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

Artikel: Stability of linear chains with third-order anharmonicity
Autor: Enz, C.P. / Hongler, M.O. / Quach Thi, C.V.
DOI: https://doi.org/10.5169/seals-114698

Nutzungsbedingungen
Die ETH-Bibliothek ist die Anbieterin der digitalisierten Zeitschriften auf E-Periodica. Sie besitzt keine Urheberrechte an den Zeitschriften und ist nicht verantwortlich für deren Inhalte. Die Rechte liegen in der Regel bei den Herausgebern beziehungsweise den externen Rechteinhabern. Das Veröffentlichen von Bildern in Print- und Online-Publikationen sowie auf Social Media-Kanälen oder Webseiten ist nur mit vorheriger Genehmigung der Rechteinhaber erlaubt. Mehr erfahren

Conditions d'utilisation
L'ETH Library est le fournisseur des revues numérisées. Elle ne détient aucun droit d'auteur sur les revues et n'est pas responsable de leur contenu. En règle générale, les droits sont détenus par les éditeurs ou les détenteurs de droits externes. La reproduction d'images dans des publications imprimées ou en ligne ainsi que sur des canaux de médias sociaux ou des sites web n'est autorisée qu'avec l'accord préalable des détenteurs des droits. En savoir plus

Terms of use
The ETH Library is the provider of the digitised journals. It does not own any copyrights to the journals and is not responsible for their content. The rights usually lie with the publishers or the external rights holders. Publishing images in print and online publications, as well as on social media channels or websites, is only permitted with the prior consent of the rights holders. Find out more

Download PDF: 25.11.2025

ETH-Bibliothek Zürich, E-Periodica, https://www.e-periodica.ch

Stability of Linear Chains with Third-order Anharmonicity

by **C. P. Enz, M. O. Hongler** and **C. V. Quach Thi**

Département de Physique Théorique, Université de Genève, 1211 Genève 4

(11. VIII. 75)

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

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

[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

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

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

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

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.

REFERENCES

[1] M. Hénon and C. Heiles, Astron. Journ. *69*, 73 (1964).
[2] P. Bocchieri, A. Scotti, B. Bearzi and A. Loinger, Phys. Rev. *A2*, 2013 (1970).
[3] L. Galgani and A. Scotti, Revista del Nuovo Cimento *2*, 189 (1972).
[4] G. H. Lunsford and J. Ford, J. Math. Phys. *13*, 700 (1972).
[5] E. Fermi, J. Pasta and S. Ulam, in *Collected Papers by E. Fermi* (Chicago, 1965), p. 978.
[6] M. Toda, Physics Letters *48A*, 335 (1974).
[7] M. O. Hongler et C .V. Quach Thi, *Travaux de diplôme*, Université de Genève, 1975 (unpublished).
[8] U. Enz, Phys. Rev. *131*, 1392 (1963); Helv. Phys. Acta *37*, 245 (1964).
[9] S. Aubry, *Première Thèse*, Université de Paris VI, 1975 (unpublished).
[10] J. A. Krumhansl and J. R. Schrieffer, Phys. Rev. *B11*, 3535 (1975).