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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 $1/4\alpha^2 \le E_c \le 1/\alpha^2$, α being the coupling constant. The bound $E_t \le 1/\alpha^2$ 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

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

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

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

with

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

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

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

$$\ddot{q}_i = -\partial U/\partial q_i \qquad i = 1, \dots, n, \tag{5}$$

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

this means that the matrix

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

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

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

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

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

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

since it implies

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

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

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

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

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

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

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

by

$$\|\tilde{X}\| = \|X\| = 0. \tag{14}$$

Here

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

and the minimum condition (8) now becomes

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

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

$$\sum_{i=1}^{n} q_i = 0 \tag{17}$$

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 $q_i \to q_i + \tau$ 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)

$$X_{ij} = W_{ij} + \frac{1}{n} \tag{18}$$

and [7]

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

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

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

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

$$M_{m} = \prod_{i=1}^{n} A_{m}$$

$$A_{1} = a_{1}, \quad A_{i} = a_{i} - b_{i-1}^{2} / A_{i-1} \qquad i \ge 2$$
(21)

from which the recursion relation

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

follows.

In the case of the FPU-model (4)

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

$$b_{i} = 1 - 2\alpha(q_{i+1} - q_{i}).$$
(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)

$$||X|| = n^2 + H_2(q) + H_3(q) + \cdots$$
 (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]

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

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

where

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

Now the condition (14) becomes

$$\frac{1}{2n} \sum_{i} (q_{i+1} - q_{i})^{2} = \bar{q}^{2}(1 - \xi)$$

$$= \frac{1}{4\alpha^{2}(n-2)} \left\{ 1 + \frac{1}{n^{2}} H_{3}(q) + \cdots \right\}$$
(27)

Since $\xi < 1$ for $\bar{q} \neq 0$ this shows that \bar{q} decreases as $n^{-1/2}$ for $n \to \infty$ 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, ..., n) defined by

$$q_{i} = \sum_{l=0}^{i-1} x_{l} \qquad i = 1, \dots, n+1$$

$$\sum_{l=0}^{n-1} (n-l)x_{l} = 0, \quad \sum_{l=1}^{n} x_{l} = 0$$
(28)

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

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

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

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

and hence [7]

$$E_c \geqslant \frac{n}{4\alpha^2(n-2)} \left(1 - \frac{1}{3}\sqrt{\frac{2}{n-2}}\right) = \frac{1}{4\alpha^2} + 0\left(\frac{1}{n^2}\right).$$
 (31)

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

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

If we require in addition

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

$$E_c \leqslant \frac{1}{2\alpha^2}.$$
(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

$$q_k = -q_{1-k} = x$$
 $k = 1, ..., l; 2 \ge 2l \ge n - 1$
all other $q_i = 0$ (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 $n \to \infty$, $l \to \infty$ the configuration (35) becomes a step function reminiscent of the soliton solution

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

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

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

$$\ddot{q}(x) = -\delta U[q]/\delta q(x) = c^2 q'' - 2\alpha c^3 q' q'' + \frac{1}{12} c^4 q^{IV} + 0(c^5).$$
(38)

This has indeed a solution (36) with

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

Since (38) is invariant under $q \to -q$, $\alpha \to -\alpha$ 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

$$U_s(\gamma) = \frac{\gamma}{6\alpha^2} \left\{ 1 - \frac{1 \mp 4}{15} \gamma^2 + 0(c^5) \right\}$$
 (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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