Zeitschrift: Helvetica Physica Acta
Band: 48 (1975)
Heft: 5-6

Artikel: Stability of linear chains with third-order anharmonicity
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DOI: https://doi.org/10.5169/seals-114698

Helvetica Physica Acta, Vol. 48 (1975), Birkhäuser Verlag, Basel

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

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

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

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

with

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

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

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

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[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

$$\| W \| = 0. \tag{7}$$

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

$$\frac{\partial U}{\partial q_i} = \lambda \frac{\partial \| W \|}{\partial q_i} \qquad i = 1, \ldots, n, \tag{8}$$

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

$$\sum_{i=1}^{n} W_{ij} = 0 \qquad i = 1, \ldots, n, \tag{10}$$

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

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

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

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

by

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

Here

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

and the minimum condition (8) now becomes

$$\partial \tilde{V}/\partial \tilde{q}_i = \lambda \frac{\partial \| \tilde{X} \|}{\partial \tilde{q}_i} \qquad i = 1, \ldots, n. \tag{16}$$

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 $\sum_i (q_i + \tau)\times(q_{i+l} + \tau)$ 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]

$$\|X\| = nM_{n-1}. \tag{19}$$

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

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

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

$$M_m = \prod_{i=1}^{n} A_m$$
$$A_1 = a_1, \quad A_i = a_i - b_{i-1}^2/A_{i-1} \qquad i \geqslant 2 \tag{21}$$

from which the recursion relation

$$M_m = a_m M_{m-1} - b_{m-1}^2 M_{m-2} \tag{22}$$

follows.

In the case of the FPU-model (4)

$$\begin{aligned} a_i &= 2 - 2\alpha(q_{i+1} - q_{i-1}), \\ b_i &= 1 - 2\alpha(q_{i+1} - q_i). \end{aligned} \tag{23}$$

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)

$$\|X\| = n^2 + H_2(q) + H_3(q) + \cdots \tag{24}$$

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]

$$\begin{aligned} H_2(q) &= \frac{n}{2}\sum_i \left.\frac{\partial M_{n-1}}{\partial q_i}\right|_{q=0} q_i \\ &= -4\alpha^2 n^2(n-2)\bar{q}^2(1-\xi) \end{aligned} \tag{25}$$

where

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

Now the condition (14) becomes

$$\frac{1}{2n} \sum_i (q_{i+1} - q_i)^2 = \bar{q}^2(1 - \xi)$$
$$= \frac{1}{4\alpha^2(n-2)} \left\{1 + \frac{1}{n^2} H_3(q) + \cdots\right\} \tag{27}$$

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 ($i = 0, \ldots, n$) defined by

$$q_i = \sum_{l=0}^{i-1} x_l \qquad i = 1, \ldots, n+1$$
$$\sum_{l=0}^{n-1} (n - l)x_l = 0, \quad \sum_{l=1}^{n} x_l = 0 \tag{28}$$

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

$$(1 - \lambda)x_l - \alpha x_l^2 = 0 \qquad l = 1, \ldots, n, \tag{29}$$

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]

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

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

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

If we require in addition

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

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]

$$E_c \leqslant \frac{1}{2\alpha^2}. \tag{34}$$

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

$$\begin{aligned} &q_k = -q_{1-k} = x \qquad k = 1,\ldots, l;\ 2 \geqslant 2l \geqslant n-1 \\ &\text{all other } q_i = 0 \end{aligned} \tag{35}$$

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 $E_t \leqslant 1/\alpha^2$ 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

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

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

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

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]

$$\begin{aligned} \ddot{q}(x) &= -\,\delta U[q]/\delta q(x) \\ &= c^2 q'' - 2\alpha c^3 q' q'' + \tfrac{1}{12} c^4 q^{\mathrm{IV}} + 0(c^5). \end{aligned} \tag{38}$$

This has indeed a solution (36) with

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

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

$$U_s(\gamma) = \frac{\gamma}{6\alpha^2}\left\{1 - \frac{1 \mp 4}{15}\gamma^2 + 0(c^5)\right\} \tag{40}$$

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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