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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 $1 / 4 \alpha^{2} \leqslant E_{c} \leqslant 1 / \alpha^{2}, \alpha$ 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

$$
\begin{equation*}
H=\frac{1}{2}\left(p_{1}^{2}+p_{2}^{2}+q_{1}^{2}+q_{2}^{2}\right)+q_{1}^{2} q_{2}-\frac{1}{3} q_{1}^{3} \tag{1}
\end{equation*}
$$

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

$$
\begin{equation*}
H=\frac{1}{2} \sum_{i=1}^{n} p_{i}^{2}+U(q) \tag{2}
\end{equation*}
$$

with

$$
\begin{equation*}
U(q)=\sum_{i=1}^{n} v\left(q_{i+1}-q_{i}\right) ; \quad q_{i+n}=q_{i} \tag{3}
\end{equation*}
$$

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'

$$
\begin{equation*}
v(x)=\frac{1}{2} x^{2}-\frac{\alpha}{3} x^{3} \tag{4}
\end{equation*}
$$

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

$$
\begin{equation*}
\ddot{q}_{i}=-\partial U / \partial q_{i} \quad i=1, \ldots, n \tag{5}
\end{equation*}
$$

$\left.{ }^{1}\right)$ References [1], [2] and [5] are abbreviated throughout the article as HH, BSBL and FPU, respectively.
this means that the matrix

$$
\begin{equation*}
W_{i j}=\partial^{2} U / \partial q_{i} \partial q_{j} \tag{6}
\end{equation*}
$$

which determines the motion of the variations $\delta q_{i}$ has negative eigenvalues. The limit of this instability is thus given by the condition

$$
\begin{equation*}
\|W\|=0 \tag{7}
\end{equation*}
$$

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

$$
\begin{equation*}
\frac{\partial U}{\partial q_{i}}=\lambda \frac{\partial\|W\|}{\partial q_{i}} \quad i=1, \ldots, n, \tag{8}
\end{equation*}
$$

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

$$
\begin{equation*}
\sum_{i=1}^{n} \partial U / \partial q_{i}=0 \tag{9}
\end{equation*}
$$

since it implies

$$
\begin{equation*}
\sum_{i=1}^{n} W_{i j}=0 \quad i=1, \ldots, n \tag{10}
\end{equation*}
$$

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

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

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

$$
\begin{equation*}
A_{i n}=n^{-1 / 2} ; \quad \tilde{q}_{n}=n^{-1 / 2} \sum_{i=1}^{n} q_{i} . \tag{12}
\end{equation*}
$$

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

$$
\begin{equation*}
\tilde{X}_{i j}=\tilde{W}_{i j}+\delta_{i n} \delta_{j n}=\frac{\partial^{2} \tilde{V}}{\partial \tilde{q}_{i} \partial \tilde{q}_{j}} \tag{13}
\end{equation*}
$$

by

$$
\begin{equation*}
\|\tilde{X}\|=\|X\|=0 \tag{14}
\end{equation*}
$$

Here

$$
\begin{equation*}
\tilde{V}(\tilde{q})=\tilde{U}(\tilde{q})+\frac{1}{2} \tilde{q}_{n}^{2} \tag{15}
\end{equation*}
$$

and the minimum condition (8) now becomes

$$
\begin{equation*}
\partial \tilde{V} / \partial \tilde{q}_{i}=\lambda \frac{\partial\|\tilde{X}\|}{\partial \tilde{q}_{i}} \quad i=1, \ldots, n . \tag{16}
\end{equation*}
$$

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

$$
\begin{equation*}
\sum_{i=1}^{n} q_{i}=0 \tag{17}
\end{equation*}
$$

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 $\sum_{i}\left(q_{i}+\tau\right) \times$ $\left(q_{i+l}+\tau\right)$ is minimum for any $l$.

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

$$
\begin{equation*}
X_{i j}=W_{i j}+\frac{1}{n} \tag{18}
\end{equation*}
$$

and [7]

$$
\begin{equation*}
\|X\|=n M_{n-1} . \tag{19}
\end{equation*}
$$

Here $M_{m}(m \leqslant n-1)$ is the determinant of the elements $W_{i j}$ 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,

$$
\begin{equation*}
W_{i j}=W_{i, j+n}=a_{i} \delta_{i j}-b_{i} \delta_{i+1, j}-b_{i-1} \delta_{i-1, j} \tag{20}
\end{equation*}
$$

$M_{m}$ can be calculated by successive annihilation of the elements below the main diagonal [7]. The result is the continued fraction expression

$$
\begin{align*}
M_{m} & =\prod_{i=1}^{n} A_{m} \\
A_{1} & =a_{1}, \quad A_{i}=a_{i}-b_{i-1}^{2} / A_{i-1} \quad i \geqslant 2 \tag{21}
\end{align*}
$$

from which the recursion relation

$$
\begin{equation*}
M_{m}=a_{m} M_{m-1}-b_{m-1}^{2} M_{m-2} \tag{22}
\end{equation*}
$$

follows.
In the case of the FPU-model (4)

$$
\begin{align*}
& a_{i}=2-2 \alpha\left(q_{i+1}-q_{i-1}\right), \\
& b_{i}=1-2 \alpha\left(q_{i+1}-q_{i}\right) \tag{23}
\end{align*}
$$

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)

$$
\begin{equation*}
\|X\|=n^{2}+H_{2}(q)+H_{3}(q)+\cdots \tag{24}
\end{equation*}
$$

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]

$$
\begin{align*}
H_{2}(q) & =\left.\frac{n}{2} \sum_{i} \frac{\partial M_{n-1}}{\partial q_{i}}\right|_{q=0} q_{i} \\
& =-4 \alpha^{2} n^{2}(n-2) \bar{q}^{2}(1-\xi) \tag{25}
\end{align*}
$$

where

$$
\begin{equation*}
\bar{q}^{2}=\frac{1}{n} \sum_{i} q_{i}^{2} ; \quad \bar{q}^{2} \xi=\frac{1}{n} \sum_{i} q_{i} q_{i+1} \tag{26}
\end{equation*}
$$

Now the condition (14) becomes

$$
\begin{align*}
\frac{1}{2 n} \sum_{i}\left(q_{i+1}-q_{i}\right)^{2} & =\bar{q}^{2}(1-\xi) \\
& =\frac{1}{4 \alpha^{2}(n-2)}\left\{1+\frac{1}{n^{2}} H_{3}(q)+\cdots\right\} \tag{27}
\end{align*}
$$

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

$$
\begin{align*}
& q_{i}=\sum_{l=0}^{i-1} x_{l} \quad i=1, \ldots, n+1 \\
& \sum_{l=0}^{n-1}(n-l) x_{l}=0, \quad \sum_{l=1}^{n} x_{l}=0 \tag{28}
\end{align*}
$$

we obtain a lower bound to $E_{c}$ by leaving out the two restrictions in (28). In this form the extremal conditions are

$$
\begin{equation*}
(1-\lambda) x_{l}-\alpha x_{l}^{2}=0 \quad l=1, \ldots, n \tag{29}
\end{equation*}
$$

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

$$
\begin{equation*}
\alpha x_{l}=1-\lambda=1 / \sqrt{2(n-2)} \tag{30}
\end{equation*}
$$

and hence [7]

$$
\begin{equation*}
E_{c} \geqslant \frac{n}{4 \alpha^{2}(n-2)}\left(1-\frac{1}{3} \sqrt{\frac{2}{n-2}}\right)=\frac{1}{4 \alpha^{2}}+0\left(\frac{1}{n^{2}}\right) \tag{31}
\end{equation*}
$$

An upper bound to $E_{c}$ is obtained from any particular point on the surface (14). Now from (20) and (23) follows

$$
\begin{equation*}
\sum_{j=1}^{n-1} W_{i j}=a_{i}-b_{i-1}-b_{i}=0 \quad i=2, \ldots, n-2 \tag{32}
\end{equation*}
$$

If we require in addition

$$
\begin{equation*}
\sum_{j=1}^{n-1} W_{1 j}=a_{1}-b_{1}=0 ; \quad \sum_{j=1}^{n-1} W_{n-1, j}=a_{n-1}-b_{n-2}=0 \tag{33}
\end{equation*}
$$

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]

$$
\begin{equation*}
E_{c} \leqslant \frac{1}{2 \alpha^{2}} \tag{34}
\end{equation*}
$$

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 LennardJones 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

$$
\begin{equation*}
q_{k}=-q_{1-k}=x \quad k=1, \ldots, l ; 2 \geqslant 2 l \geqslant n-1 \tag{35}
\end{equation*}
$$

all other $q_{i}=0$
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 $n \rightarrow \infty, l \rightarrow \infty$ the configuration (35) becomes a step function reminiscent of the soliton solution

$$
\begin{equation*}
q_{s}(x, t)=q_{0} \tanh \left[(x-v t) / x_{0}\right] \tag{36}
\end{equation*}
$$

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

$$
\begin{equation*}
U[q]=\int \frac{d x}{c} v(q(x+c)-q(x)) \tag{37}
\end{equation*}
$$

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]

$$
\begin{align*}
\ddot{q}(x) & =-\delta U[q] / \delta q(x)  \tag{38}\\
& =c^{2} q^{\prime \prime}-2 \alpha c^{3} q^{\prime} q^{\prime \prime}+\frac{1}{12} c^{4} q^{\mathrm{IV}}+0\left(c^{5}\right)
\end{align*}
$$

This has indeed a solution (36) with

$$
\begin{equation*}
q_{0}=-\frac{\gamma}{2 \alpha} ; \quad x_{0}=\frac{c}{\gamma} ; \quad \gamma=\sqrt{3\left(v^{2} / c^{2}-1\right)}>0 . \tag{39}
\end{equation*}
$$

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

$$
\begin{equation*}
U_{s}(\gamma)=\frac{\gamma}{6 \alpha^{2}}\left\{1-\frac{1 \mp 4}{15} \gamma^{2}+0\left(c^{5}\right)\right\} \tag{40}
\end{equation*}
$$

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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