have plotted the combined harmonic energy plus anharmonic self-energy of mode 1 [17].

The superperiod recurrence in the seven-particle quartic chain can also be understood using the shifted-frequency perturbation scheme. It can easily be verified from the linear frequencies of this system that there is a resonance between modes 1 and 7 that does not appear in other chains, $5\omega_1 - \omega_7 \simeq 0$. These two frequencies are in fact closer to exact resonance than the linear frequencies of modes 1 and 3. Although a $\cos(5\Omega_1 - \Omega_7)t$ component does not appear in the energy of mode 1 up to the orders that we have explicitly calculated, it is expected to appear at higher orders. The closeness of the resonance between the two modes in this case accentuates the corresponding amplitude of the component and causes a long period recurrence that is entirely independent of the FPU recurrence. Calculation of the theoretically predicted period of this recurrence,

$$T_{\text{sup}} = 2\pi/(5\Omega_1 - \Omega_7), \tag{42}$$

shows excellent agreement with numerically measured values (Fig. 7), even though Ω_7 has only been calculated to first order.

It is possible that other quartic chains exhibit superperiod recurrences arising from a similar mechanism. We have numerically simulated all chains with $N < 30$ that have unusual resonances in the linear frequencies (for example, when $N = 15$, modes 1 and 11 are close to resonance). None of these chains, apart from $N = 7$, had any clearly detectable long-period recurrence in addition to the FPU recurrence. Heuristically, we can understand this as follows; as the number that multiplies the frequen-

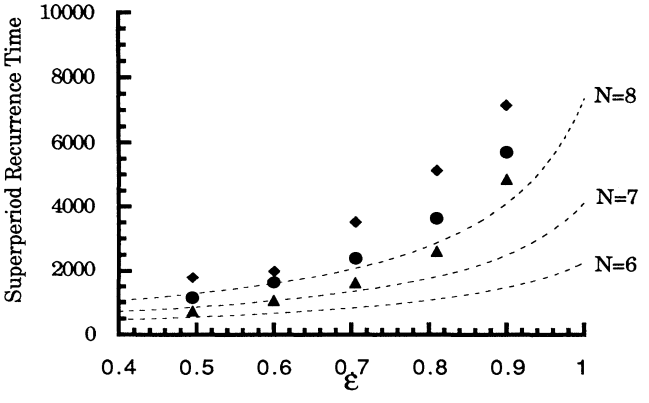

FIG. 5. The superperiod recurrence time in cubic chains as a function of ϵ. The dashed lines are theoretical results from Eq. (41); measurements from numerical simulations are represented by ▲ ($N = 6$), ● ($N = 7$), and ◆ ($N = 8$).

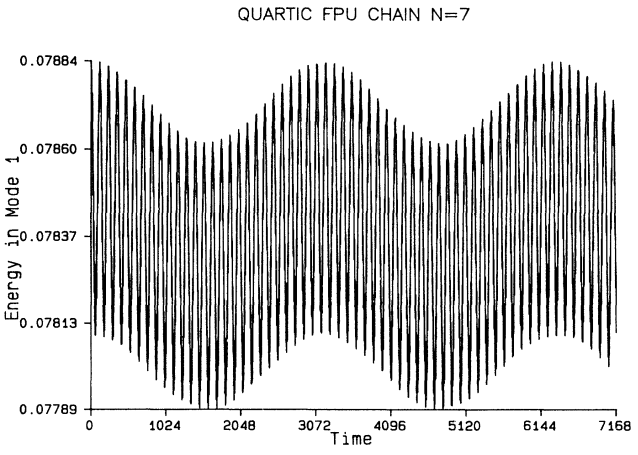

FIG. 6. The energy in mode 1 as a function of time for the quartic FPU chain with $N = 7$ and $\epsilon = 2.5$. The fast oscillations are the FPU recurrences. Two full superperiods are shown.

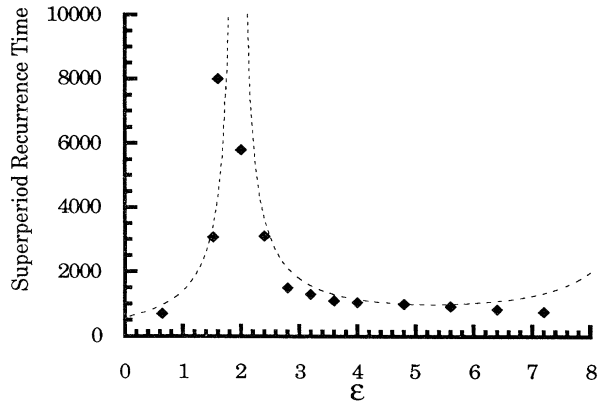

FIG. 7. The superperiod recurrence time in the quartic chain with $N=7$ as a function of ϵ. The dashed line shows theoretical results from Eq. (42); measurements from numerical simulations are represented by ♦.

cies in the resonance relation increases, so does the order at which the associated long-period component first appears in the expansion of the mode energy. Hence, as this number becomes larger, the frequencies must be increasingly close to exact resonance in order for the long-period component to have an observable amplitude.

The superperiod and FPU recurrences are not the only long-period components that are present in FPU chains. The perturbation expansions suggest that, in general, a large variety of long-period terms can exist due to the many resonances that occur between the frequencies of the modes. However, most of these terms have very small amplitudes and are not seen in numerical simulations. The shifted-frequency perturbation scheme provides a means to investigate these other recurrences.

VII. CONVERGENCE OF THE PERTURBATION SCHEME

It is difficult to rigorously determine where the shifted-frequency perturbation scheme is convergent. At low orders in the expansions, resonant denominators appear that cause the long-period recurrences observed in FPU chains. At higher orders in the expansions, the variety of linear combinations of frequencies that appear increases. When combinations of arbitrarily large numbers of frequencies are considered, resonance denominators that are arbitrarily small can be constructed. In general, we expect the presence of these denominators at very high orders in the perturbation expansions causes the formal divergence of the series almost everywhere in phase space. Nevertheless, by truncating the expansions at low orders, these divergences are avoided and the series yield apparently accurate approximations.

The reasons for this behavior can be understood in terms of the properties of nonlinear Hamiltonian systems. Numerical results suggest that discrete FPU chains are nonintegrable [17]; that is, no analytic global constants of the motion of these chains exist apart from the total energy. However, the shifted-frequency perturbation scheme amounts to trying to assign action-angle variables to the chain to which it is applied. If these coordinates do not exist globally, the expansions arising from the perturbation scheme are formally divergent in most parts of phase space.

The only initial conditions for which the perturbation scheme may possibly yield formally convergent expansions are those with truly quasiperiodic trajectories, such as initial conditions that lie on Kolmogorov-Arnold-Moser (KAM) tori [2]. It is expected that these invariant tori have a finite measure for sufficiently small nonlinearities, but that densely interweaved among them are initial conditions that allow Arnold diffusion [18]. However, numerical simulations of chains with small nonlinearities have shown that almost all initial conditions show quasiperiodic behavior over the time scales for which accurate simulations are possible. This means that if any of these quasiperiodic trajectories lie in the Arnold web, their diffusion is extremely slow; the quasiperiodic behaviors arise because the trajectories are "trapped" in the vicinity of the invariant KAM tori. It is not possible to use the shifted-frequency perturbation scheme to determine whether the initial condition lies on a KAM tori or lies within the Arnold web.

As was demonstrated in Figs. 1, 3, 5, and 7, the perturbation scheme gives accurate predictions for values of ϵ larger than 1. At first this may appear strange; however, it is important to point out that the shifted-frequency perturbation scheme is quite generally applicable in the regime where the linear energy in the chain is large compared to the nonlinear energy in the chain. In this regime the harmonic approximation is a good zeroth-order approximation—a requirement of the shifted-frequency scheme. The relative size of the linear to nonlinear energy depends on the magnitude of ϵE in the case of the quartic chain and $\epsilon^2 E$ in the case of the cubic chain. It is a simple scaling exercise to show that the linear energy is much larger than the nonlinear energy if $\epsilon E \ll 1$ in the case of the quartic chain, and $\epsilon^2 E \ll 1$ in the case of the cubic chain. For the initial conditions that we have used, $E \simeq \omega_1^2/2$. All of the results that we have presented here are within the above "linear" regimes.

An explicitly convergent perturbation scheme, which can be used to find periodic orbits in systems of coupled oscillators such as FPU chains, has been developed by Eminhizer and co-workers [19]. This scheme constructs initial conditions that satisfy specified periodicity requirements. The initial conditions do not appear as free parameters. The method is therefore unsuitable for the investigation of phenomena that arise from a definite initial state such as the recurrence behaviors examined here, although it is useful in other contexts.

VIII. CONCLUSION

We have employed the shifted-frequency perturbation scheme to obtain expressions for the long-time recurrence periods in cubic and quartic chains when the chains are initially excited with all the energy in the lowest-frequency mode. All mode interactions have been included in our perturbation-theory treatment and we have ob-

tained solutions for chains of arbitrary length. The FPU recurrence is shown to be a generic feature of cubic and quartic chains with arbitrary numbers of particles. Our perturbation studies have revealed new scaling properties of the FPU recurrence times that are not suggested by soliton theories. Our expressions for the FPU recurrence periods have been found to be in excellent agreement with reproducible measurements from numerical simulations.

We have also used the shifted-frequency perturbation scheme to investigate superperiod recurrences in FPU chains. A beat mechanism has been proposed to explain the superperiod phenomena in cubic FPU chains. This mechanism, which is generic in cubic chains but not in quartic chains, provides superperiod recurrence times that are in agreement with numerical studies. Furthermore, numerical simulations have shown that superperiod recurrences are readily observable in all cubic, but not all quartic, chains. An exceptional superperiod, which occurs in quartic chains with $N=7$, has been accounted for by a resonance mechanism that is unique to this chain.

The calculations reported in this study confirm the usefulness of the shifted-frequency perturbation scheme in providing reliable estimates of long-period recurrences in weakly nonlinear FPU chains. Our calculations were carried out on chains with clamped ends, but the perturbation scheme can also be readily applied to chains with other boundary conditions. Other initial conditions can also be studied within this framework provided that the nonlinear energy is not comparable in magnitude to the linear energy of the chain.

ACKNOWLEDGMENTS

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APPENDIX A

We list here for completeness the definitions of some of the amplitude coefficients necessary to describe the expansion derived for the quartic FPU chain. The coefficients used in the solutions of modes 1 and 3 at second order are

$$B_{1,1}=-\sum_{p=2}^{6}B_{1,p},$$

$$B_{1,2}=\frac{3A_{1113}}{32\Omega_1^2}(2A_{3,3}+A_{3,2}),$$

$$B_{1,3}=\frac{3}{96\Omega_1^2}(A_{1111}A_{1,1}+A_{1113}A_{1,3}),$$

$$B_{1,4}=\frac{-3A_{1113}A_{3,1}}{2(\Omega_1^2-\Omega_3^2)},$$

$$B_{1,5}=\frac{-3A_{1113}A_{3,1}}{4[\Omega_1^2-(\Omega_3-2\Omega_1)^2]},$$

$$B_{1,6}=\frac{-3A_{1113}A_{3,1}}{4[\Omega_1^2-(\Omega_3+2\Omega_1)^2]},$$

$$B_{3,1}=-\sum_{p=2}^{6}B_{3,p},$$

$$B_{3,2}=\frac{3}{4(\Omega_3^2-\Omega_1^2)}[2A_{1113}A_{1,1}-A_{3311}(A_{3,2}+A_{3,3})],$$

$$B_{3,3}=\frac{-3}{4(\Omega_3^2-9\Omega_1^2)}(A_{1113}A_{1,1}+A_{3311}A_{3,2}),$$

$$B_{3,4}=\frac{-3}{4(\Omega_3^2-25\Omega_1^2)}(A_{1113}A_{1,1}+A_{3311}A_{3,3}),$$

$$B_{3,5}=\frac{-3A_{3311}A_{3,1}}{4[\Omega_3^2-(\Omega_3-2\Omega_1)^2]},$$

$$B_{3,6}=\frac{-3A_{3311}A_{3,1}}{[\Omega_3^2-(\Omega_3+2\Omega_1)^2]}.$$

At third order in the equation of motion, the solution for mode 1 is

$$a_{1,3}=\epsilon^3[C_{1,1}\cos\Omega_1 t+C_{1,2}\cos3\Omega_1 t+C_{1,3}\cos5\Omega_1 t+C_{1,4}\cos7\Omega_1 t+C_{1,5}\cos\Omega_3 t+C_{1,6}\cos(\Omega_3-2\Omega_1)t+C_{1,7}\cos(\Omega_3+2\Omega_1)t+C_{1,8}\cos(\Omega_3-4\Omega_1)t+C_{1,9}\cos(\Omega_3+4\Omega_1)t+C_{1,10}\cos(2\Omega_3-\Omega_1)t+C_{1,11}\cos(2\Omega_3+\Omega_1)t],$$

where the amplitude coefficients are defined by

$$C_{1,1}=-\sum_{p=2}^{1}C_{1,p},$$

$$C_{1,2}=\frac{9}{32\Omega_1^2}[A_{1111}(B_{1,1}+B_{1,3}-2A_{1,1}^2)+3A_{1133}(A_{3,2}^2+4A_{3,2}A_{3,3})+A_{1113}(2B_{3,3}+B_{3,2}+B_{3,4}-A_{3,2}A_{1,1}-5A_{3,3}A_{1,1})],$$

$$C_{1,3}=\frac{-3}{96\Omega_1^2}[A_{1111}(B_{1,2}-A_{1,1}^2)+A_{1133}(A_{3,3}^2+2A_{3,2}A_{3,3})+A_{1113}(B_{3,3}+2B_{3,4}+2A_{3,2}A_{1,1})],$$

$$C_{1,4}=\frac{-3}{192\Omega_1^2}[A_{1111}(A_{1,1}^2+B_{1,3})+A_{1133}A_{3,3}^2+A_{1113}(2A_{1,1}+B_{3,4})],$$

$$C_{1,5}=\frac{-3}{4(\Omega_1^2-\Omega_3^2)}[A_{1111}(B_{1,5}+B_{1,6})+4A_{1133}A_{3,1}A_{3,2}+A_{1113}(2B_{3,1}+B_{3,5}+B_{3,6}-4A_{3,1}A_{1,1})],$$

$$C_{1,6}=\frac{-3}{4[\Omega_1^2-(\Omega_3-2\Omega_1)^2]}[A_{1111}B_{1,4}+A_{1113}(2B_{3,5}+B_{3,1})+2A_{1113}A_{3,1}(A_{3,2}+A_{3,3})],$$

$$C_{1,7}=\frac{-3}{4[\Omega_1^2-(\Omega_3+2\Omega_2)^2]}[A_{1111}(B_{1,4}+2B_{1,6}-2B_{1,5})+A_{1113}(2B_{3,6}+B_{3,1})+2A_{1133}A_{3,1}(A_{3,2}+A_{3,3})],$$

$$C_{1,8}=\frac{-3}{4[\Omega_1^2-(\Omega_3-4\Omega_1)^2]}[A_{1111}B_{1,5}+A_{1113}(2A_{3,1}A_{1,1}+B_{3,5})+2A_{1133}A_{3,1}A_{3,3}],$$

$$C_{1,9}=\frac{-3}{4[\Omega_1^2-(\Omega_3+4\Omega_1)^2]}[A_{1111}B_{1,6}+A_{1113}(2A_{3,1}A_{1,1}+B_{3,6})+2A_{1133}A_{3,1}A_{3,3}],$$

$$C_{1,10}=\frac{-3A_{1133}A_{3,1}^2}{4[\Omega_1^2-(2\Omega_3-\Omega_1)^2]},$$

$$C_{1,11}=\frac{-3A_{1133}A_{3,1}^2}{4[\Omega_1^2-(2\Omega_3+\Omega_1)^2]}.$$

APPENDIX B

The coefficients used to describe the solution of the cubic FPU chain to second order are

$$A_{2,1}=-A_{2,2}-A_{2,3},$$

$$A_{2,2}=-\frac{3A_{211}}{2\Omega_2^2},$$

$$A_{2,3}=-\frac{3A_{211}}{2(\Omega_2^2-4\Omega_1^2)},$$

$$B_{1,1}=-\sum_{p=2}^{4}B_{1,p},$$

$$B_{1,2}=\frac{3A_{112}A_{2,3}}{8\Omega_1^2},$$

$$B_{1,3}=-\frac{3A_{112}A_{2,1}}{2\Omega_1\Omega_2-\Omega_2^2},$$

$$B_{1,4}=\frac{3A_{112}A_{2,1}}{2\Omega_1\Omega_2+\Omega_2^2},$$

$$B_{3,1}=-\sum_{p=2}^{5}B_{3,p},$$

$$B_{3,2}=-\frac{6A_{321}(A_{2,2}+\frac{1}{2}A_{2,3})}{\Omega_3^2-\Omega_1^2},$$

$$B_{3,3}=-\frac{3A_{321}A_{2,3}}{\Omega_3^2-9\Omega_1^2},$$

$$B_{3,4}=-\frac{3A_{321}A_{2,1}}{\Omega_3^2-(\Omega_1-\Omega_2)^2},$$

$$B_{3,5}=-\frac{3A_{321}A_{2,1}}{\Omega_3^2-(\Omega_1+\Omega_2)^2}.$$

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