Nanopteron-Stegoton Traveling Waves in Mass and Spring Dimer Fermi-Pasta-Ulam-Tsingou Lattices

Timothy E. Faver & J. Douglas Wright

Drexel University

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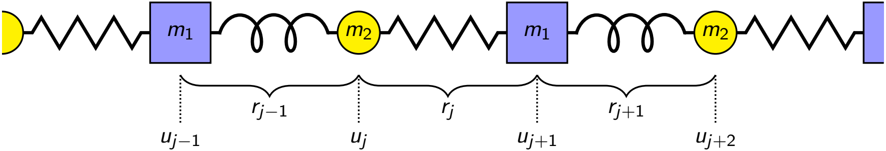
The dimer FPUT lattice



$$m_j = \text{mass of } j\text{th particle} = \begin{cases} m_1, & j \text{ is odd} \\ m_2, & j \text{ is even} \end{cases}$$

$$\begin{aligned} F_j(r) &= \text{force exerted by } j\text{th spring when stretched a distance } r \\ &= \varkappa_j r + \beta_j r^2 + \mathcal{O}(r^3) = \begin{cases} F_1(r), & j \text{ is odd} \\ F_2(r), & j \text{ is even} \end{cases} \end{aligned}$$

$$u_j = \text{position of } j\text{th particle}$$

$$r_j = \text{relative displacement} = u_{j+1} - u_j$$

Newton's law: $m_j \ddot{u}_j = F_j(u_{j+1} - u_j) - F_{j-1}(u_j - u_{j-1})$

Mass and spring dimers

Mass dimer

$$m_j = \begin{cases} w > 1, & j \text{ is odd} \\ 1, & j \text{ is even} \end{cases} \qquad F_j(r) = F(r) = r + r^2$$

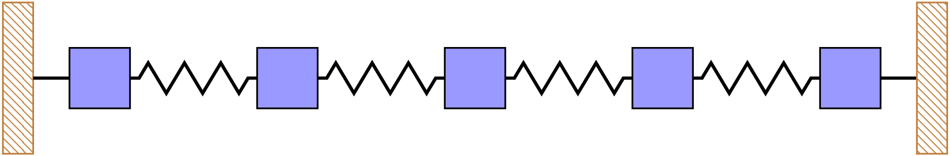
Spring dimer

$m_j = 1$

$F_{2j}(r) = r + r^2$

$F_{2j+1}(r) = \varkappa r + \beta r^2$
$\varkappa > 1$

• Fermi, Pasta, Ulam, & Tsingou (1955): numerical experiments suggest that the energy of finite monatomic lattices with *nonlinear* spring forces does not "thermalize" over long times but instead exhibits periodic "recurrence."



• Zabusky & Kruskal (1965+): the Korteweg-de Vries (KdV) equation

$$u_t + 6uu_x + u_{xxx} = 0$$

is a good *formal* "continuum limit" for monatomic FPUT.

- Friesecke & Wattis (1994): variational arguments establish that for certain wave speeds, the monatomic lattice has **solitary wave** solutions.

- Friesecke & Pego (1999): the monatomic lattice has solitary wave solutions for all speeds slightly greater than the lattice's "speed of sound."

- Schneider & Wayne (2000): solutions to certain KdV equations are good approximations to the solutions to the equations of motion for monatomic FPUT over long times.

- Gaison, Moskow, Wright, & Zhang (2014): solutions to certain KdV equations are good approximations to solutions of the equations of motion for **polymer** FPUT lattices over long times.

Theorem

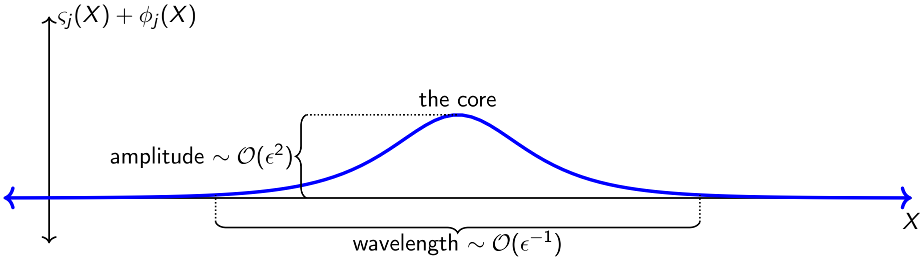
Let $\varkappa > 1$ and $\beta \neq -\varkappa^3$. There is a lower threshold $c_\varkappa > 0$ (the "speed of sound") such that for wave speeds c slightly greater than $c_\varkappa$, there is a traveling wave solution for the spring dimer equations of motion (in terms of relative displacement) with wave speed c as

$$r_j(t) = \underbrace{\text{exponentially decaying term}}_{\varsigma_j(j-ct)} + \underbrace{\text{periodic term}}_{\phi_j(j-ct)}.$$

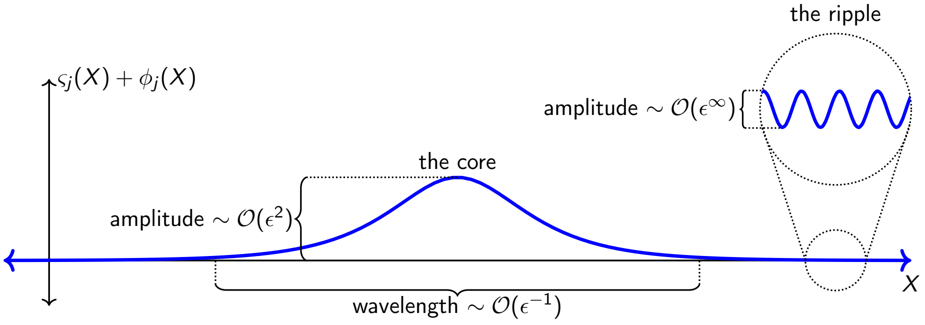
where

- ς_j is an exponentially decaying perturbation of a sech^2-type profile for a KdV traveling wave equation;
- ς_j has amplitude $\sim \epsilon^2 := c^2 - c_\varkappa^2$ and wavelength $\sim 1/\epsilon$;
- ϕ_j is periodic with amplitude small beyond all orders of ϵ and frequency $\mathcal{O}(1)$ in ϵ.

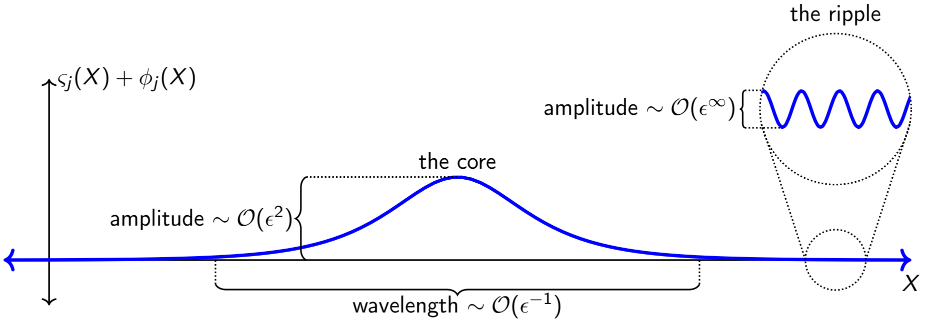
The nanopteron



The nanopteron



ϵ^∞ = small beyond all orders of ϵ

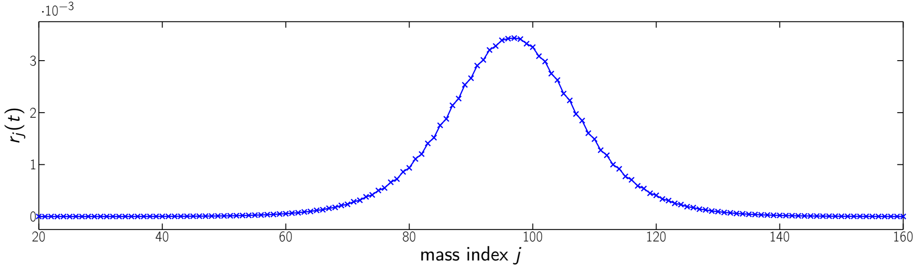


ϵ^∞ = small beyond all orders of ϵ

Boyd (1998): the **nanopteron** is a "coherent structure which approximately satisfies the classical definition of a solitary wave" and which "asymptotes to a small amplitude oscillation" at infinity (nanopteron = dwarf-wing = core + ripple).

Fix a time t. How do successive relative displacements, all at t, compare to each other?

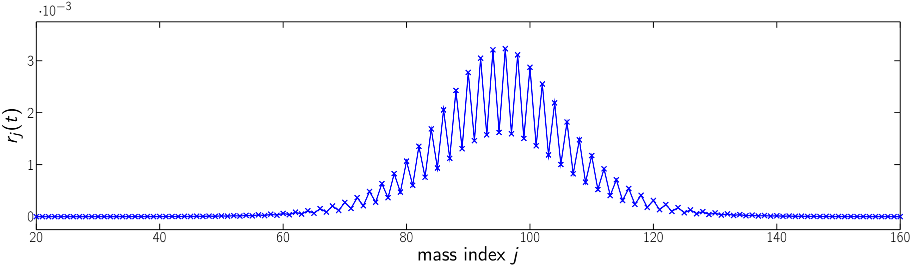
Mass Dimer



$$r_j(t) = C_w \epsilon^2 \operatorname{sech}^2(\epsilon(j - ct)) + \mathcal{O}(\epsilon^3)$$

Fix a time t. How do successive relative displacements, all at t, compare to each other?

Spring Dimer



$$r_j(t) = \varkappa^{((-1)^j+1)/2}\epsilon^2 \operatorname{sech}^2(\epsilon(j-ct)) + \mathcal{O}(\epsilon^3)$$

The traveling wave problem

Set

$$r_j(t) = \begin{cases} p_1(j - ct), & j \text{ is odd} \\ p_2(j - ct), & j \text{ is even}. \end{cases}$$

Newton's law for the lattice becomes

$$c^2 \partial_x^2 \mathbf{p} + L_\varkappa \mathbf{p} + L_\beta \mathbf{p}^{.2} = 0, \qquad \mathbf{p}(x) = \begin{pmatrix} p_1(x) \\ p_2(x) \end{pmatrix},$$

where the operators $L_\varkappa$ and L_β are Fourier multipliers constructed chiefly from shift operators.

An analysis of the eigenvalues of $L_{\varkappa}$ produces $c_{\varkappa} > 0$ with the property that if

$$\mathbf{p}(x) = \epsilon^2 \boldsymbol{\theta}(\epsilon x), \qquad \boldsymbol{\theta}(X) = (\theta_1(X), \theta_2(X)),$$

$$c^2 = c_\epsilon^2 := c_{\varkappa}^2 + \epsilon^2,$$

then we can diagonalize $L_{\varkappa}$ and make a "cancelation" in the p_1 equation to convert our system for the profiles $\mathbf{p}$ into

$$\boldsymbol{\Theta}_\epsilon(\boldsymbol{\theta}) = \underbrace{\begin{bmatrix} 1 & 0 \\ 0 & \mathcal{T}_\epsilon \end{bmatrix}}_{\mathcal{D}_\epsilon} \boldsymbol{\theta} + \mathcal{Q}_\epsilon(\boldsymbol{\theta}) = 0.$$

Here the operator $\mathcal{T}_\epsilon := \epsilon^2 c_\epsilon^2 \partial_X^2 + \lambda_+^\epsilon$ is **singularly perturbed**.

Taking $\epsilon = 0$ and defining the operator $\mathbf{\Theta}_0$ correctly, we find that for a certain sech^2-type KdV traveling wave solution σ, we have

$$\mathbf{\Theta}_0(\boldsymbol{\sigma}) = 0, \qquad \boldsymbol{\sigma} := \begin{pmatrix} \sigma \\ 0 \end{pmatrix}.$$

Can we solve $\mathbf{\Theta}_\epsilon(\boldsymbol{\theta}) = 0$ by perturbing from $\boldsymbol{\sigma}$? Try setting

$$\boldsymbol{\theta} = \boldsymbol{\sigma} + \boldsymbol{\xi},$$

where $\boldsymbol{\xi} = (\xi_1, \xi_2)$ is exponentially decaying.

We aim for a fixed point problem and find

$$\mathbf{\Theta}_\epsilon(\boldsymbol{\sigma} + \boldsymbol{\xi}) = 0 \iff \begin{cases} \xi_1 = -\sigma - \mathcal{Q}_{1,\epsilon}(\boldsymbol{\sigma} + \boldsymbol{\xi}) \\ \\ \mathcal{T}_\epsilon \xi_2 = -\mathcal{Q}_{2,\epsilon}(\boldsymbol{\sigma} + \boldsymbol{\xi}). \end{cases}$$

We can suss out a unique number ω_ϵ with the property that

$$\widehat{\mathcal{T}_\epsilon f}(\omega_\epsilon) = 0$$

for any function f. This means that $\mathcal{T}_\epsilon$ cannot be surjective (and thus is not invertible).

And if we want to solve

$$\mathcal{T}_\epsilon \xi_2 = -\mathcal{Q}_{2,\epsilon}(\boldsymbol{\sigma} + \boldsymbol{\xi}),$$

this forces $\boldsymbol{\xi}$ to satisfy the additional *third* equation

$$\mathfrak{F}[\mathcal{Q}_{2,\epsilon}(\boldsymbol{\sigma} + \boldsymbol{\xi})](\omega_\epsilon) = 0.$$

We resolve the problem of "two unknowns, three equations" by looking not for solitary waves but **nonlocal** solitary waves (**nanopterons**): instead of the ansatz

$$\boldsymbol{\theta} = \boldsymbol{\sigma} + \boldsymbol{\xi},$$

we let

$$\boldsymbol{\theta} = \boldsymbol{\sigma} + \boldsymbol{\varphi}_\epsilon^a + \boldsymbol{\eta},$$

where

- $\boldsymbol{\varphi}_\epsilon^a$ is periodic with amplitude $\sim a$ and solves $\boldsymbol{\Theta}_\epsilon(\boldsymbol{\varphi}_\epsilon^a) = 0$;
- $\boldsymbol{\eta} = (\eta_1, \eta_2)$ is an exponentially decaying remainder.

Then our three variables are a, η_1, and η_2.

We take this ansatz from Beale's work on exact traveling wave solutions for gravity-capillary waves (see also Amick & Toland).

Theorem

There exist $\epsilon_{\text{per}} > 0$ and $a_{\text{per}} > 0$ such that for all $\epsilon \in (0, \epsilon_{\text{per}})$ and $a \in (-a_{\text{per}}, a_{\text{per}})$, there is $\boldsymbol{\varphi}_\epsilon^a \in \mathcal{C}^\infty_{\text{per}} \times \mathcal{C}^\infty_{\text{per}}$ with $\boldsymbol{\Theta}_\epsilon(\boldsymbol{\varphi}_\epsilon^a) = 0$.

Proof. Bifurcation from a simple eigenvalue (Crandall-Rabinowitz-Zeidler).

We are solving

$$\boldsymbol{\Theta}_\epsilon(\boldsymbol{\sigma} + \boldsymbol{\varphi}_\epsilon^a + \boldsymbol{\eta}) = 0 \qquad (*)$$

for $a \in \mathbb{R}$ and $\boldsymbol{\eta} = (\eta_1, \eta_2)$ exponentially decaying, i.e.,

$$\eta_1, \eta_2 \in H_q^1 := \left\{ f \in H^1 \;\middle|\; \cosh(q\cdot)f \in H^1 \right\}.$$

Using the structure of our first perturbation attempt, we can successfully rewrite $(*)$ as a fixed point problem of the form

$$\boldsymbol{\mathcal{N}}_\epsilon(\boldsymbol{\eta}, a) = (\boldsymbol{\eta}, a).$$

Theorem

There exist $\epsilon_\star > 0$ and $q_\star > 0$ such that for all $\epsilon \in (0, \epsilon_\star)$, there exists a unique $(\boldsymbol{\eta}_\epsilon, a_\epsilon) \in \cap_{r=1}^\infty H_{q_\star}^r \times H_{q_\star}^r \times \mathbb{R}$ such that $\boldsymbol{\Theta}_\epsilon(\boldsymbol{\sigma} + \boldsymbol{\varphi}_\epsilon^{a_\epsilon} + \boldsymbol{\eta}_\epsilon) = 0$. Also, for all $r \in \mathbb{N}$, there is $C_r > 0$ such that $|a_\epsilon| \le C_r \epsilon^r$ for all $\epsilon \in (0, \epsilon_\star)$.

Questions for future consideration

1. How small is small? We know $|a_\epsilon| \leq C_r \epsilon^r$ for all $r \in \mathbb{N}$. Do we have

$$a_\epsilon = Ce^{-p/\epsilon}?$$

2. Is the ripple really there? Can we have $a_\epsilon = 0$?

3. The dreaded **general dimer**: what happens when masses **and** springs alternate?