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Stability of Linear Chains with Third-order Anharmonicity

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Abstract. A n -particle chain with third-order coupling and periodic boundary condition is analyzed with respect to orbital instability (critical energy E_c) and mechanical instability (threshold E_t). For E_c the bounds found for large n are $1/4\alpha^2 \leq E_c \leq 1/\alpha^2$, α being the coupling constant. The bound $E_t \leq 1/\alpha^2$ is found for a configuration which in the continuum limit corresponds to a supersonic (or tachyonic) solitons which, however, is physically not realizable.

In the computer analysis of integrals of galactic motion Henin and Heiles [1]¹⁾ discovered that the classical orbits determined by the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2 + q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3} q_1^3 \quad (1)$$

are stochastically distributed above a critical energy $E_c \cong 0.11$ but ordered below. Similar behaviour has been found by Bocchieri, Scotti, Bearzi and Loinger [2] and others [3] in translation-invariant anharmonic linear chains defined by the Hamiltonian

$$H = \frac{1}{2} \sum_{i=1}^n p_i^2 + U(q) \quad (2)$$

with

$$U(q) = \sum_{i=1}^n v(q_{i+1} - q_i); \quad q_{i+n} = q_i. \quad (3)$$

Using a Lennard-Jones form for v , BSBL found a critical energy E_c proportional to the number n of particles in the chain. These two results are connected, since (1) can be shown [4] to be equivalent with (2) and (3) for $n = 3$ and with the form

$$v(x) = \frac{1}{2} x^2 - \frac{\alpha}{3} x^3, \quad (4)$$

analyzed by Fermi, Pasta and Ulam [5] with fixed boundary conditions.

Recently, Toda [6] has interpreted the critical energy in the HH-model as energy of exponential instability, defined by the condition that above E_c neighbouring orbits diverge exponentially. In terms of the equations of motion

$$\ddot{q}_i = -\partial U / \partial q_i \quad i = 1, \dots, n, \quad (5)$$

¹⁾ References [1], [2] and [5] are abbreviated throughout the article as HH, BSBL and FPU, respectively.

this means that the matrix

$$W_{ij} = \partial^2 U / \partial q_i \partial q_j, \quad (6)$$

which determines the motion of the variations δq_i has negative eigenvalues. The limit of this instability is thus given by the condition

$$\|W\| = 0. \quad (7)$$

Toda defines E_c as the energy contour $U(q) = E_c$ which touches the surface (7), that is by

$$\frac{\partial U}{\partial q_i} = \lambda \frac{\partial \|W\|}{\partial q_i} \quad i = 1, \dots, n, \quad (8)$$

together with (7). He finds $E_c = \frac{1}{12}$ in fair agreement with the numerical value of HH.

The question arises whether the BSBL-result $E_c \propto n$, also follows, for large n , with Toda's definition of E_c . Applied to the translation-invariant potential (3) a complication arises from the identity

$$\sum_{i=1}^n \partial U / \partial q_i = 0 \quad (9)$$

since it implies

$$\sum_{i=1}^n W_{ij} = 0 \quad i = 1, \dots, n, \quad (10)$$

and hence $\|W\| = 0$. In order to apply condition (7) it is necessary, therefore, to eliminate one coordinate by a canonical transformation

$$q = A\tilde{q}; \quad W = A\tilde{W}A^T; \quad A^T A = 1 \quad (11)$$

such that all $q_{i+1} - q_i$ are independent of \tilde{q}_n (for $n = 3$ this leads to (1), see Ref. [4]); thus

$$A_{in} = n^{-1/2}; \quad \tilde{q}_n = n^{-1/2} \sum_{i=1}^n q_i. \quad (12)$$

Since \tilde{W} has all but zeros in the last line and column the stability limit (7) is given in terms of the matrix

$$\tilde{X}_{ij} = \tilde{W}_{ij} + \delta_{in}\delta_{jn} = \frac{\partial^2 \tilde{V}}{\partial \tilde{q}_i \partial \tilde{q}_j} \quad (13)$$

by

$$\|\tilde{X}\| = \|X\| = 0. \quad (14)$$

Here

$$\tilde{V}(\tilde{q}) = \tilde{U}(\tilde{q}) + \frac{1}{2}\tilde{q}_n^2 \quad (15)$$

and the minimum condition (8) now becomes

$$\partial \tilde{V} / \partial \tilde{q}_i = \lambda \frac{\partial \|\tilde{X}\|}{\partial \tilde{q}_i} \quad i = 1, \dots, n. \quad (16)$$

Indeed, for $i = n$ this implies, according to (12),

$$\sum_{i=1}^n q_i = 0 \quad (17)$$

so that $V = U$. Equation (17) corresponds to the initial condition of a fixed center of mass and also fixes the constant in the translation $q_i \rightarrow q_i + \tau$ such that $\sum_i (q_i + \tau) \times (q_{i+1} + \tau)$ is minimum for any l .

Applying the inverse of (11) to (13) one finds with (12)

$$X_{ij} = W_{ij} + \frac{1}{n} \quad (18)$$

and [7]

$$\|X\| = nM_{n-1}. \quad (19)$$

Here M_m ($m \leq n-1$) is the determinant of the elements W_{ij} with $i, j = 1, \dots, m$. Since, according to (3) and (6), the only non-vanishing elements of W are on and adjacent to the main diagonal,

$$W_{ij} = W_{i,j+n} = a_i \delta_{ij} - b_i \delta_{i+1,j} - b_{i-1} \delta_{i-1,j} \quad (20)$$

M_m can be calculated by successive annihilation of the elements below the main diagonal [7]. The result is the continued fraction expression

$$M_m = \prod_{i=1}^n A_m$$

$$A_1 = a_1, \quad A_i = a_i - b_{i-1}^2/A_{i-1} \quad i \geq 2 \quad (21)$$

from which the recursion relation

$$M_m = a_m M_{m-1} - b_{m-1}^2 M_{m-2} \quad (22)$$

follows.

In the case of the FPU-model (4)

$$a_i = 2 - 2\alpha(q_{i+1} - q_{i-1}),$$

$$b_i = 1 - 2\alpha(q_{i+1} - q_i). \quad (23)$$

Because of the linearity of these functions an explicit expression for $\|X\|$ up to second order in the q_i can be obtained [7]. Indeed, because of symmetry and of (17)

$$\|X\| = n^2 + H_2(q) + H_3(q) + \dots \quad (24)$$

where H_l is a homogeneous symmetric polynomial of degree l . By one iteration of (22) it is straightforward to calculate $\partial M_{n-1}/\partial q_{n-1}$ making use of (23). Then [7]

$$H_2(q) = \frac{n}{2} \sum_i \left. \frac{\partial M_{n-1}}{\partial q_i} \right|_{q=0} q_i$$

$$= -4\alpha^2 n^2 (n-2) \bar{q}^2 (1 - \xi) \quad (25)$$

where

$$\bar{q}^2 = \frac{1}{n} \sum_i q_i^2; \quad \bar{q}^2 \xi = \frac{1}{n} \sum_i q_i q_{i+1}. \quad (26)$$

Now the condition (14) becomes

$$\begin{aligned} \frac{1}{2n} \sum_i (q_{i+1} - q_i)^2 &= \bar{q}^2(1 - \xi) \\ &= \frac{1}{4\alpha^2(n-2)} \left\{ 1 + \frac{1}{n^2} H_3(q) + \dots \right\} \end{aligned} \quad (27)$$

Since $\xi < 1$ for $\bar{q} \neq 0$ this shows that \bar{q} decreases as $n^{-1/2}$ for $n \rightarrow \infty$ and hence justifies the development (24).

E_c is now obtained by minimizing $U(q)$ under the conditions (27) and (17). Going over to variables x_i ($i = 0, \dots, n$) defined by

$$\begin{aligned} q_i &= \sum_{l=0}^{i-1} x_l \quad i = 1, \dots, n+1 \\ \sum_{l=0}^{n-1} (n-l)x_l &= 0, \quad \sum_{l=1}^n x_l = 0 \end{aligned} \quad (28)$$

we obtain a lower bound to E_c by leaving out the two restrictions in (28). In this form the extremal conditions are

$$(1 - \lambda)x_l - \alpha x_l^2 = 0 \quad l = 1, \dots, n, \quad (29)$$

λ being the Lagrange multiplier for condition (27) which, by insertion of (29), yields

$$\alpha x_l = 1 - \lambda = 1/\sqrt{2(n-2)} \quad (30)$$

and hence [7]

$$E_c \geq \frac{n}{4\alpha^2(n-2)} \left(1 - \frac{1}{3} \sqrt{\frac{2}{n-2}} \right) = \frac{1}{4\alpha^2} + o\left(\frac{1}{n^2}\right). \quad (31)$$

An upper bound to E_c is obtained from any particular point on the surface (14). Now from (20) and (23) follows

$$\sum_{j=1}^{n-1} W_{ij} = a_i - b_{i-1} - b_i = 0 \quad i = 2, \dots, n-2. \quad (32)$$

If we require in addition

$$\sum_{j=1}^{n-1} W_{1j} = a_1 - b_1 = 0; \quad \sum_{j=1}^{n-1} W_{n-1,j} = a_{n-1} - b_{n-2} = 0 \quad (33)$$

then $M_{n-1} = 0$. But (33) has the particular solution $q_1 = q_{n-1} = \frac{1}{2}\alpha$, all other $q_i = 0$, which inserted into $U(q)$ yields [7]

$$E_c \leq \frac{1}{2\alpha^2}. \quad (34)$$

This bound is independent of n , in apparent contradiction with the numerical result of BSBL. However, the property (32) is a direct consequence of the linearity of the functions (23); in other words, it holds for the FPU-model (4) but not for the Lennard-Jones potential used by BSBL. It is interesting also that in the case $n = 3$ of the HH-

model the bound (34) is actually reached. Indeed, this value corresponds, in the units of HH, to Toda's result $E_c = \frac{1}{12}$.

The fact that the leading power in the FPU-potential (4) is odd makes this model mechanically unstable above a threshold E_t . An upper bound to E_t is obtained for the particular configuration

$$\begin{aligned} q_k &= -q_{1-k} = x & k = 1, \dots, l; 2 \geq 2l \geq n-1 \\ \text{all other } q_i &= 0 \end{aligned} \quad (35)$$

which satisfies (17). In this case $U(q) = x^2(3 - 2\alpha x)$ which has a maximum $1/\alpha^2$ at $x = 1/\alpha$. For larger x the potential energy becomes negative and unbounded so that the chain must break between particles n and 1. This maximum leads to $E_t \leq 1/\alpha^2$ which might indicate a connection with E_c .

It is interesting that in the limit $n \rightarrow \infty$, $l \rightarrow \infty$ the configuration (35) becomes a step function reminiscent of the soliton solution

$$q_s(x, t) = q_0 \tanh[(x - vt)/x_0] \quad (36)$$

of certain one-dimensional continuum models [8-10]. The continuum limit of (3) is simplest in the form

$$U[q] = \int \frac{dx}{c} v(q(x+c) - q(x)) \quad (37)$$

which has to be understood as an expansion in powers of c , the inter-particle distance. With (4) the equations of motion (5) become [7]

$$\begin{aligned} \ddot{q}(x) &= -\delta U[q]/\delta q(x) \\ &= c^2 q'' - 2\alpha c^3 q' q'' + \frac{1}{12} c^4 q^{IV} + O(c^5). \end{aligned} \quad (38)$$

This has indeed a solution (36) with

$$q_0 = -\frac{\gamma}{2\alpha}; \quad x_0 = \frac{c}{\gamma}; \quad \gamma = \sqrt{3(v^2/c^2 - 1)} > 0. \quad (39)$$

Since (38) is invariant under $q \rightarrow -q$, $\alpha \rightarrow -\alpha$ the opposite sign of q_0 is also a solution. The potential energy (37) corresponding to these two solutions can be calculated by elementary integrations, it is

$$U_s(\gamma) = \frac{\gamma}{6\alpha^2} \left\{ 1 - \frac{1 \mp 4}{15} \gamma^2 + O(c^5) \right\} \quad (40)$$

This shows that the positive step, $q_0 > 0$, which is the continuum limit of the configuration (35), leads to a negative and unbounded $U_s(\gamma)$. Of course, the relations (39) are quite different from the Lorentz-covariance relations of normal solitons [8, 9]: They describe supersonic (or tachyonic) solitons in the sense that the soliton velocity $v > c$. This fact seems to indicate that the mechanical instability of the configuration (35) is dynamically irrelevant since the supersonic solitons are physically not realizable.

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