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

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

\[ F_j(r) = \text{force exerted by } j\text{th spring when stretched a distance } r \]

\[ = \kappa_j r + \beta_j r^2 + \mathcal{O}(r^3) = \begin{cases} 
  F_1(r), & j \text{ is odd} \\
  F_2(r), & j \text{ is even}
\end{cases} \]

\[ u_j = \text{position of } j\text{th particle} \]

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

**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

\[
m_j = \begin{cases} 
  w > 1, & j \text{ is odd} \\
  1, & j \text{ is even}
\end{cases}
\]

\[F_j(r) = F(r) = r + r^2\]

Spring dimer

\[m_j = 1\]

\[F_{2j}(r) = r + r^2\]

\[F_{2j+1}(r) = \kappa r + \beta r^2\]

\[\kappa > 1\]
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.
Contemporary lattice results

• 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.
Main result for the spring dimer

Theorem

Let \( \kappa > 1 \) and \( \beta \neq -\kappa^3 \). There is a lower threshold \( c_\kappa > 0 \) (the “speed of sound”) such that for wave speeds \( c \) slightly greater than \( c_\kappa \), 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

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

\[ \xi_j(X) + \phi_j(X) \]

amplitude \( \sim \mathcal{O}(\epsilon^2) \)

wavelength \( \sim \mathcal{O}(\epsilon^{-1}) \)

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The nanopteron

\[ s_j(X) + \phi_j(X) \]

amplitude \( \sim \mathcal{O}(\epsilon^2) \)

wavelength \( \sim \mathcal{O}(\epsilon^{-1}) \)

amplitude \( \sim \mathcal{O}(\epsilon^\infty) \)

the core

the ripple

\[ \epsilon^\infty = \text{small beyond all orders of } \epsilon \]
The nanopteron

\[ \phi_j(X) + \varsigma_j(X) \]

amplitude \( \sim \mathcal{O}(\epsilon^2) \)

wavelength \( \sim \mathcal{O}(\epsilon^{-1}) \)

amplitude \( \sim \mathcal{O}(\epsilon^\infty) \)

\( \epsilon^\infty = \text{small beyond all orders of } \epsilon \)

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?

$$r_j(t) = C_w \epsilon^2 \text{sech}^2(\epsilon(j - ct)) + O(\epsilon^3)$$
Fix a time $t$. How do successive relative displacements, all at $t$, compare to each other?

\[ r_j(t) = \kappa^{(-1)^j+1/2} \epsilon^2 \text{sech}^2(\epsilon(j - ct)) + O(\epsilon^3) \]
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

\[ c^2 \partial_x^2 p + L_\kappa p + L_\beta p \cdot 2 = 0, \quad p(x) = \begin{pmatrix} p_1(x) \\ p_2(x) \end{pmatrix}, \]

where the operators \( L_\kappa \) and \( L_\beta \) are Fourier multipliers constructed chiefly from shift operators.
An analysis of the eigenvalues of $L_\kappa$ produces $c_\kappa > 0$ with the property that if

$$p(x) = \epsilon^2 \theta(\epsilon x), \quad \theta(X) = (\theta_1(X), \theta_2(X)),$$

$$c^2 = c_\epsilon^2 := c_\kappa^2 + \epsilon^2,$$

then we can diagonalize $L_\kappa$ and make a “cancelation” in the $p_1$ equation to convert our system for the profiles $p$ into

$$\Theta_\epsilon(\theta) = \begin{bmatrix} 1 & 0 \\ 0 & T_\epsilon \end{bmatrix} \theta + Q_\epsilon(\theta) = 0.$$

Here the operator $T_\epsilon := \epsilon^2 c_\epsilon^2 \partial^2_X + \lambda^\epsilon\epsilon$ is singularly perturbed.
Taking $\epsilon = 0$ and defining the operator $\Theta_0$ correctly, we find that for a certain sech$^2$-type KdV traveling wave solution $\sigma$, we have

$$\Theta_0(\sigma) = 0, \quad \sigma := \begin{pmatrix} \sigma \\ 0 \end{pmatrix}.$$ 

Can we solve $\Theta_\epsilon(\theta) = 0$ by perturbing from $\sigma$? Try setting

$$\theta = \sigma + \xi,$$

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

We aim for a fixed point problem and find

$$\Theta_\epsilon(\sigma + \xi) = 0 \iff \begin{cases} 
\xi_1 = -\sigma - Q_{1,\epsilon}(\sigma + \xi) \\
T_\epsilon \xi_2 = -Q_{2,\epsilon}(\sigma + \xi).
\end{cases}$$
The operator $\mathcal{T}_\epsilon$

We can suss out a unique number $\omega_\epsilon$ with the property that

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

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

And if we want to solve

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

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

$$\mathcal{F}[Q_{2,\epsilon}(\sigma + \xi)](\omega_\epsilon) = 0.$$
We resolve the problem of “two unknowns, three equations” by looking not for solitary waves but nonlocal solitary waves (nanopterons): instead of the ansatz

$$\theta = \sigma + \xi,$$

we let

$$\theta = \sigma + \varphi^a + \eta,$$

where

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

Then our three variables are $a$, $\eta_1$, and $\eta_2$.

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

**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 $\varphi_{\epsilon}^a \in C_{\text{per}}^\infty \times C_{\text{per}}^\infty$ with $\Theta_{\epsilon}(\varphi_{\epsilon}^a) = 0$.

**Proof.** Bifurcation from a simple eigenvalue (Crandall-Rabinowitz-Zeidler).
The nanopteron equations

We are solving

\[ \Theta_\epsilon(\sigma + \varphi^a_\epsilon + \eta) = 0 \]  \hspace{1cm} (\ast)

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

\[ \eta_1, \eta_2 \in H^{1}_{q} := \{ f \in H^{1} \mid \cosh(q \cdot f) \in H^{1} \} . \]

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

\[ \mathcal{N}_\epsilon(\eta, a) = (\eta, a). \]

**Theorem**

There exist \( \epsilon_{\ast} > 0 \) and \( q_{\ast} > 0 \) such that for all \( \epsilon \in (0, \epsilon_{\ast}) \), there exists a unique \( (\eta_\epsilon, a_\epsilon) \in \bigcap_{r=1}^{\infty} H^{r}_{q_{\ast}} \times H^{r}_{q_{\ast}} \times \mathbb{R} \) such that

\[ \Theta_\epsilon(\sigma + \varphi^a_\epsilon + \eta_\epsilon) = 0. \]

Also, for all \( r \in \mathbb{N} \), there is \( C_r > 0 \) such that \( |a_\epsilon| \leq C_r \epsilon^r \) for all \( \epsilon \in (0, \epsilon_{\ast}) \).
Questions for future consideration

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

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

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

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