Pressure Fronts in 1D Damped Nonlinear Lattices

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The propagation of pressure fronts (impact solutions) in 1D chains of atoms coupled by anharmonic potentials between nearest neighbor and submitted to damping forces preserving uniform motion, is investigated. Travelling fronts between two regions at different uniform pressures are found numerically and well approximate analytically. It is proven that there are three analytical relations between the impact velocity, the compression, the front velocity and the energy dissipation which only depend on the coupling potential and are independent of the damping. Such travelling front solutions cannot exist without damping.

I. THE MODEL

This study was motivated for understanding sonoluminescence (see refs. 1,2) observed for example when water saturated with rare gas is submitted to an intense ultrasonic field. Spherical bubbles of rare gas expand and collapse periodically at supersonic or nearly supersonic speed emitting simultaneously a short and intense broadband light pulse at impact on the bubble core (sonoluminescence). We suggested more generally that light emission is systematically generated at strong enough impacts still below the range for generating plasmas at impact on the bubble core (sonoluminescence). We suggested more generally that light emission is systematically generated at strong enough impacts still below the range for generating plasmas but providing they become highly nonlinear. This situation occurs when the hard core of the atoms (which prevent volume elements to become negative), is involved that is for supersonic or nearly supersonic impacts. We suggest now a new remark for amending our early theory. Since condensed matter is made of bonded charged particles, sharp accelerations of these charges at strong enough impact may be sufficient to generate an intense (Abrahams-Lorentz) electromagnetic (em) radiation visible as sonoluminescence and generating damping (note that a charged hard sphere model would produce a diverging radiation!). We do not discuss here the physical validity of this suggestion but we only focus on some preliminary mathematical aspects of shocks in simple 1D model with damping.

FPU lattices are 1D chains of atoms coupled by anharmonic springs with Hamiltonian

$$\mathcal{H} = \sum_n \left( \frac{1}{2} p_n^2 + V(u_{n+1} - u_n) \right)$$

where $u_n(t)$ is the scalar coordinate of atom $n$, $p_n = \dot{u}_n$ is the associated conjugate variable and $V(v)$ is the coupling potential which depends on the distance $v_n = u_{n+1} - u_n$ between nearest neighbor atoms $n + 1$ and $n$.

We are interested in moving pressure fronts between two regions at different pressure obtained from initial conditions corresponding to an impact which are for example: $u_n(0) = n v$ and $\dot{u}_n(0) = -V_P$ for $n > 0$, $\dot{u}_n(0) = +V_P$ for $n < 0$ and $u_0(0) = 0$. The chain at equilibrium is initially moving uniformly for positive $n$ and at the opposite velocity for negative $n$ ($V_P$ is the impact velocity). Since by symmetry arguments, atom 0 remains immobile at all time ($u_0(t) = 0$), it is equivalent to consider that the positive part of the chain $n > 0$) impacts a fixed rigid wall at $u_0(0) = 0$ or in the framework of the center of mass of the half chain that atom 0 in the chain initially at rest is pushed by a piston $u_0(t) = V_P t$. Studies were already devoted to pressure fronts in lattice models without damping3,4. The same model with damping preserving uniform motion (as in for a Toda potential) is described by eqs.

$$\ddot{u}_n - \gamma (\dot{u}_{n+1} + \dot{u}_{n-1} - 2\dot{u}_n) - V'(u_{n+1} - u_n) + V'(u_n - u_{n-1}) = 0 \quad \text{or} \quad (2)$$

$$\ddot{v}_n - \gamma \Delta \dot{v}_n - \Delta V'(v_n) = 0 \quad (3)$$

where operator $\Delta$ is defined by $\Delta F_n = F_{n+1} + F_{n-1} - 2F_n$ and $\gamma > 0$ is the damping constant. A solution of eq(3) is $u_n(t) = v$ where $v$ is an arbitrary constant. The linearized equations for $|v_n(t) - v|$ small at $\gamma = 0$, yield plane wave solutions $v_n(t) = v + A \cos(qn - \omega(q)t - \alpha)$ where $\omega^2(q) = 4V''(v) \sin^2 q/2 \approx s^2(v)q^2$ for small $q$. For avoiding more complex situations where the front breaks into several fronts (phase separation), it is convenient (and physically reasonable) to assume that the square of the sound velocity $s^2(v) = V''(v)$ is a monotone decreasing function of $v$ that is $V''(v) < 0$. 

II. CONTINUOUS MODEL

Since continuous model are often used for describing fluids, we investigate first the continuous version of this model which will appear physically inconsistent but nevertheless will reveal interesting features. Assuming \( |u_{n+1} - u_n| \) small that is \( u_n(t) \) is a slowly varying function of \( n = x \) (while the variation of \( u_n(t) \) is not necessarily small), the PDE

\[
\begin{align*}
\frac{\partial^2 u}{\partial x^2} - \gamma \frac{\partial^3 u}{\partial x \partial t} - \frac{\partial \mathcal{V}'(\partial u)}{\partial x} &= 0 \\
\frac{\partial^2 v}{\partial x^2} - \gamma \frac{\partial^3 v}{\partial x \partial t} - \frac{\partial^2 \mathcal{V}'(v)}{\partial x^2} &= 0
\end{align*}
\]

(4)

(5)
describes \( u_n(t) = u(x, t) \) or \( v_n(t) = v(x, t) = \frac{\partial u}{\partial x} \). Eq. 4 exhibits exact step front solutions \( u(x, t) = u_{-\infty} + (v_{+\infty} - v_{-\infty})Y(x - ct) \) (with fast variation!) corresponding to \( u(x, t) = u_{-\infty} + (v_{+\infty} - v_{-\infty})(x - ct)Y(x - ct) \). \((Y(x) \) is the Heavyside function \((Y(x) = 0 \) for \( x < 0 \) and \( Y(x) = 1 \) for \( x > 0 \)). The square of the front velocity \( c \)

\[
e^2(v_{-\infty}, v_{+\infty}) = \frac{\mathcal{V}'(v_{+\infty}) - \mathcal{V}'(v_{-\infty})}{v_{+\infty} - v_{-\infty}}
\]

(6)
is a only function of the atomic compression at infinities \( v_{+\infty} \) and \( v_{-\infty} \). The difference \( V_P = \dot{u}(-\infty, t) - \dot{u}(+\infty, t) \) is the impact velocity

\[
V_P = c(v_{+\infty} - v_{-\infty})
\]

(7)

Considering the energy of a finite but long part of the chain containing the front \( \Phi(t) = \int_{-L}^{L} (\frac{1}{2}\dot{u}^2 + \mathcal{V}(\frac{\partial u}{\partial x})) \) \( dx \), we readily obtain for any solution \( u(x, t) \) of eq 4 with smooth second derivatives that the rate of energy variation of the system per unit time \( \dot{\Phi} = \dot{\Phi}_0 \) where \( \dot{\Phi}_0 = \mathcal{V}'(u(L, t))\dot{u}(L, t) - \mathcal{V}'(u(-L, t))\dot{u}(-L, t) \) is the power delivered by the pressure at the edge of the system (energy conservation). When the second derivatives of \( u(x, t) \) are not smooth but involve Dirac functions, there is generally no energy conservation! An explicit calculation of the energy \( \Phi \) for the step front solution (using eq. 8) yields the dissipated power

\[
D = \dot{\Phi} - \dot{\Phi}_0 = -c \left( \mathcal{V}(v_{+\infty}) - \mathcal{V}(v_{-\infty}) - \frac{1}{2}(v_{+\infty} - v_{-\infty})(\mathcal{V}'(v_{+\infty}) + \mathcal{V}'(v_{-\infty})) \right)
\]

(8)

which may be written again in a simpler form as

\[
D = \frac{c}{4}(v_{+\infty} - v_{-\infty})^3S(v_{+\infty}, v_{-\infty})
\]

(9)

where \( S(x, y) = \frac{\partial R(x, y)}{\partial x} \) is the x-derivative of \( R(x, y) \) defined by the equation \( \mathcal{V}(x) = \mathcal{V}(y) + (x - y)\mathcal{V}'(y) + \frac{1}{2}(x - y)^2(\mathcal{V}''(y) + R(x, y)) \). We remark that

\[
R(x, y) = \frac{x - y}{3} \int_{y}^{x} \left[ \int_{y}^{\xi_2} \left( \int_{y}^{\xi_1} \mathcal{H}''(\xi) d\xi \right) d\xi_2 \right] d\xi_1
\]

is non vanishing only when potential \( \mathcal{V} \) is anharmonic. Then, the above assumption \( \mathcal{V}''(x) \) negative readily implies \( (x - y)R(x, y) < 0 \) and \( (x - y)S(x, y) < 0 \). Thus, we have spontaneous energy dissipation when \( c(v_{+\infty} - v_{-\infty}) > 0 \) or energy creation in the opposite case!

Because of this lack of energy conservation, this continuous model is not physically acceptable for a correct description of impacts. Where this energy would go (or come from)? This continuous equation at zero damping has another flaw we do not detail here. There are smooth initial conditions which spontaneously develop a singularity (a divergence of the derivative \( \frac{\partial u}{\partial x}(x, t) \)) within a finite time by the standard Rankine-Hugoniot mechanism. Actually, the pressure fronts in lattice models without damping are not step-like but exhibit a puzzling behavior with an expanding intermediate region and backward oscillations extending to \(-\infty\) where nearest neighbor atoms are in antiphase. Despite the inconsistencies of this continuous model, we prove now that formula 7, 8 and 9 which relates the impact velocity \( V_P = -\dot{u}_{+\infty} + \dot{u}_{-\infty} \), the compression \( v_{+\infty} \) and \( v_{-\infty} \) at infinity, the front velocity \( c \) and the power dissipated by the front, are the same for the discrete case when damping is present but independently of this damping.
III. PRESSURE FRONTS IN DISCRETE MODEL: EXACT RELATIONS

We assume in the discrete model with $\gamma > 0$, there are travelling front solution $v_n(t) = g(n - ct)$ described by a smooth steplike hull function $g(x)$ fulfilling $\lim_{x \to -\infty} g(x) = v_{\infty}$, $\lim_{x \to \infty} g'(x) = 0$ and

$$c^2 \ddot{g}'' + \gamma c \Delta g'(x) - \Delta \nabla' g(x) = 0$$

(10)

(Operator $\Delta$ is defined by $\Delta F(x) = F(x+1) + F(x-1) - 2F(x)$.)

For proving eq.10 we consider the length $L_{-N,+N}(t) = u_N(t) - u_{-N}(t) = \sum_{n=-N}^{N-1} v_n(t) = \sum_{n=-N}^{N-1} g(n - ct)$ of the chain between far sites $-N$ and $+N$. We have $\lim_{n \to \infty} L_{-N,+N}(t) = \lim_{n \to \infty} (u_N(n) - u_{-N}(n)) = \dot{u}_{\infty} = -V_F$. Otherwise, because of the existence of the hull function $g(x)$, the rate of variation of the length $c(L_{-N,+N}(t+1/c) - L_{-N,+N}(t))$ between time $t$ and $t + 1/c$ is also equal to $c(\dot{g}(N - ct) + g(-N - 1 - ct)) = c(-v_{N} + v_{N-1})$. Then, $\lim_{n \to \infty} \left(L_{-N,+N}(t)\right) = -c(v_{\infty} - v_{-\infty}) = -V_F$ which yields eq.10.

For proving eq.9 we consider the momentum $M_{-N,+N}(t) = \sum_{n=-N}^{N-1} \dot{u}_n(t)$ of the chain between far sites $-N$ and $+N$. Eq.8 yields $\dot{M}_{-N,+N} = \gamma (\dot{v}_{N} - \dot{v}_{N-1}) + \dot{\gamma} V_{-N}(v_{N}) - \dot{\gamma} V_{-N}(v_{N-1})$ and then $\dot{M} = \lim_{n \to \infty} \dot{M}_{-N,+N} = \dot{M}'(v_{\infty}) - \dot{M}'(v_{-\infty})$.

Finally, for proving eq.11 we consider the energy of the chain $\Phi_{-N,+N} = \sum_{n=-N}^{N-1} \frac{1}{2} \dot{u}_n^2 + \sum_{n=-N}^{N-1} V(u_{n+1} - u_{n})$ between sites $-N$ and $+N$. We readily obtain $\dot{\Phi}_{-N,+N} = \sum_{n=-N}^{N-1} \dot{u}_n^2 + \sum_{n=-N}^{N-1} \dot{V}(u_{n+1} - u_{n})$ of the energy provided by the external pressure to the finite chain. We have for the infinite chain $\dot{\Phi}_{-N,+N} = \dot{M}'(v_{\infty})\dot{u}_{\infty} + \dot{M}'(v_{-\infty})\dot{u}_{-\infty}$. Then, using eq.2 we readily obtain $\dot{\Phi}_{-N,+N} - \dot{\Phi}_{-N,+N} = -\gamma \sum_{n=-N}^{N-1} (\dot{u}_{n+1} - \dot{u}_n)^2 + (\dot{u}_{N+1} - \dot{u}_N)\dot{u}_{N} - (\dot{u}_{N} - \dot{u}_{N-1})\dot{u}_{N-1}$ since $\lim_{n \to \infty} \dot{u}_{N+1} = 0$, we obtain that the power dissipated by the damping force in the infinite system $D = \lim_{n \to \infty} (\dot{\Phi}_{N,+N} - \dot{\Phi}_{-N,+N}) < 0$ is

$$D = -\gamma \sum_{n=-\infty}^{\infty} (\dot{u}_{n+1} - \dot{u}_n)^2$$

(11)

This dissipate power may be calculated differently since we assume that the solution is described by a hull function $v_n(t) = g(n - ct)$ implying $\dot{u}_n = F(n - ct)$. Then, we have $\Phi_{-N,+N}(t) = \sum_{n=-N}^{N-1} \frac{1}{2} \dot{u}_n^2 + \sum_{n=-N}^{N-1} V(u_{n+1} - u_{n})$ so that we readily obtained similarly as above, the rate of variation over an interval of time $1/c$ of the energy $c(\Phi_{-N,+N}(t+1/c) - \Phi_{-N,+N}(t)) = c\left(\dot{V}(F(-N - 1 - ct) - F(N - 1 - ct)) + \dot{V}(g(-N - 1 - ct)) - \dot{V}(g(N - 1 - ct))\right)$ which for $N \to +\infty$ becomes $c\left(\dot{u}_{\infty} - \dot{u}_{-\infty}\right) + \dot{V}(v_{-\infty}) - \dot{V}(v_{+\infty}) = \Phi = \lim_{n \to \infty} \dot{\Phi}_{-N,+N}$ which is time constant. Consequently, we obtain for the infinite chain, $D = \dot{\Phi} - \dot{\Phi}(0) = c\left(\dot{u}_{-\infty} - \dot{u}_{\infty})(\dot{u}_{-\infty} + \dot{u}_{\infty}) + \dot{V}(v_{-\infty}) - \dot{V}(v_{+\infty})\right) - \dot{V}(v_{-\infty})\dot{u}_{-\infty} + \dot{V}(v_{+\infty})\dot{u}_{+\infty}$. Using $V_F = \dot{u}_{-\infty} - \dot{u}_{+\infty}$ and eq.7 and 8 the dissipated power $D$ defined by eq.11 is found to fulfill eq.8.

As a consequence, there is no stationary travelling front solutions $g(x)$ in the harmonic system with damping $\gamma \neq 0$ because eq.8 yields $D = 0$ while eq.11 yields $D \neq 0$. There is also no stationary travelling front solutions when the system is anharmonic and $\gamma = 0$ because eq.8 yields $D \neq 0$ while eq.11 yields $D = 0$. Otherwise, since $D$ has to be negative, front solutions may only exist when they propagate from larger toward the lower pressure region ($c > 0$ when $v_{-\infty} < v_{\infty}$).

Assuming the existence of a hull function, $g(x)$, it is straightforward to extend the same proofs for formulae 9, 10 and 11 to any other kind of damping forces preserving the uniform motion of the chain for example the Abrahams-Lorentz force proportional to the third time derivative $\ddot{u}_n$. 

obtained as the separatrix solution of this equation such that the rate of convergence slows down while the stationary front solution develops backward oscillations which diverges. At strong damping the damping constant \( \gamma > 0 \) is non zero, \( T^p(X) \) systematically converges for \( p \rightarrow +\infty \) to a fixed point which corresponds to a solution \( v_n(t) = g(n - ct) \). Plots of an example of calculation of this hull function is shown fig. 1 for several damping constants. At strong damping \( \gamma \approx > 1 \), convergence is obtained within few iterations only and the hull function is step like. For smaller damping, the rate of convergence slows down while the stationary front solution develops backward oscillations which diverges at \( \gamma = 0 \). At zero damping, there is no convergence at all. Actually, this problem was already investigated in the literature.

At nonvanishing damping, \( g(x) \) may be well approximate as a solution of a differential equation describing an anharmonic oscillator with damping. We apply operator \( 1 - Q \) where \( Q = Q(z) \) with \( Q(z) = 1 - \frac{2z^2}{2/(\cosh z - 1)} = \sum_{n=0}^{\infty} \frac{z^n}{2n+1} \) to the left member of eq.10. Since \( \Delta = L(\frac{dz}{dx}) \) where \( L(z) = \frac{2z^2}{1-Q(z)} \), eq.10 becomes \( \frac{dz}{dx} (c^2(1-Q)g + \gamma cg' - \mathcal{V}'(g)) = 0 \) and after two integrations \( c^2Qg - \gamma cg' + \mathcal{V}'(g) = -c^2g^2 - bg \). Since we search for (physical) solutions \( g(x) \) which are bounded at \( \pm \infty \), we must have \( a = 0 \). Then, defining potential \( \mathcal{W}(g) = \mathcal{V}(g) - \frac{1}{2}c^2g^2 - bg \), eq.11 takes the form

\[
\begin{align*}
c^2Qg - \gamma cg' + \mathcal{W}'(g) &= 0 \\
c^2g'' - \gamma cg' + \mathcal{W}'(g) &\approx 0
\end{align*}
\]

for the lowest order approximation \( Q(z) \approx \frac{1}{17} z^2 \). Eq.13 may be viewed as the equation of a negatively damped particle with coefficient \( -\gamma \) and mass \( c^2/12 \) in the effective potential \( \mathcal{W}(g) \). There are non diverging solutions for \( x \rightarrow \pm \infty \) only when \( \mathcal{W}(g) \) has at least two extrema and then the solution is asymptote to each of these extrema. Actually since \( \mathcal{W}'(g) = \mathcal{V}'(g) - c^2 \) is monotone decreasing, \( \mathcal{W}(g) \) has at most a maximum at \( g = v^\pm_\infty \) and a minimum at \( g = v_\infty \) which are determined by \( b \) and \( c^2 \) and then eq.6 is fulfilled. Fig. 1 (right) shows a fit of the hull function obtained as the separatrix solution of this equation such that \( \lim_{x \rightarrow -\infty} g(x) = v_\infty \) is the minimum of \( \mathcal{W}(x) \) and

**IV. NUMERICAL CALCULATION OF PRESSURE FRONTS**

The hull function \( g(x) \) at nonvanishing damping can be numerically calculated at computer accuracy. We start form initial conditions where a half chain is at rest \( u_n(0) = \frac{n}{v^+_{\infty}} \) and \( u_n(0) = 0 \) for \( n > 0 \) while the edge site \( u_0(t) = V_Pt \) is constrained to have a uniform motion at velocity \( V_P > 0 \) (piston or impact velocity). The front velocity \( c(V_P, v^+_{\infty}) \) is determined as a function of the impact velocity \( V_P \) and \( v^+_{\infty} \) through eqs.\( \color{red}{6} \) and \( \color{red}{7} \) which yields the implicit equation \( c = (\mathcal{V}'(v^+_{\infty}) - \mathcal{V}'(v^+_{\infty} - V_P/c))/V_P \). It is a monotone increasing function of \( V_P \) because \( \mathcal{V}'' \) is assumed to be monotone decreasing. At \( V_P = 0 \), \( c^2(0, v^+_{\infty}) = \mathcal{V}'(v^+_{\infty}) = s^2(v^+_{\infty}) \) becomes the sound square velocity. The map

\[
\begin{align*}
\{v_n+1(1/c) \} \\
\{\bar{v}_n+1(1/c) \}
\end{align*}
\]

defined by integration of eq.\( \color{red}{2} \) or \( \color{red}{3} \) over the period of time \( 1/c \) and a shift of the indices, is iterated by numerically from the initial conditions \( X \) defined above. It is found that when the damping constant \( \gamma > 0 \) is non zero, \( T^p(X) \) systematically converges for \( p \rightarrow +\infty \) to a fixed point which corresponds to a solution \( v_n(t) = g(n - ct) \). Plots of an example of calculation of this hull function is shown fig. 1 for several damping constants. At strong damping \( \gamma \approx > 1 \), convergence is obtained within few iterations only and the hull function is step like. For smaller damping, the rate of convergence slows down while the stationary front solution develops backward oscillations which diverges at \( \gamma = 0 \). At zero damping, there is no convergence at all. Actually, this problem was already investigated in the literature.

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\[
\lim_{x \to +\infty} g(x) = v_{+\infty}
\]
is the maximum. The error is negligible at large \( \gamma \) but appears mostly as a phase shift in the tail for small \( \gamma \) visible fig.1 right.

In summary, the most important result of this paper is that the energy dissipated at an impact is independent of the physical origin of the damping and of its value providing it preserves the translational motion of the system (as it should in physical models). It only depends through formula (9) on the anharmonic part of the potential between the compressions ahead and backward the front and is proportional to the front velocity. This result would formally determine the emitted power of sonoluminescence if one believes our physical interpretation. It is then straightforward to check that the emitted power is negligible for nearly harmonic impacts but in principle could approach 100% of the input power when \( \mathcal{V} \) is a hardcore potential diverging at some \( v_c < v \) and for strong impacts where \( v_{-\infty} \approx v_c \).

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