Physics Letters A 381 (2017) 87–93

Contents lists available at ScienceDirect

Physics Letters A

www.elsevier.com/locate/pla

Improved models of dense anharmonic lattices

P. Rosenau *, A. Zilburg

School of Mathematical Sciences, Tel-Aviv University, Tel Aviv 69978, Israel

ARTICLE INFO

Article history:
Received 12 July 2016
Received in revised form 26 October 2016
Accepted 27 October 2016
Available online 2 November 2016
Communicated by C.R. Doering

Keywords:
Anharmonic lattices
Compactons
Improved PDE description
Quartic and Hertz potentials

ABSTRACT

We present two improved quasi-continuous models of dense, strictly anharmonic chains. The direct expansion which includes the leading effect due to lattice dispersion, results in a Boussinesq-type PDE with a compacton as its basic solitary mode. Without increasing its complexity we improve the model by including additional terms in the expanded interparticle potential with the resulting compacton having a milder singularity at its edges. A particular care is applied to the Hertz potential due to its non-analyticity. Since, however, the PDEs of both the basic and the improved model are ill posed, they are unsuitable for a study of chains dynamics. Using the bond length as a state variable we manipulate its dispersion and derive a well posed fourth order PDE.

1. Introduction

A wide variety of physical systems are described by anharmonic lattices that on the macroscopic length-scale involve many unit cells [1] and thus in a first approximation are modeled using the continuum limit given in terms of partial differential equation(s) (PDE), with the discrete effects being completely washed away. Since, however, with few notable exceptions [7], the continuum limit leads to gradients catastrophe, the leading effect due to the discreteness was retained to yield a quasi-continuum PDE description of the lattice. The resulting solitary mode – the compacton [2] – is an example of energy-storing, essentially nonlinear entity and is both of fundamental importance and of longstanding interest [1, 3–5,11]. Note that although, in principle, lattices governed by Newton's laws immediately spread any information posed over a finite domain, the purely anharmonic interparticle interaction creates a genuine screening effect beyond which there is no measurable excitation. In fact the quasi-continuum limit correctly predicts the main span of the discreton – the solitary solution of the anharmonic chain, which decays at a *doubly exponential rate*.

In spite of the desired features of the compacton, the underlying PDE model hardly solves our quest for an analytically accessible model to study interactions on the lattice. For not only is the expansion not asymptotic and its utility unknown a priori, but the PDE itself is ill posed (occasionally referred to as a bad-Boussinesq Equation). Its main use was to extract an approximate shape of the underlying compacton to be used as an input in the original lattice.

Yet the fundamental importance of the dynamics on the lattice and, apart from few exceptions, our inability to analyze it, makes it highly desirable to derive a usable model. Note that the asymptotic procedure devised by Kruskal which resulted in the rebirth of the KdV, is applicable only to weakly anharmonic lattices. With these issues in mind we reexamine a class of purely and almost purely anharmonic lattices and demonstrate how a judicious use of the expanded interparticle potential and the discreteness begets equations with compactons which have an improved level of regularity and provide a better rendition of their discrete antecedents. However, to overcome the ill-posedness of the PDE models based on a direct expansion, we adopt another maneuver which begets a well posed fourth order PDE (capable of handling two sided propagation and head on collisions) which is then optimized for the best L^1 fit of its solitary waves with their discrete antecedents. This approach has two main drawbacks, it is limited to 1-D chains and the tails decay at the conventional exponential rate missing the screening effect of their discrete antecedents.

In passing we stress again that our goal is not to duplicate the discrete profile of traveling waves (an exact solution profile can be computed following [13], see also the Appendix) but to derive a better PDE model of lattices dynamics which hopefully will enable a better handle on lattices dynamics. In fact with few notable exceptions the dynamics of nonlinear dense chains is beyond our ability to analyze it and apart from brute force simulation of the lattice, modelization via a PDE seems at this time to be the only tool available to us.

* Corresponding author.
E-mail address: rosenau@post.tau.ac.il (P. Rosenau).

http://dx.doi.org/10.1016/j.physleta.2016.10.051

2. Equations of motion and PDE approximation

Consider the Hamiltonian

$$H_{\text{disc}} = h\left\{\sum_{n=-N}^{N}\frac{\rho \dot{y}_n^2}{2} + P\left(\tfrac{y_{n+1}-y_n}{h}\right)\right\} \tag{1}$$

describing a chain of $2N+1$ particles of equal density $\rho = m/h$, equal spatial separation h and P being the interaction potential.

The equations of motion are

$$\ddot{y}_n = \tfrac{1}{h}\left[P'\left(\tfrac{y_{n+1}-y_n}{h}\right) - P'\left(\tfrac{y_n-y_{n-1}}{h}\right)\right] \tag{2}$$

or for $u_n = \frac{y_n - y_{n-1}}{h}$

$$\ddot{u}_n = \frac{1}{h^2}\left[P'(u_{n+1}) - 2P'(u_n) + P'(u_{n-1})\right]. \tag{3}$$

To approximate by a continuum we fix the total length $L = 2Nh$ while letting $h \downarrow 0$ (and hence $N \uparrow \infty$) which yields the continuum limit

$$H_{\text{cont}} = \int\left\{\frac{\rho y_t^2}{2} + P(y_x)\right\} dx. \tag{4}$$

We eliminate ρ by rescaling t yielding a nonlinear wave equation

$$y_{tt} = \tfrac{\partial}{\partial x}P'(y_x), \quad P'(S) \geq 0. \tag{5}$$

In the strict continuum limit not only do the solitary waves observed on a lattice disappear but, as is well known, for any reasonable initial excitation, the second derivatives of solutions may become infinite in a finite time for it is the dispersion due to the discrete lattice which prevents this blow-up, *hence its singular effect on the dynamics.* The nonlinear spatial gradients are a major change from the linear wave equation; for now we are in a realm typical for quasilinear wave equations.

So the issue facing us is to construct an equation which incorporates the discrete effects in an adequate manner. However, since the problem is essentially nonlinear which amounts to saying that it has no phonons, there is no weakly nonlinear regime and an asymptotic expansion associated with it. With that in mind, we expand the potential $P\left(\frac{y_{n+1}-y_n}{h}\right)$ in h (see Eq. (10)). Keeping the leading order correction and assuming $P''(s) \geq 0$ and smooth we get

$$y_{tt} = \tfrac{\partial}{\partial x}P'(y_x) + \tfrac{h^2\partial}{12\partial x}\left[\sqrt{P''(y_x)}\tfrac{\partial}{\partial x}\sqrt{P''(y_x)}y_{xx}\right] + \mathcal{O}(h^4). \tag{6}$$

Define $u = y_x$, $\beta = h^2/12$, differentiate once and rescale

$$(x,t) = (\sqrt{\beta}z, \sqrt{\beta}\tau) \tag{7}$$

to obtain

$$u_{\tau\tau} = \tfrac{\partial^2}{\partial z^2}P'(u) + \tfrac{\partial^2}{\partial z^2}\left[\sqrt{P''(u)}\tfrac{\partial}{\partial z}\sqrt{P''(u)}u_z\right]. \tag{8}$$

Unfortunately, Eq. (8) has two flaws

1) It is ill posed.
2) The expansion leading to Eq. (8) is not asymptotic.

The first feature is well known and can be deduced either by inspecting the extended Hamiltonian

$$H_{\text{qc}} = \int\left\{\frac{\rho y_t^2}{2} + P(y_x) - \frac{h^2}{24}P''(y_x)(y_{xx})^2\right\} dx \tag{9}$$

which unlike its discrete antecedent is no longer bounded from below, or by inspection of the linearized dispersion. Actually this fact is by now well known, and for $P''(s) \sim const.$ the resulting equation of motion is referred to as the "bad" Boussinesq equation [14,15]. Originally it has already emerged in the very first analytical treatment of the FPU problem by Kruskal wherein P was a cubic polynomial and the nonlinearity was assumed to be weak. This resulted in $P'' \sim const.$ rendering the leading fourth order term linear. Kruskal circumvented the ill-posedness by deriving the one sided KdV equation as a leading asymptotic approximation of the weakly nonlinear regime. However, surprisingly enough, in the present genuinely nonlinear case there is no small parameter. In fact, the scaling which eliminates h in (8) eliminates h in all higher order terms of the expansion as well! The size of h is thus irrelevant and the problem has no genuinely small parameter. The termination of the expansion at any level beyond the strict continuum, as done for example in Eq. (6), can be judged only a posteriori according to its utility in describing the sought after phenomena. That being the case, one may turn things around and rather than to terminate the expansion at a given power of h, to terminate it *at a given level of complexity*, which in the present context will mean that no derivatives of order higher than the second will be kept in the Hamiltonian. Consequently, the resulting equation of motion shall have no derivatives of order higher than fourth. To carry out this program we expand the potential. Integration by parts and elimination of null divergences begets

$$\begin{aligned}
&P\left(\tfrac{y_{n+1}-y_n}{h}\right) \Rightarrow P(y_x) + \\
&+ a_2h^2P''(y_{xx})^2 + a_4h^4P^{(4)}(y_{xx})^4 + a_6h^6P^{(6)}(y_{xx})^6 + \ldots \\
&+ b_2h^4P''(y_{3x})^2 + b_4h^8P^{(4)}(y_{3x})^4 + b_6h^{12}P^{(6)}(y_{3x})^6 + \ldots \\
&+ c_2h^6P''(y_{4x})^2 + \ldots \\
&+ \ldots
\end{aligned} \tag{10}$$

where $a_2 = -1/24$, $a_4 = -1/(10 \cdot 24^2)$, $b_2 = 1/6!$, etc. Clearly this expansion assumes an analytic P. In the following we will present two concrete examples: one where this assumption is satisfied and another where it is not [6] and further measures should be taken. If P is a polynomial of order 2K, $P^{(2K+1)} = 0$ and each row terminates after K terms. First row terms render a fourth order term in the PDE, the second row begets a sixth order term, and so on. To keep complexity in check we shall not venture beyond a fourth order PDE, which amounts to using only the first row in the expansion of P. First, let us define

$$P_{2m} \doteq P(y_x)^{(2m)} \quad \text{and} \quad \tilde{a}_{2m} \doteq (2m-1)a_{2m}.$$

Thus

$$P\left(\tfrac{y_{n+1}-y_n}{h}\right) \cong P(y_x) + \sum_{m=1}\frac{\tilde{a}_{2m}h^{2m}}{2m-1}P_{2m}(y_{xx})^{2m}. \tag{11}$$

$$\begin{aligned}
2m&\left\{P_{2m}^{\frac{2m-1}{2m}}(y_{xx})^{2m-2}\tfrac{\partial}{\partial x}\left(y_{xx}P_{2m}^{\frac{1}{2m}}\right)\right\} \\
&\qquad = \frac{1}{y_{xx}}\tfrac{\partial}{\partial x}\left[(y_{xx})^{2m}P_{2m}\right]
\end{aligned} \tag{12}$$

which enables to represent the resulting equation of motion in the form

$$y_{tt} = \tfrac{\partial}{\partial x}P'(y_x) - \tfrac{\partial}{\partial x}\frac{1}{y_{xx}}\tfrac{\partial}{\partial x}\sum_{2m}\tilde{a}_{2m}h^{2m}\left[(y_{xx})^{2m}P_{2m}\right]. \tag{13}$$

Rescaling à la (7), we have in terms of $u = y_x$