Fermi-Pasta-Ulam-Tsingou nonlinear lattice

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Boussinesq equation

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Korteweg – de Vries equation

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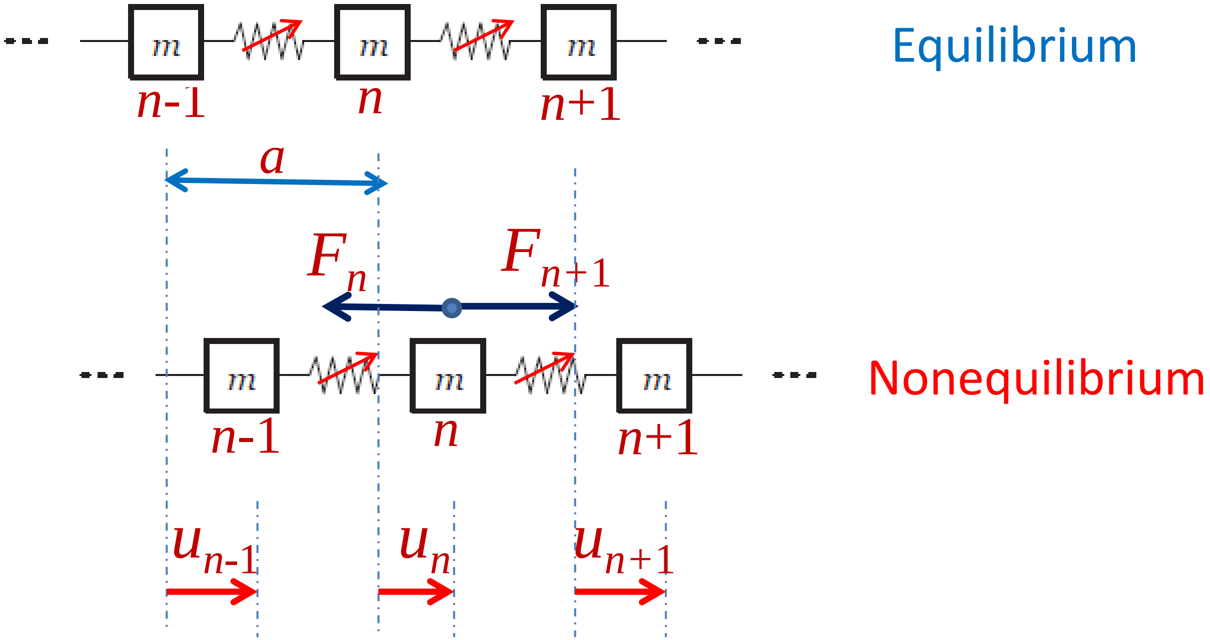
The Fermi-Pasta-Ulam-Tsingou lattice

Consider a nonlinear lattice with the **force law**: $\boxed{F = G(\Delta + \kappa\Delta^2)}$

where $\boldsymbol{\Delta}$ is the **displacement** between the masses, $\boldsymbol{G}$ is the **spring constant** and $\boldsymbol{\kappa}$ is the nonlinear coefficient.



- **Newton's 2nd law:** $\boxed{m\ddot{u}_n = -F_n + F_{n+1}}$

Force that particle ***i*-1** exerts on particle ***i***

Lattice dynamics - equations of motion

Newton's 2nd law:

Force law nonlinear response:

$$\left.\begin{aligned} m\ddot{u}_n &= -F_n + F_{n+1} \\ F_n &= G(u_n - u_{n-1}) + \kappa(u_n - u_{n-1})^2 \end{aligned}\right\} \Rightarrow$$

$$m\ddot{u}_n = -\left[G(u_n - u_{n-1}) + \kappa(u_n - u_{n-1})^2\right] + G\left[(u_{n+1} - u_n) + \kappa(u_{n+1} - u_n)^2\right] \Rightarrow$$

$$m\ddot{u}_n = G\left(u_{n+1} - 2u_n + u_{n-1}\right) + \kappa G \underbrace{\left[(u_{n+1} - u_n)^2 - (u_n - u_{n-1})^2\right]}$$

Simplifying the difference between the two squares, we obtain:

$$\boxed{m\ddot{u}_n = \underbrace{G\left(u_{n+1} - 2u_n + u_{n-1}\right)}_{\text{Linear discrete wave equation}} + \underbrace{\kappa G\left(u_{n+1} - 2u_n + u_{n-1}\right)\left(u_{n+1} - u_{n-1}\right)}_{\text{Nonlinear correction}}}$$

The continuous limit

As in the linear case, we seek for solutions of the nonlinear DDE:

$$m\ddot{u}_n = G\left(u_{n+1} - 2u_n + u_{n-1}\right) + \kappa G\left(u_{n+1} - 2u_n + u_{n-1}\right)\left(u_{n+1} - u_{n-1}\right)$$

with a ***width >> lattice spacing*** ***a*** $\rightarrow$ **continuum approximation**

We treat $x_n = na$ as a continuous variable, $x_n = na \rightarrow x$, so that:

$$u_n(t) \equiv u(x_n, t) = u(na, t) \rightarrow u(x, t)$$

We can then expand the solution in a **Taylor series**, around ***x***, as:

$$u_{n\pm1}(t) = u(n(a\pm1), t) = u(x\pm a, t)$$

$$\approx u(x,t) \pm u_x(x,t)a + \frac{1}{2}u_{xx}(x,t)a^2 \pm \frac{1}{6}u_{xxx}(x,t)a^3 + \frac{1}{24}u_{xxxx}(x,t)a^4 + O(a^5)$$

Keeping O(a^4) terms, the **nonlinear term of the DDE** is found as:

$$u_{n+1} - 2u_n + u_{n-1} \approx a^2 u_{xx} + \frac{a^4}{12}u_{xxxx}, \qquad u_{n+1} - u_{n-1} \approx 2au_x + \frac{a^3}{3}u_{xxx}$$

$$\left(u_{n+1} - 2u_n + u_{n-1}\right)\left(u_{n+1} - u_{n-1}\right) = 2a^3 u_x u_{xx} + O(a^5)$$

The Boussinesq equation

We thus obtain, at O(a^4), the following **nonlinear dispersive PDE**:

$$\boxed{u_{tt} - c^2\left(u_{xx} + \frac{a^2}{12}u_{xxxx} + 2\kappa a\, u_x u_{xx}\right) = 0,} \qquad \boxed{c^2 = Ga^2/m}$$

Using the transformation $w = u_x$ (where w is analogous to strain in continuous mechanics) we differentiate wrt. to x and obtain:

$$\left.\begin{array}{r} w_{tt} - c^2\left(w_{xx} + \frac{a^2}{12}w_{xxxx} + 2\kappa a\left(ww_x\right)_x\right) = 0 \\ ww_x = (1/2)\left(w^2\right)_x \end{array}\right\} \Rightarrow$$

$$\boxed{w_{tt} - c^2\left(w_{xx} + \frac{a^2}{12}w_{xxxx} + \kappa a\left(w^2\right)_{xx}\right) = 0}$$

Boussinesq equation

(derived by **Joseph Boussinesq (1871)** in the context of **shallow water waves**)

Boussinesq equation

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Korteweg – de Vries equation

Structure of the Boussinesq equation

We rewrite the Boussinesq equation in the general form:

$$u_{tt} - c^2 u_{xx} - \alpha u_{xxxx} - \beta (u^2)_{xx} = 0$$

In the FPUT lattice: $c^2 = Ga^2 / m, \quad \alpha = c^2 a^2 / 12, \quad \beta = \kappa a c^2$

The Boussinesq equation is a **bidirectional model** featuring both dispersion and (quadratic) nonlinearity:

$$\boxed{\underbrace{u_{tt} - c^2 u_{xx}}_{\text{2nd-order wave equation}} - \underset{\text{dispersion}}{\underset{\searrow}{\alpha u_{xxxx}}} - \underset{\text{nonlinearity}}{\underset{\searrow}{\beta (u^2)_{xx}}} = 0}$$

Dispersion relation: $D(k, \omega) = -\omega^2 + c^2 k^2 - \alpha k^4 = 0$

$$\boxed{\omega = \pm c k \left(1 - \frac{\alpha k^2}{c^2} \right)^{1/2} \qquad \text{± for right -or left-going waves}}$$

The long-wavelength approximation (I)

Dispersion relation: $D(k,\omega) = -\omega^2 + c^2k^2 - \alpha k^4 = 0$

$$\omega = \pm ck\left(1 - \frac{\alpha k^2}{c^2}\right)^{1/2}$$

± for right -or left-going waves

We focus on **right-going waves**, and consider **long waves and weak dispersion**, such that: $\underline{\alpha k^2/c^2 \ll 1.}$

Then, use the approximation:

$$(1 - \alpha k^2/c^2)^{1/2} \approx 1 - \alpha k^2/(2c^2)$$

and express the **dispersion relation** as:

$$\boxed{\omega \approx ck - \frac{\alpha}{2c}k^3}$$

The long-wavelength approximation (II)

Since the **dispersion relation** reads: $\omega \approx ck - \frac{\alpha}{2c}k^3$

the phase $\theta = kx - \omega t$ of the plane wave $u = u_0 \exp(i\theta)$

becomes: $\theta \approx kx - \left(ck - \frac{\alpha}{2c}k^3\right)t = \boxed{k(x-ct) + \frac{\alpha k^3}{2c}t}$

In compliance with our assumption for **long waves**, we now assume that **the wavenumber k is of the order $O(\varepsilon^p)$**, with $0 < \varepsilon \ll 1$ and $p > 0$.

The choice of p is not important as will be seen below, so we can **arbitrarily choose** $p = 1/2$.

The slow (or "stretched") variables

Substituting $\underline{k \to \epsilon^{1/2} k}$ in: $\theta \approx k(x - ct) + \frac{\alpha k^3}{2c} t$

we obtain:

$$\theta \approx k\left[\boxed{\epsilon^{1/2}(x - ct)}\right] - \frac{\alpha k^3}{2c}\left[\boxed{\epsilon^{3/2} t}\right]$$

This suggests the introduction of the **slow variables:**

$$\boxed{\xi = \epsilon^{1/2}(x - ct), \quad T = \epsilon^{3/2} t}$$

Next, **express the Boussinesq equation in terms of these slow variables** by using the chain rule:

$$\partial_x = \epsilon^{1/2} \partial_\xi, \quad \partial_t = -\epsilon^{1/2} c \partial_\xi + \epsilon^{3/2} \partial_T$$

The asymptotic expansion

In terms of ξ and T, the Boussinesq equation:

$$u_{tt} - c^2 u_{xx} - \alpha u_{xxxx} - \beta(u^2)_{xx} = 0$$

becomes:

$$\epsilon^3 u_{TT} - 2\epsilon^2 c u_{\xi T} - \epsilon^2 \alpha u_{\xi\xi\xi\xi} - \epsilon\beta(u^2)_{\xi\xi} = 0$$

As a final step, assume a **perturbation expansion of $u(x,t)$ with respect to** ε of the form:

$$u = \epsilon^q u_1 + \epsilon^{q+1} u_2 + \ldots, \quad q > 0$$

Substituting into the Boussinesq equation we obtain:

$$\epsilon^{3+q}(u_1 + \epsilon u_2 + \ldots)_{TT} - 2\epsilon^{2+q} c(u_1 + \epsilon u_2 + \ldots)_{\xi T}$$
$$-\epsilon^{2+q}\alpha(u_1 + \epsilon u_2 + \ldots)_{\xi\xi\xi\xi} - \epsilon^{2q+1}\beta\left(u_1^2 + 2\epsilon u_1 u_2 + \ldots\right)_{\xi\xi} = 0$$

Balance between dispersion-nonlinearity

Here, q **should not be chosen arbitrarily**: to derive the KdV, where dispersion and nonlinearity terms are **of the same order** **–a fact that gives rise to soliton solutions–** the **dispersion** and **nonlinearity** terms should also be of the same **order.**

$$\epsilon^{3+q}(u_1+\epsilon u_2+\ldots)_{TT}-2\epsilon^{2+q}c(u_1+\epsilon u_2+\ldots)_{\xi T}$$

$$\underbrace{-\epsilon^{2+q}\alpha(u_1+\epsilon u_2+\ldots)_{\xi\xi\xi\xi}}_{\text{dispersion terms}}\;\underbrace{-\epsilon^{2q+1}\beta\left(u_1^2+2\epsilon u_1u_2+\ldots\right)_{\xi\xi}}_{\text{nonlinearity terms}}=0.$$

- Leading-order **dispersion** term: $O(\epsilon^{2+q})$
- Leading-order **nonlinearity** term: $O(\epsilon^{2q+1})$

$$2+q=2q+1$$

Hence: $q=1$

The KdV equation

For $q = 1$, the equation:

$$\epsilon^{3+q}(u_1+\epsilon u_2+\ldots)_{TT} - 2\epsilon^{2+q}c(u_1+\epsilon u_2+\ldots)_{\xi T}$$
$$-\epsilon^{2+q}\alpha(u_1+\epsilon u_2+\ldots)_{\xi\xi\xi\xi} - \epsilon^{2q+1}\beta\left(u_1^2+2\epsilon u_1 u_2+\ldots\right)_{\xi\xi} = 0$$

becomes: $\underline{\cancel{\varepsilon^4 u_{1TT}} \boxed{-2\varepsilon^3 c u_{1\xi T} - \varepsilon^3 \alpha u_{1\xi\xi\xi\xi} - \varepsilon^3 \beta (u_1)_{\xi\xi}} = \cancel{O(\varepsilon^5)}}$

Thus, after an integration wrt. ξ, we obtain the **KdV equation:**

$$\boxed{2cu_{1T} + \alpha u_{1\xi\xi\xi} + 2\beta u_1 u_{1\xi} = 0}$$

To conclude, starting from the **FPU lattice**, we can derive – **in the continuum limit** – the **Boussinesq equation**; then, employing a **multiscale expansion method**, we can derive the **"far field"** of Boussinesq equation, i.e., **the KdV equation**

Some additional comments (I)

- We have introduced the slow variables

$$\xi = \epsilon^{1/2}(x - ct), \quad T = \epsilon^{3/2} t$$

based on the form of the **phase of plane waves** in the long-wavelength approximation.

- This choice is **consistent** with the **long-time behavior of the solution of the linearized Boussinesq equation**:

$$u(x,t) \approx \frac{f(0)}{\sqrt[3]{(3/2)\alpha t}} \mathrm{Ai}(z), \quad z \equiv \frac{x\text{-}ct}{\sqrt[3]{(3/2)\alpha t}}$$

- Thus, the proposed scales are the same along the **characteristics** $z = (x\text{-}ct)/t^{1/3} =$ **const.** of the solution as $t \to \infty$

Some additional comments (II)

- The **Boussinesq** equation is a **bidirectional model**, while the **KdV equation** is a **unidirectional** one.

- It can be shown that using the slow variables:

$$\xi = \epsilon^{1/2}(x - ct), \quad \eta = \epsilon^{1/2}(x + ct), \quad T = \epsilon^{3/2}t,$$

and the same asymptotic expansion as before,

$$u = \varepsilon u_1(\xi,\eta,t) + \varepsilon^2 u_2(\xi,\eta,t) + \ldots$$

One can derive, to the leading-order in ε, the equation:

$$u_1 = f(\xi) + g(\eta)$$

Superposition of a left- and a right-going wave

where:

$$\begin{aligned} 2cf_T + \alpha f_{\xi\xi\xi} + 2\beta f f_\xi &= 0 \\ -2cg_T + \alpha g_{\eta\eta\eta} + 2\beta g g_\eta &= 0 \end{aligned}$$

two KdV equations!