MOVING EXCITATIONS IN CATION LATTICES

Juan FR Archilla
Group of Nonlinear Physics Lineal (GFNL)
Sevilla, Spain

With Yury Kosevich
Semenov Institute of Chemical Physics,
Moscow, Russia

Noé Jiménez, Víctor Sánchez-Morcillo and Lluis García Raffi
Institute of Pure and Applied Mathematics, Valencia, Spain

Inspiration of **Mike Russell**, Heriot-Watt University, Edinburgh, UK

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PROBLEMS OF THEORETICAL PHYSICS
dedicated to Alexander Davydov 100th birthday
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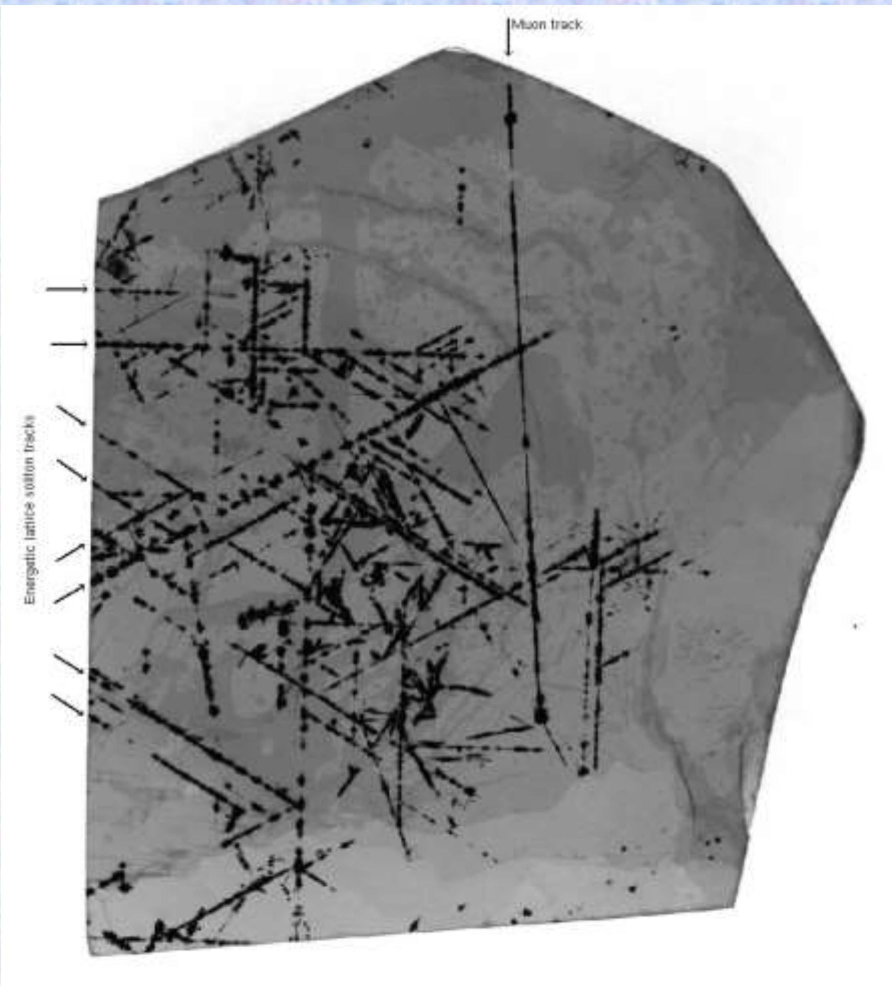
Sketch of the talk

- Why are we interested in cation lattices?
- What evidence is there of moving excitations in cation lattices?
- Which is our model?
- Kinks in cation lattices
- Theoretical and numerical results

Record of moving excitations in mica muscovite: quodons (Russell)



- 0.1% of the tracks are explained because of charged particles, like muons.
- 99.9% of the tracks are supposed to be lattice localized exitations or quodons
- They travel along lattice directions
- They travel long distances (mm)
- They have enough energy to eject an atom

Schlößer, D., Kroneberger, K., Schosnig, M., **Russell, F.M**. & Groeneveld, K.O. (1994). Search for solitons in solids. *Radiation Measurements* 23, 209-213.

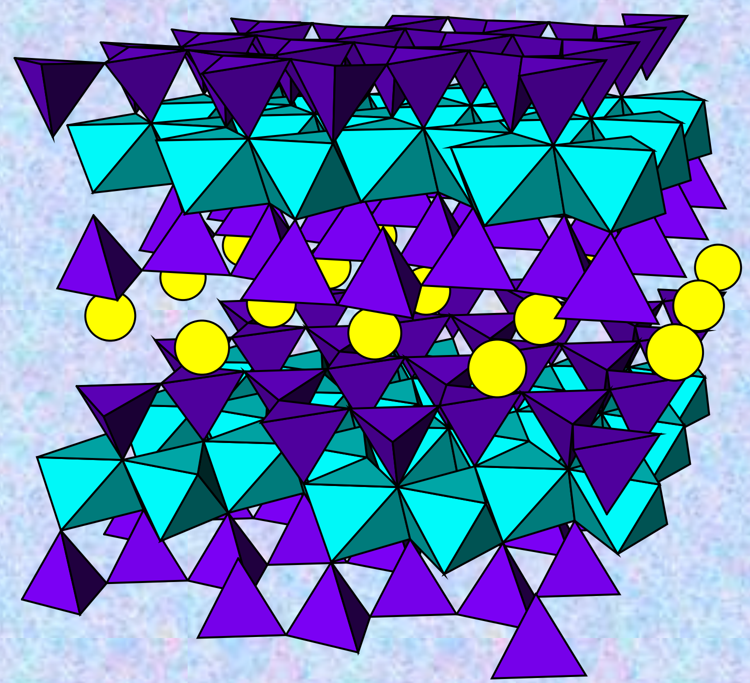
Experimental evidence of travelling excitations in mica muscovite

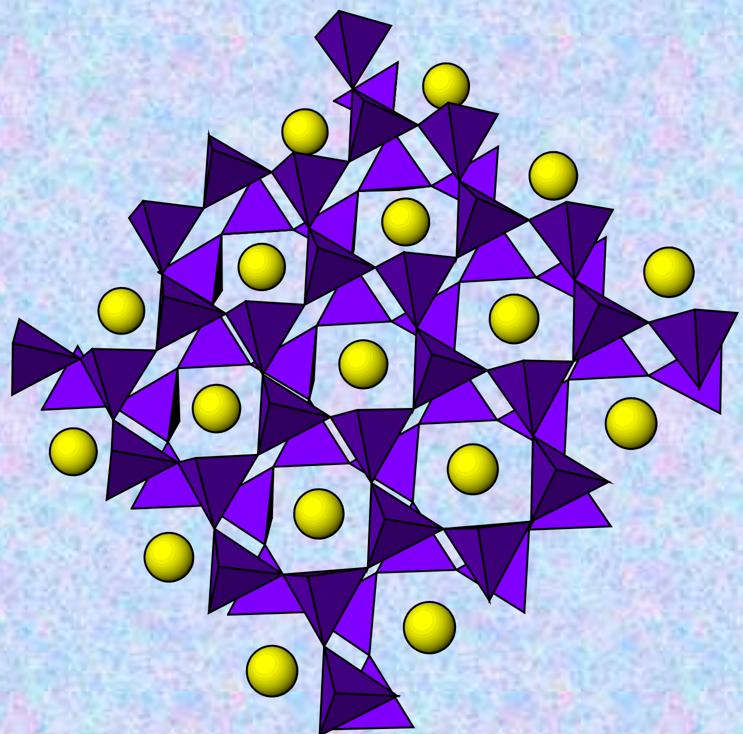
Trajectories along lattice directions within the K^+ layer

Russell, F.M., Eilbeck, J.C. (2007). Evidence for moving breathers in a layered crystal insulator at 300K. *Europhysics Letters* 78, 1004, 1-5.

Mica muscovite. Cation layers

$K_2[Si_6Al_2]^{IV}[Al_4]^{VI}O_{20}(OH)_4$



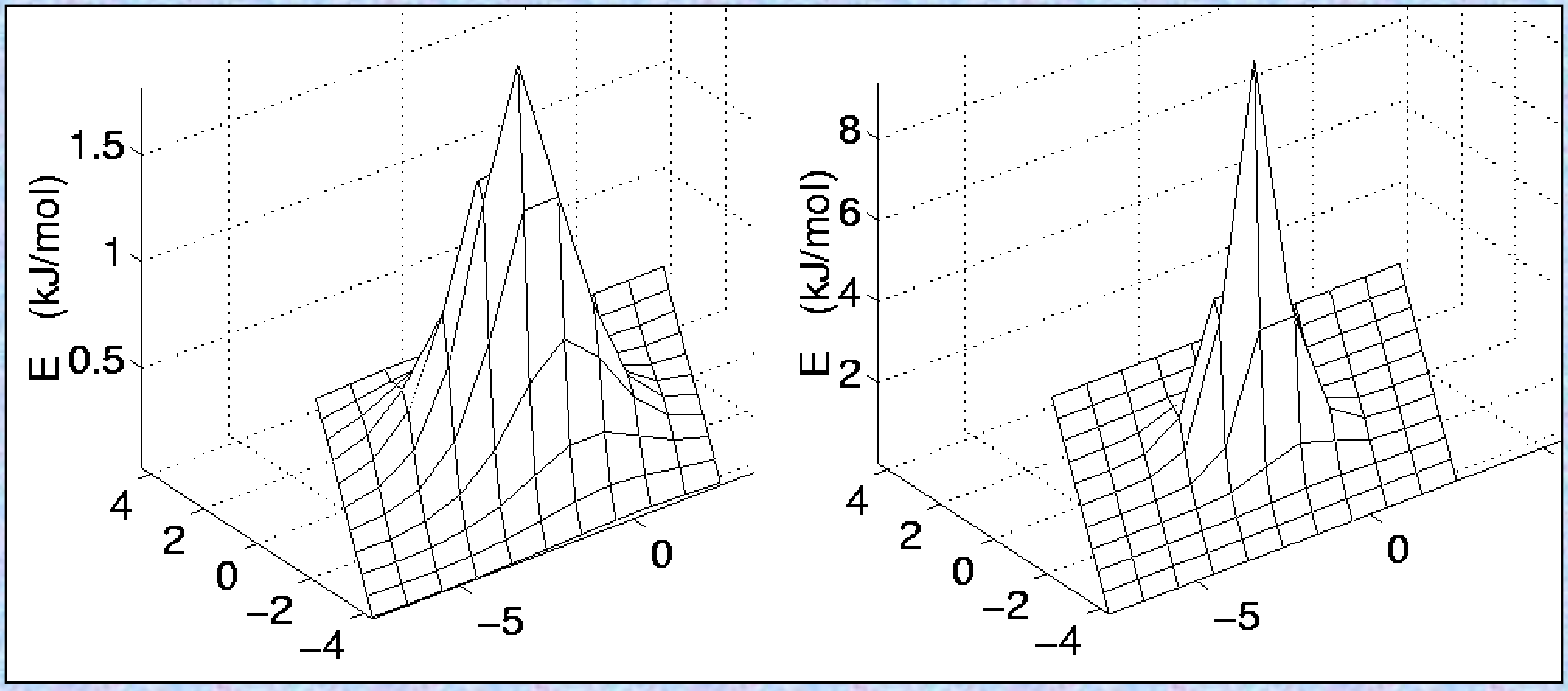


K^+

Transversal breathers have low energies and move slowly

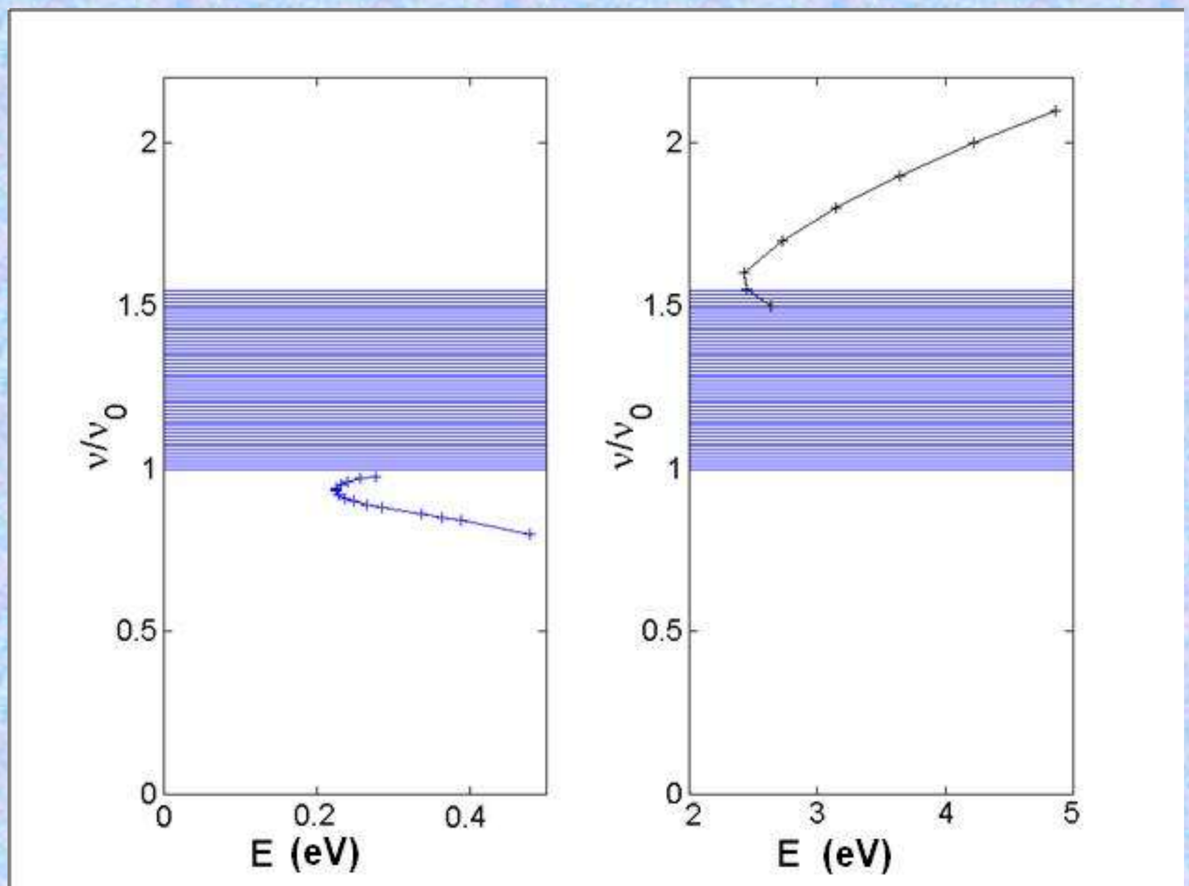
Soft breather, E=0.2~0.4 eV $\nu \sim 5\cdot10^{12}$ Hz

Hard breather. E ~0.36eV



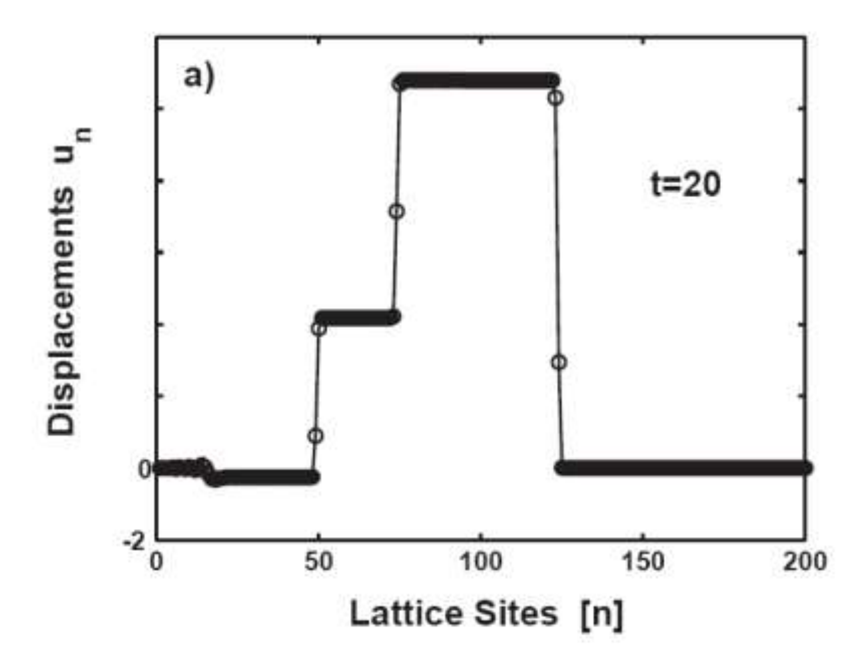
Dubinko, V.I., Selyshchev, P.A. & Archilla, J.F.R. (2011). Reaction-rate theory with account of the crystal anharmonicity. *Phys. Rev.* E 83, 041124, 1-13

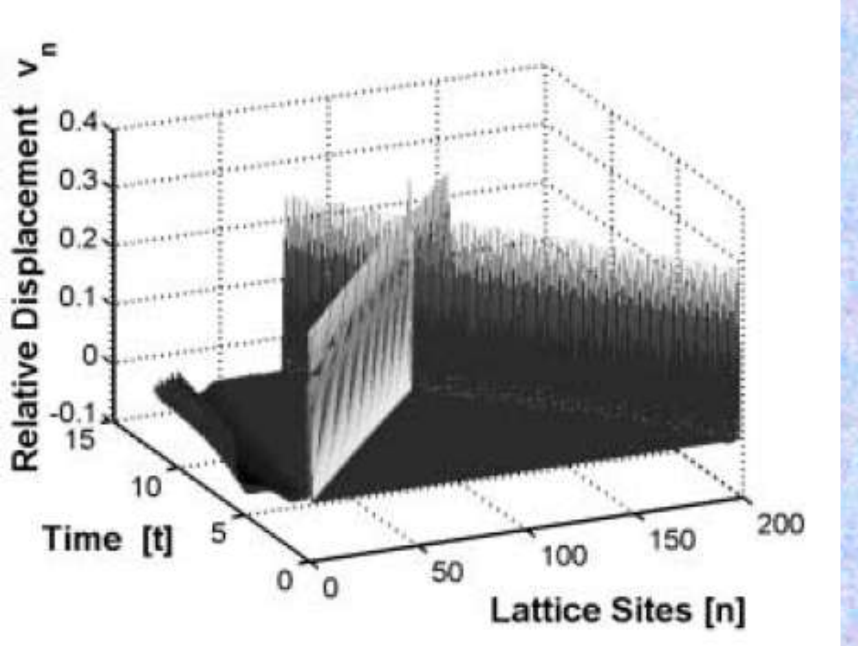
Transversal soft and hard breather spectra



ν_0= 167.5cm^{-1}
~ 5·10^{12} Hz
~20 meV

Supersonic kinks move very fast and have large energies.

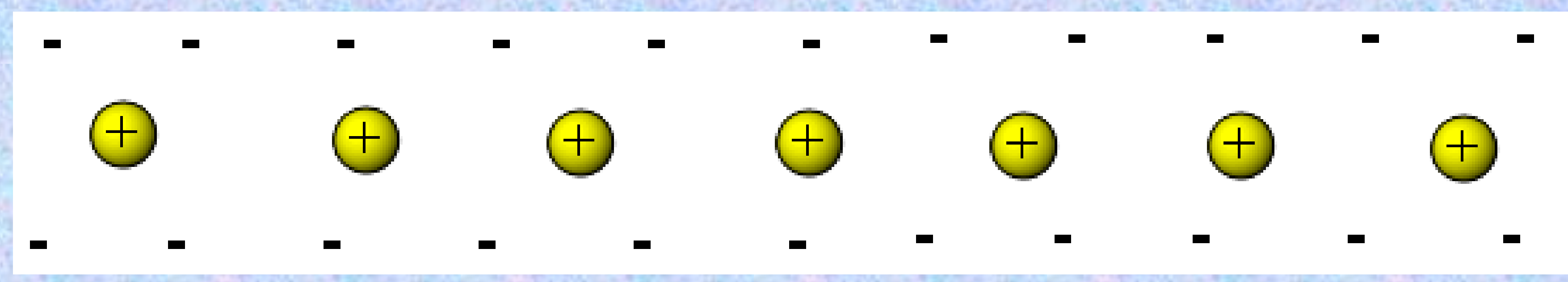




Transversal kinks in a beta FPU lattice

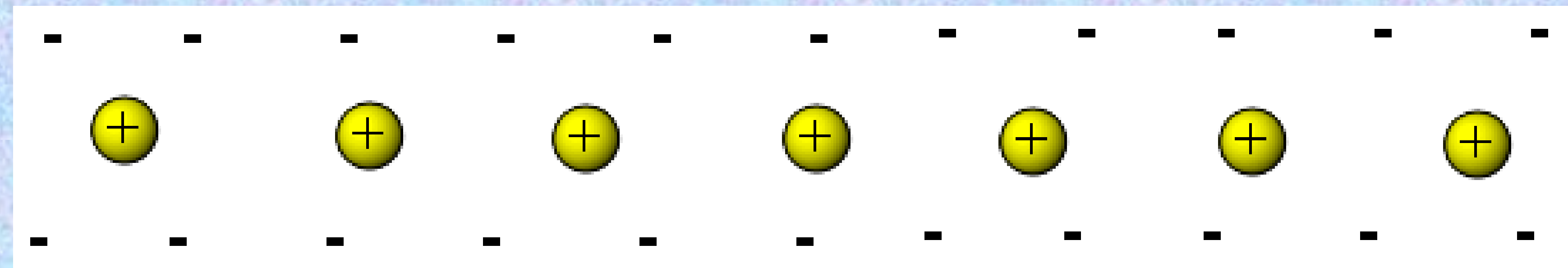
Yu A Kosevich, c, R & Ruffo, S. (2004). Supersonic discrete kink-solitons and sinusoidal patterns with "magic" wave number in anharmonic lattices. *Europhys. Lett.*, 66, 21–27.

Coulomb’s chains



- Longitudinal perturbations
- Cations are in a negative medium so:
  - Coulomb’s repulsion is rapidly screened
  - The system does not explode
  - We discard long range and more than nearest neighbour interactions.
- Negative charge at the borders keep cations inside
- Obstacle to movement would come from steric effects given by weak Van der Waals forces and electric ones by Pauli repulsion, given by overlapping electron orbitals

Model with fixed ends

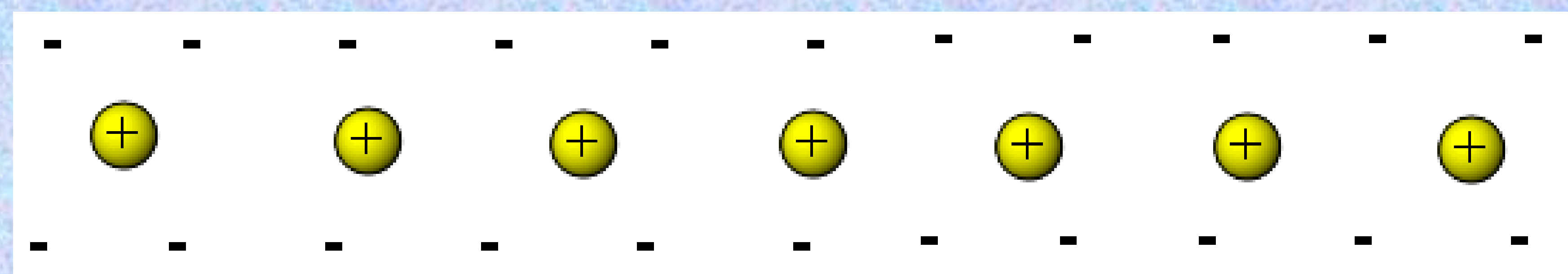


$$m_K \frac{\mathrm{d}^2 x_n}{\mathrm{d}t^2} = -\frac{Ke^2}{(x_{n+1}-x_n)^2} + \frac{Ke^2}{(x_n - x_{n-1})^2}$$

$$\ddot{u}_n = -\frac{1}{(1+u_{n+1}-u_n)^2} + \frac{1}{(1+u_n-u_{n-1})^2}$$

$$\text{Units:}\quad \mathrm{a} = 5.19\,\mathrm{A},\quad \tau = \frac{1}{\omega_0} = \sqrt{\frac{m_K a^3}{2Ke^2}} \cong 0.2\,\mathrm{ps}$$

What's spetial about Coulomb's repulsión?



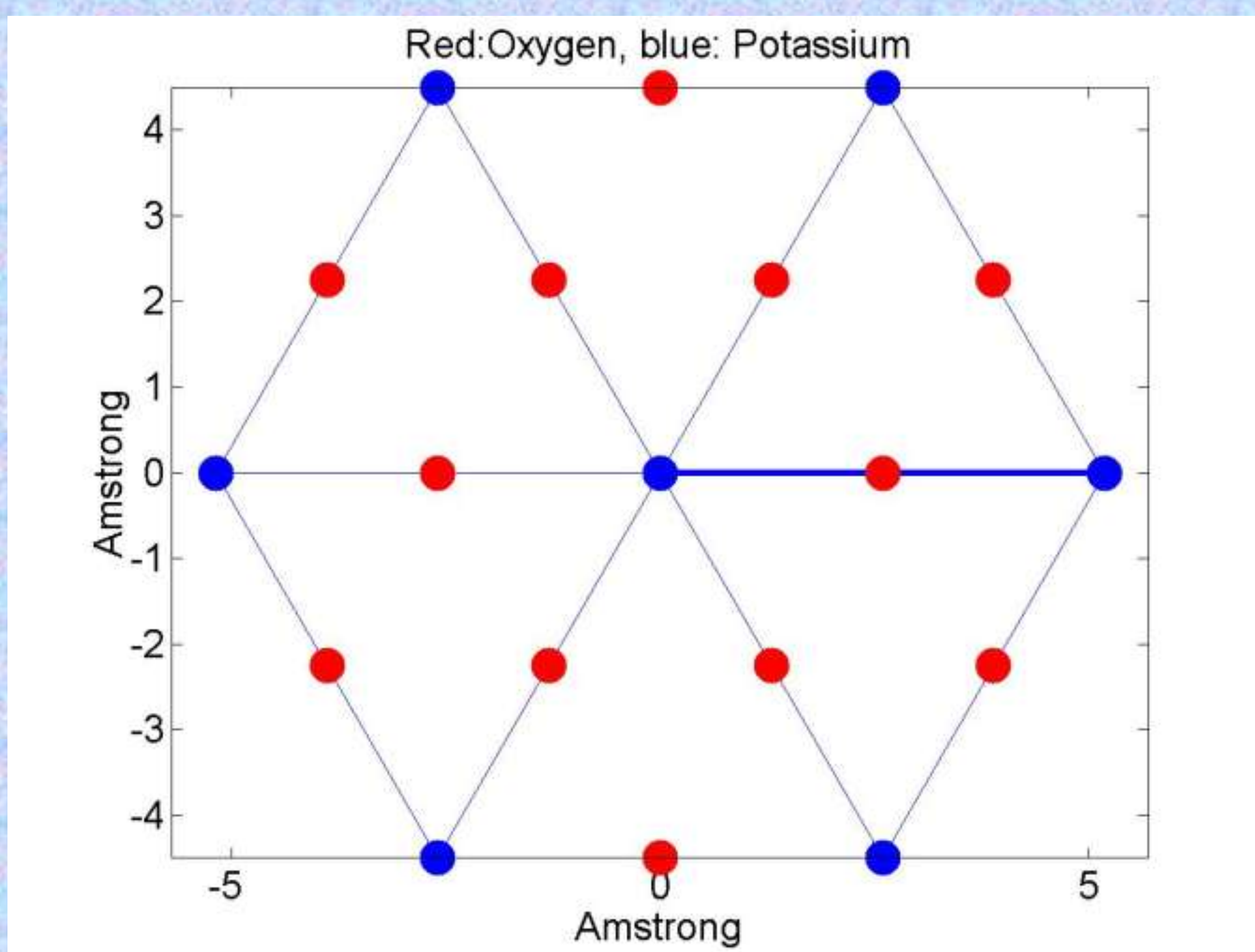
- Forces decay, fewer phonons as compared with harmonics.

- We now that it is there

- There is not a potential well

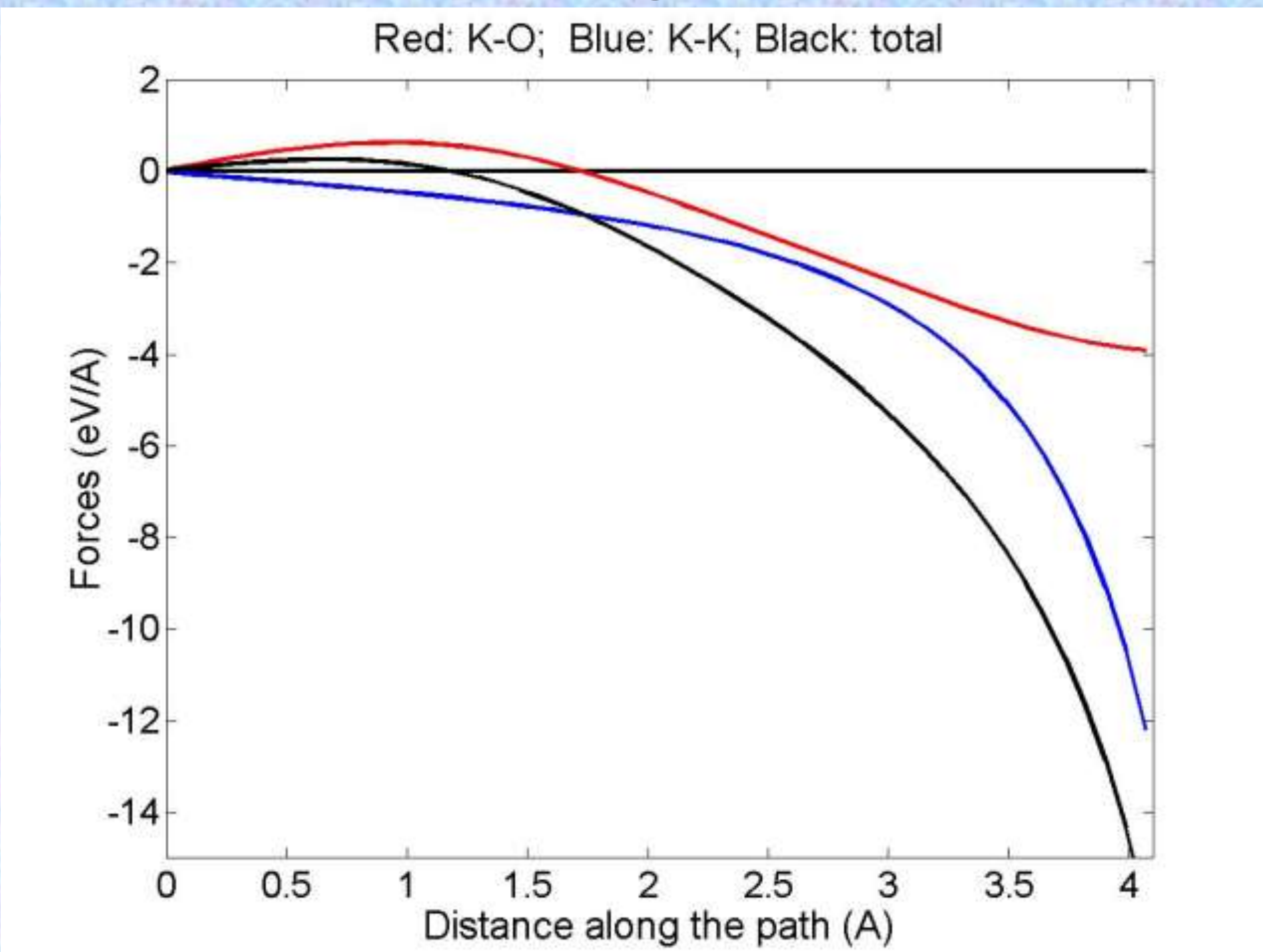
- Forces that increase with the distance are not a good physical description for this system with large perturbations.

Is the model absurd?



Muscovite empirical potentials

Short range K-O: $U = 65269.7\exp(-\frac{r}{0.213\text{A}})\text{eV}$



Coulomb interaction

$K^+ - O^{-2}$ and $K^+ - K^+$

Phonon spectrum

Linearized equation:

$$\ddot{u}_n = c^2(u_{n+1} + u_{n-1} - 2u_n)$$

$c = \sqrt{2}$ speed of sound

$$\omega_{\rm ph} = \omega_{\rm M} \sin(\frac{q}{2})$$

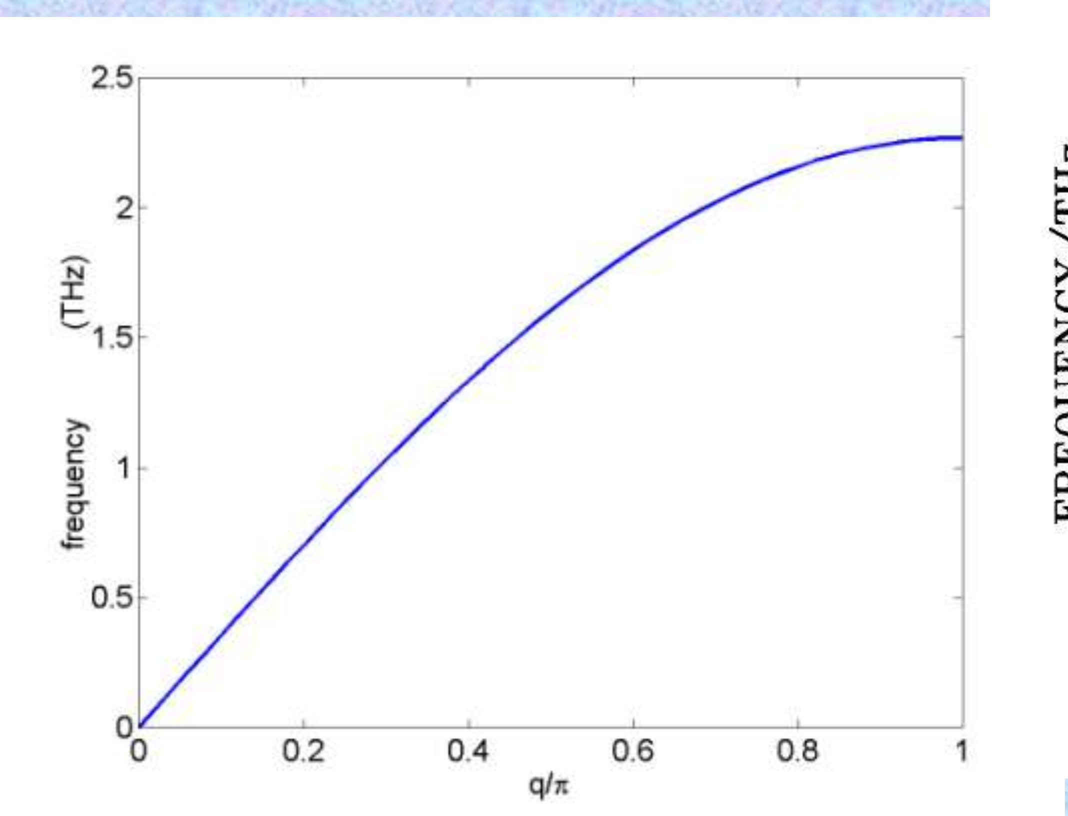
Maximum phonon frequency $\omega_{\rm M} = 2c$

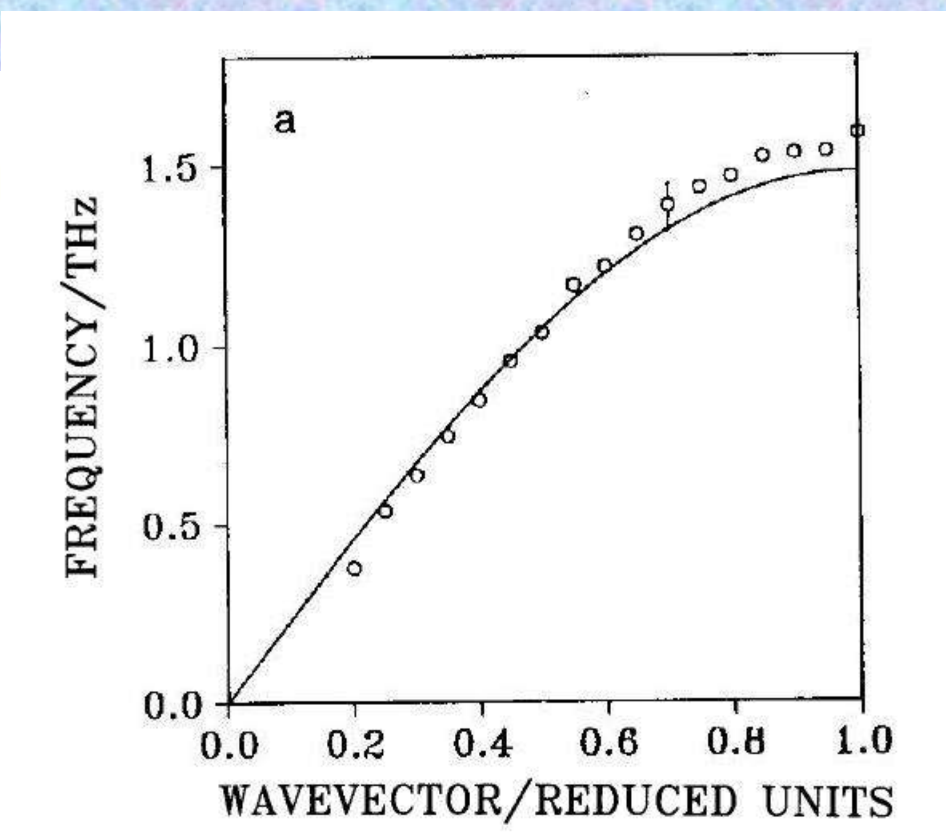
$$V_{\rm ph} = \frac{2c\sin(\frac{q}{2})}{q} \quad ; \quad V_{\rm group} = c\cos(\frac{q}{2})$$

$$V_{\rm ph,\,max} = V_{\rm group,\,max} = c$$

How they compare with experiments?

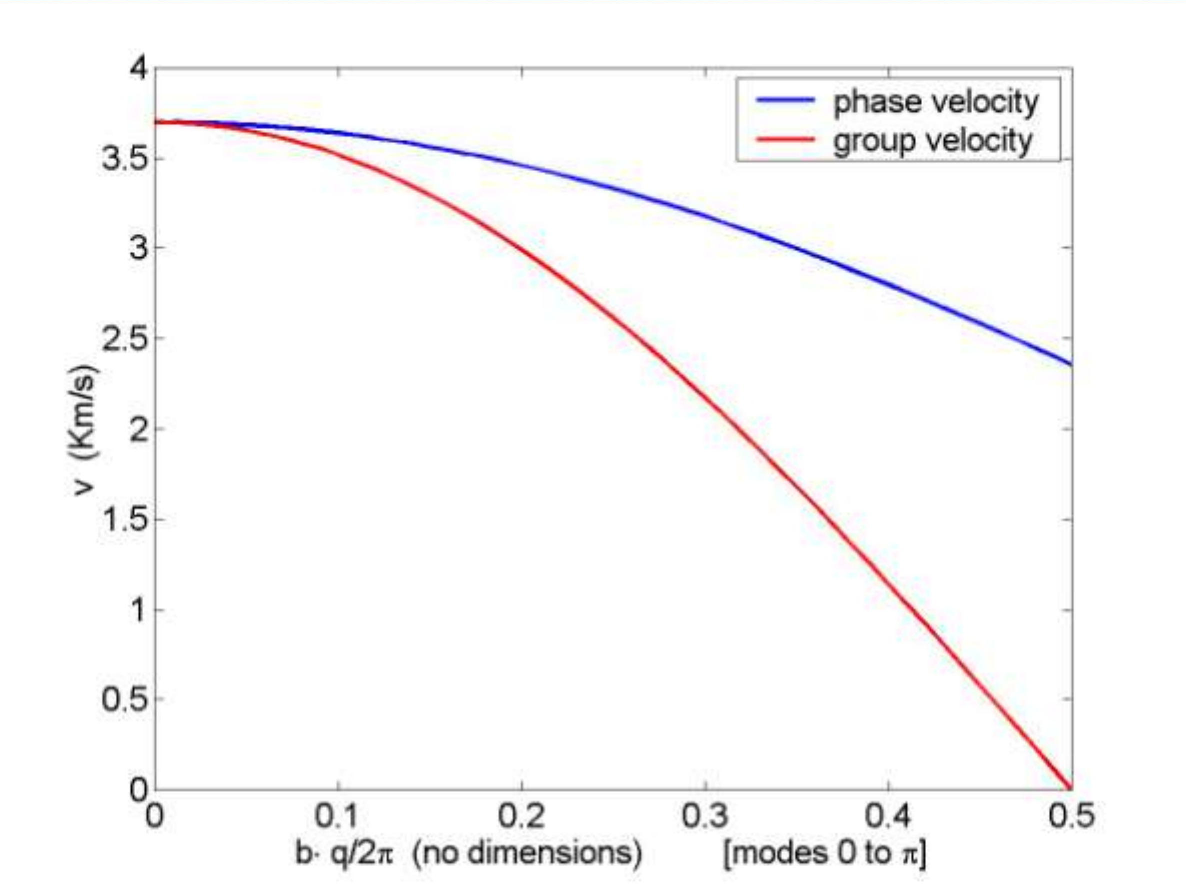
Phonon spectrum





D.R. Collins, W.G. Stirling , C.R.A. Catlow and G. Rowbotham Determination of Acoustic Phonon Dispersion Curves in Layer Silicates by Inelastic Neutron Scattering.and Computer Simulation Techniques. *Phys. Chem. Minerals.* 19: 520-527 (1993) .

Speed of sound



$$V_{\text{phys}} = \frac{a}{\tau} V_{\text{adim}}$$

Esperimental speed of sound: 3.4-3.7 km/s

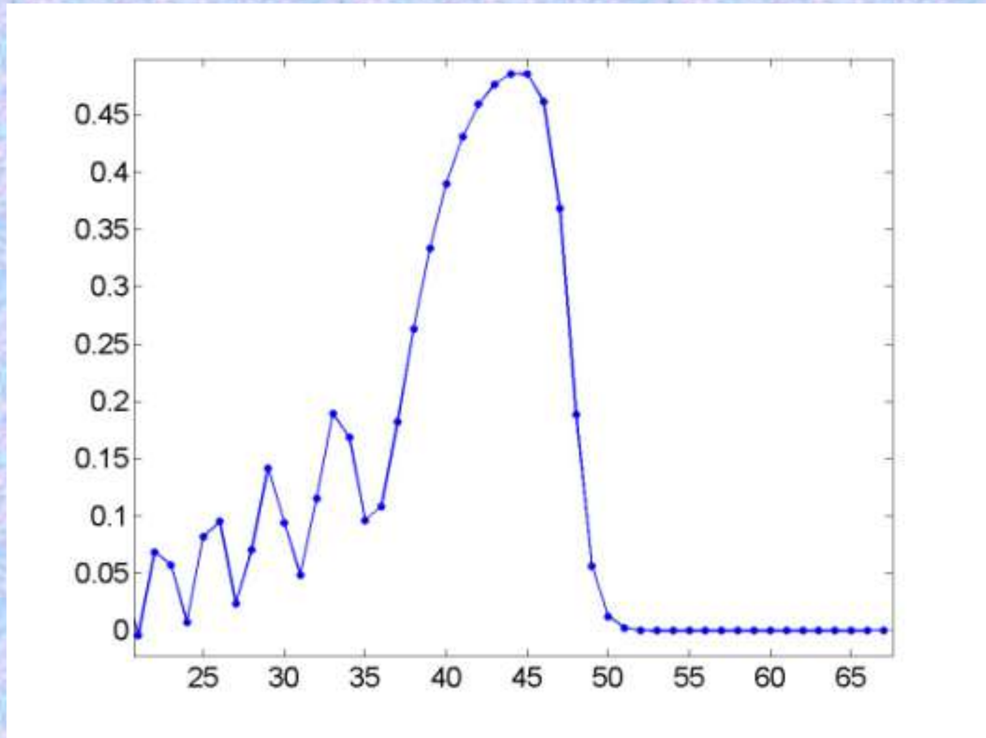
G. Brudeylins, D. Schmicker, Elastic and inelastic helium atom scattering at a cleaved mica sheet. *Surface Science*, 333: 237-242 (1995).

Tail analysis. What kind of excitation we might expect?

Tail: the small perturbation at the front abide the linear equation

$$\ddot{u}_n = c^2(u_{n+1} + u_{n-1} - 2u_n)$$

c: speed of sound



Proposed tail solution:

$$u_n = \exp(n - Vt)\exp(\mathrm{i}(\xi\,\mathrm{n} - \omega \mathrm{t}))$$

Tail analysis. Different solutions

Tail dispersion relation and velocity:

$$\omega = 2c\cosh(\frac{\xi}{2})\sin(\frac{q}{2}); \qquad V = \frac{2c}{\xi}\sinh(\frac{\xi}{2})\cos(\frac{q}{2});$$

Stationary oscillating localized solutions (**stationary breathers**)

$$\omega \neq 0; \xi \neq 0; V = 0 \Rightarrow q = \pi \qquad \omega = 2c\cos(\frac{\xi}{2});$$

Stationary breathers have frequency above the phonon band with mode $q = \pi$

Tail analysis. Moving breathers

$$\omega \neq 0; \xi \neq 0; V \neq 0 \Rightarrow q \neq 0; q \neq \pi$$

$$\boxed{\omega = 2c\cosh(\frac{\xi}{2})\sin(\frac{q}{2});} \qquad \boxed{V = \frac{2c}{\xi}\sinh(\frac{\xi}{2})\cos(\frac{q}{2});}$$

We need $\omega > 2\kappa = \max(\omega_{\text{phonon}})$ for stability

The mode $q = \pi$ is stable but does not move

The mode $q = 0$ moves faster but it's unstable

Too large localization ξ is unrealistic

$$v > \kappa \Rightarrow \xi > 6.5 \Rightarrow \quad u_{n+1} \approx 0.001 x_n \text{ and } \omega > 6.5 \max(\omega_{\text{phonon}})$$

This is unrealistic, then: **Moving breathers are subsonic**

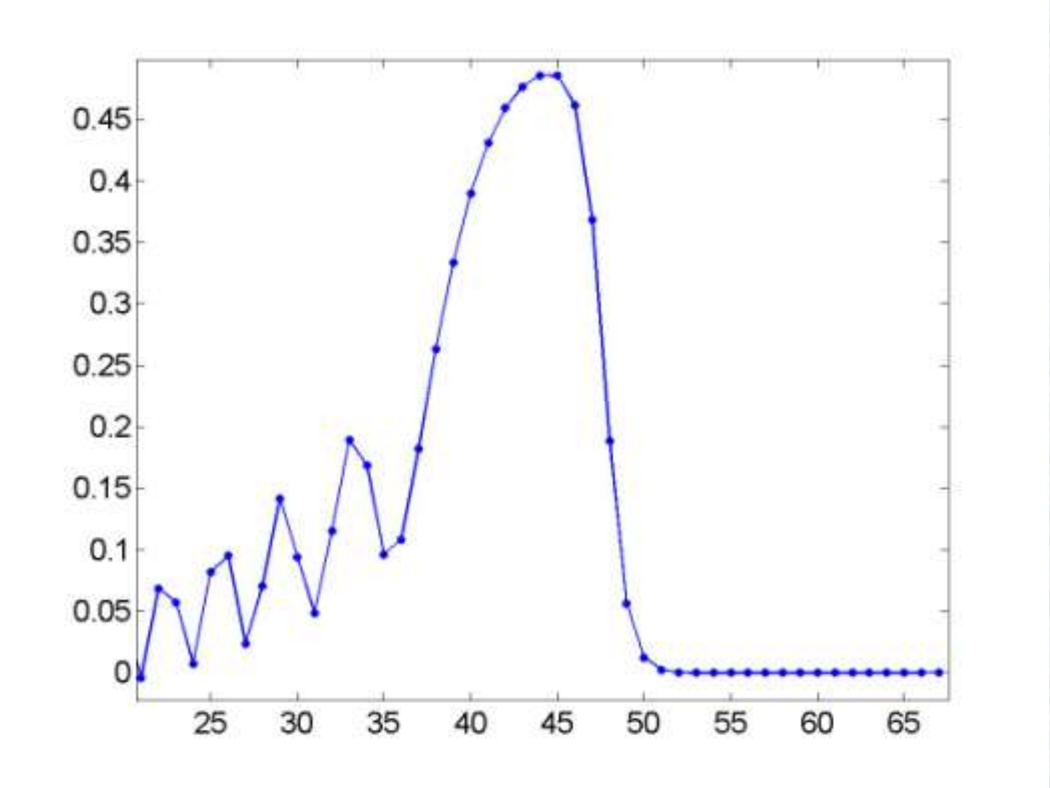
Supersonic solitons: moving, localized, non-oscillating solutions

$$\omega = 0; \xi \neq 0; V \neq 0 \Rightarrow q = 0$$

$$V = \frac{2c}{\xi}\sinh(\frac{\xi}{2});$$

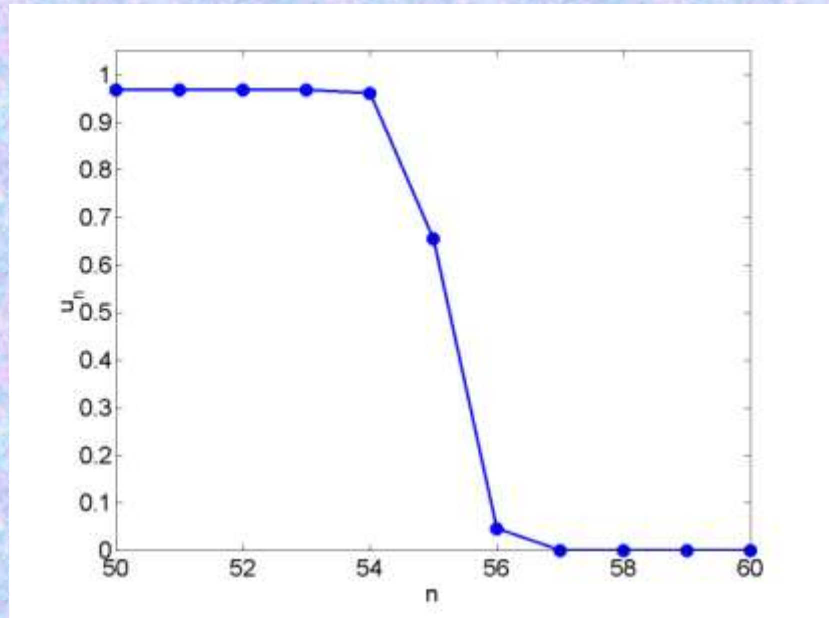
v is alway larger than the sound velocity.

Solitons are supersonic



Kinks

Moving, very steep, non-oscillating wave front



The equation in the relative displacements:

$$\ddot{v}_n = 2F_n - F_{n+1} - F_{n-1} \text{ with } F_n = \frac{1}{(1+v_n)^2} \text{ and } v_n = u_n - u_{n-1}$$

We propose the following solution for the *magic* wave number: $q = \dfrac{2\pi}{3}$, with only three particles perturbed.

$$v_n = -\frac{A}{2}(1+\cos(qn-\omega t)) \text{ if } \quad -\pi < qn - \omega t < \pi$$

$$v_n = 0 \quad \text{otherwise.}$$

Kinks with the rotating wave approximation (RWA)

Reduction to the first harmonic in $\cos(\theta)$, with $\theta = qn - \omega t$

$$-\omega^2 A\cos(\theta) = a_1 \cos(\theta), \text{ with}$$

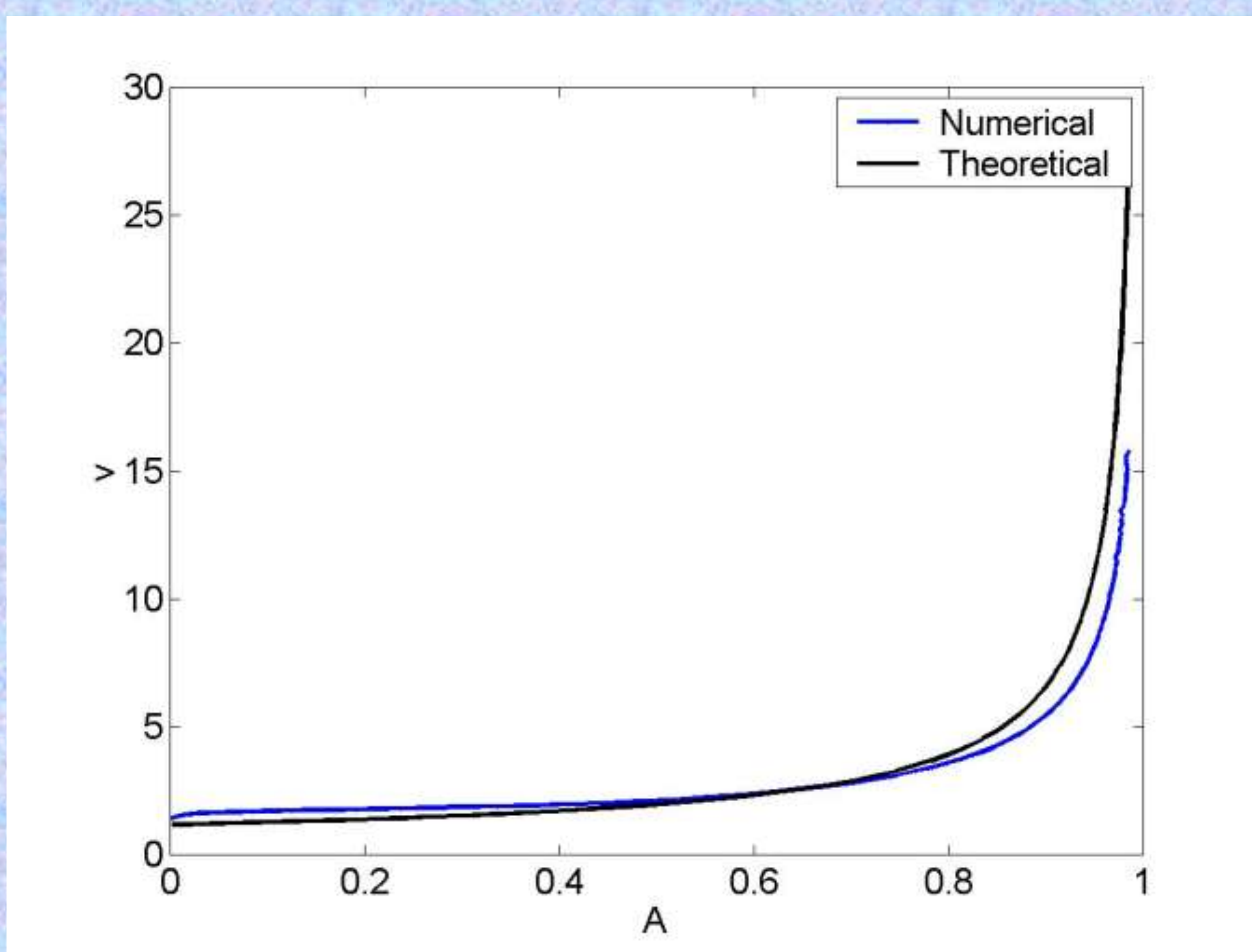
$$a_1 = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2} (F_n - F_{n+1} - F_{n-1})\cos(\theta)\,\mathrm{d}\theta$$

$$\boxed{\omega = \frac{2c}{(1-A)^{3/4}}\sin(q/2); \quad \mathrm{V} = \frac{\omega}{q} = \frac{2c}{(1-A)^{3/4}}\frac{\sin(q/2)}{q}}$$

Kinks are also supersonic

Kinks RWA, velocity versus amplitude

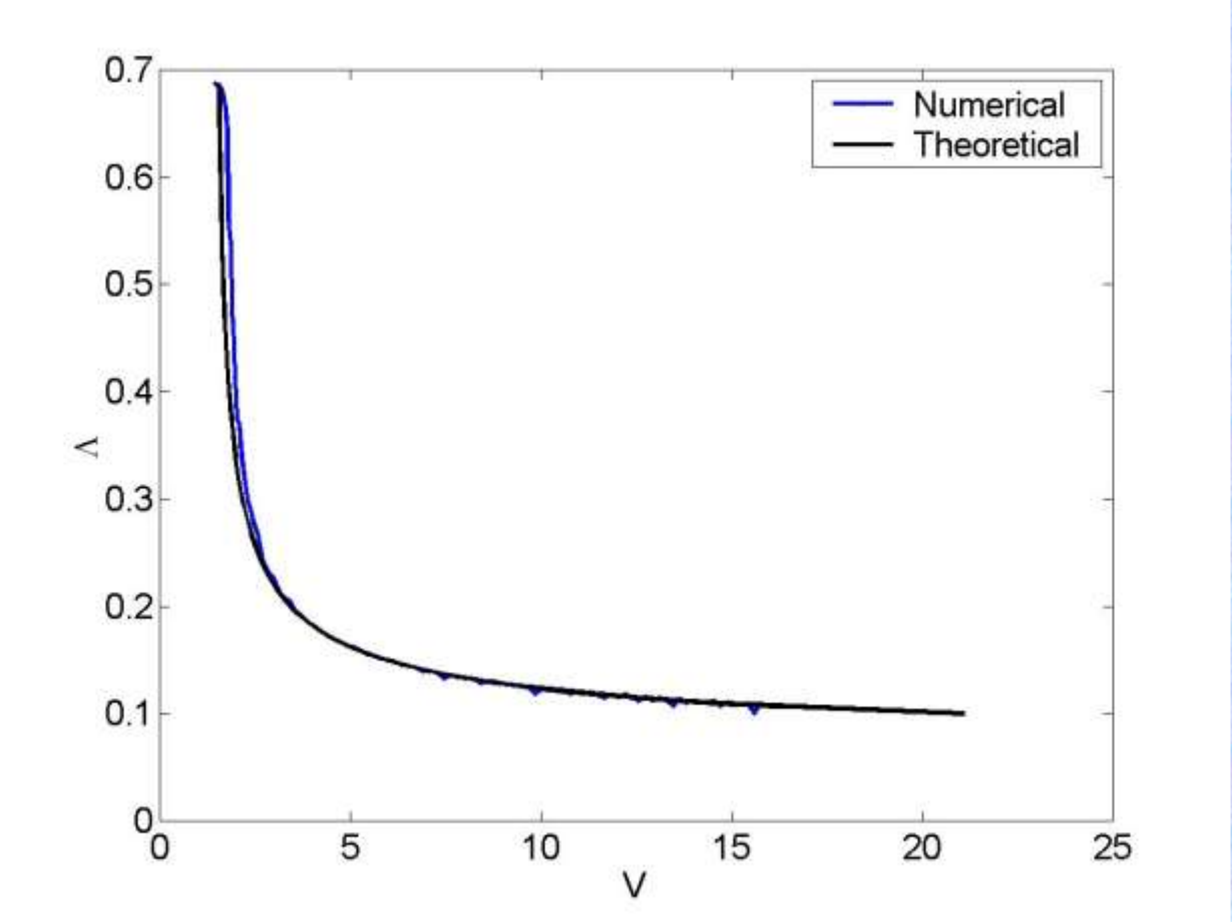
$$V = \frac{3\sqrt{3}c}{2\pi(1-A)^{3/4}}$$



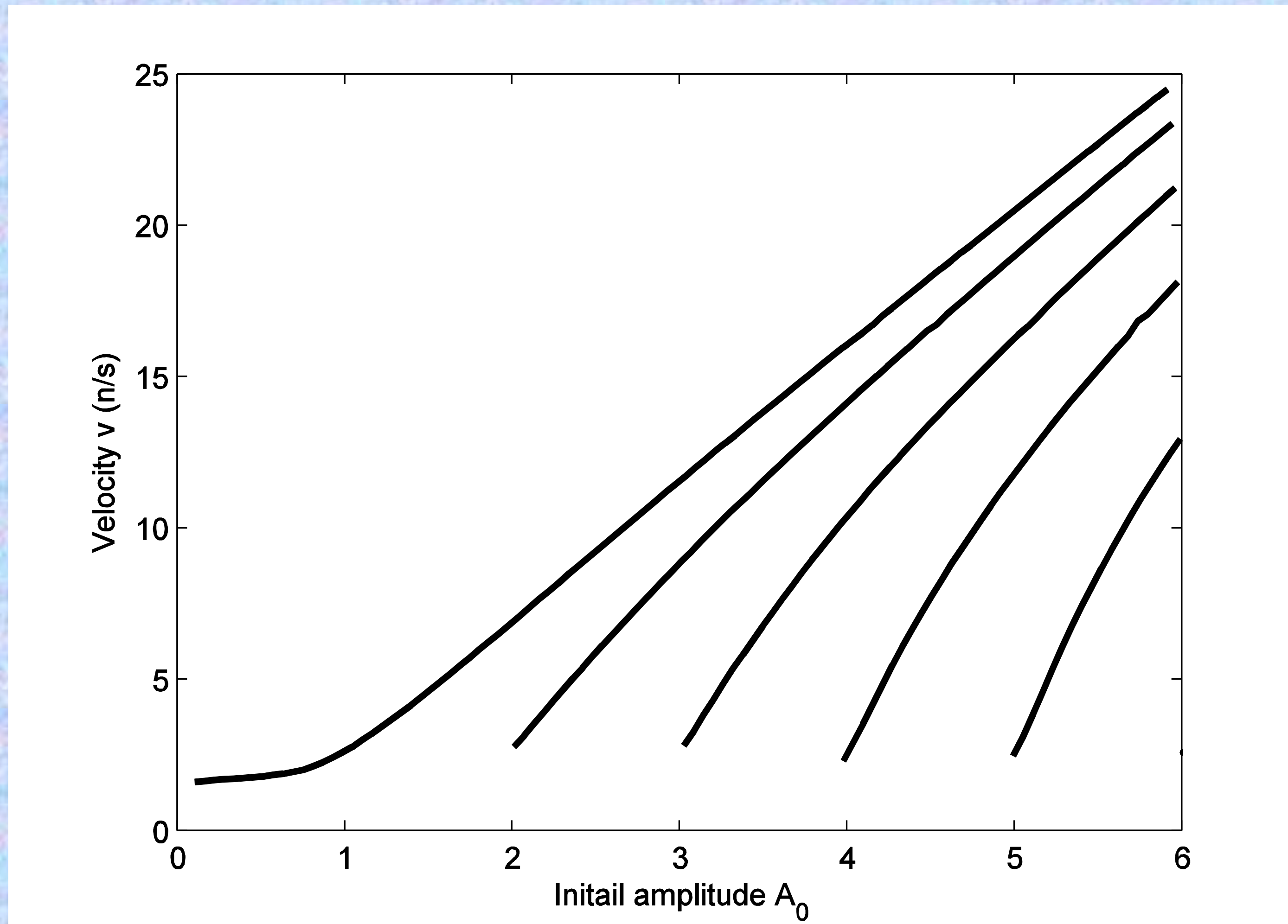
Kinks tails, decay lenght versus velocity

$$V = 2\Lambda c \sinh\left(\frac{1}{2\Lambda}\right)$$

with $\Lambda = \dfrac{1}{\xi}$

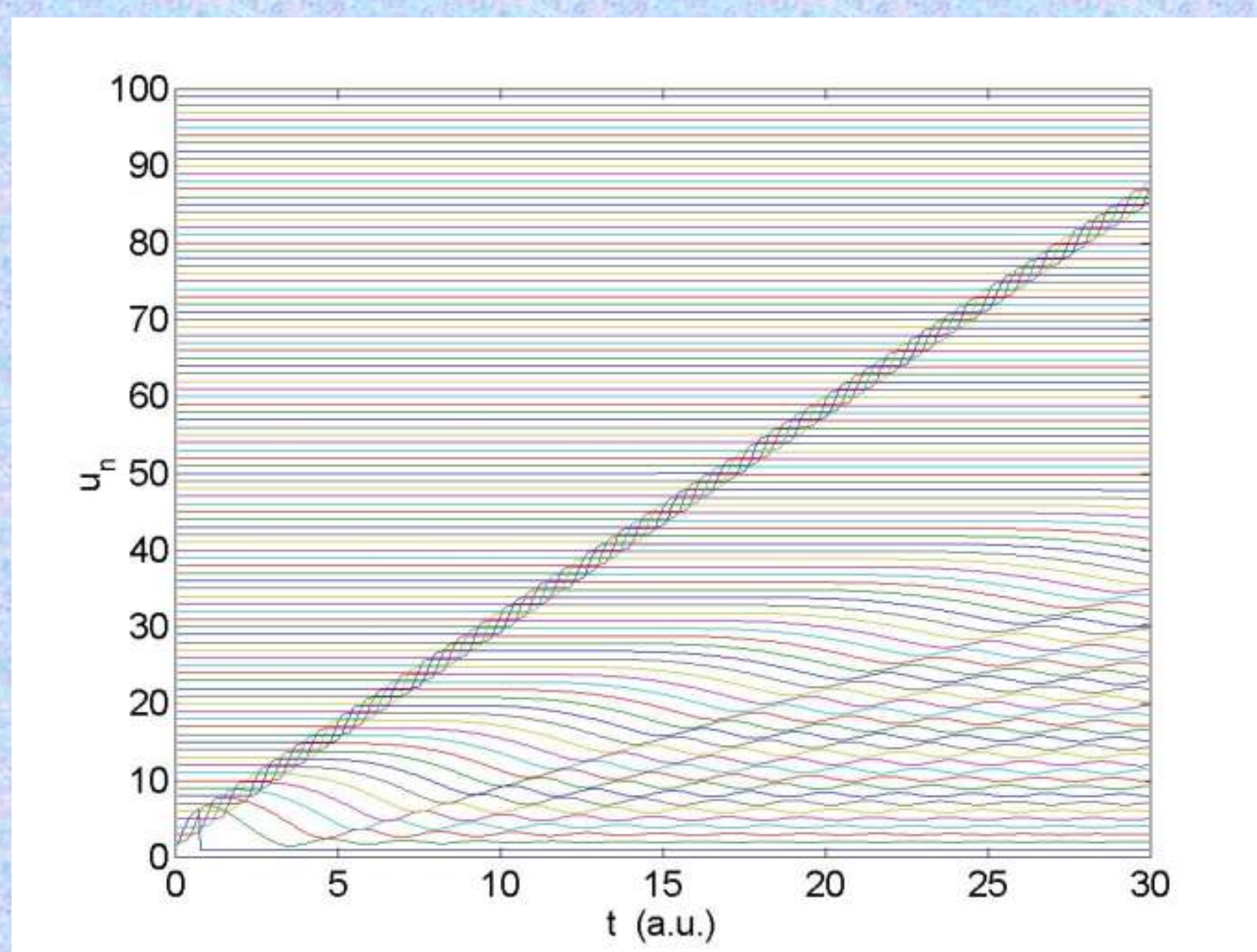


Kink simulation, Velocity-Initial amplitude



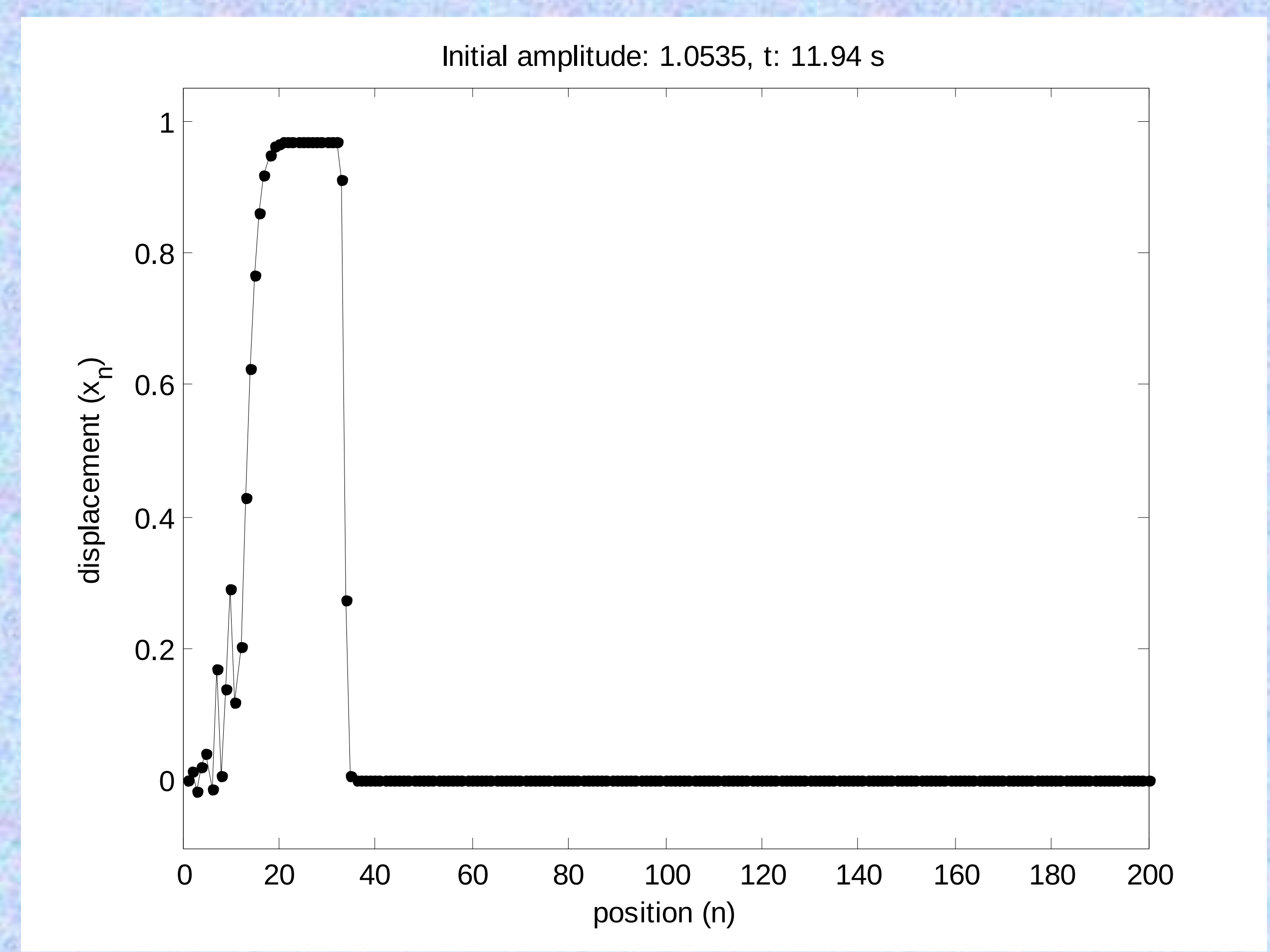
Single supersonic kink. Simulation

$V = 2c$



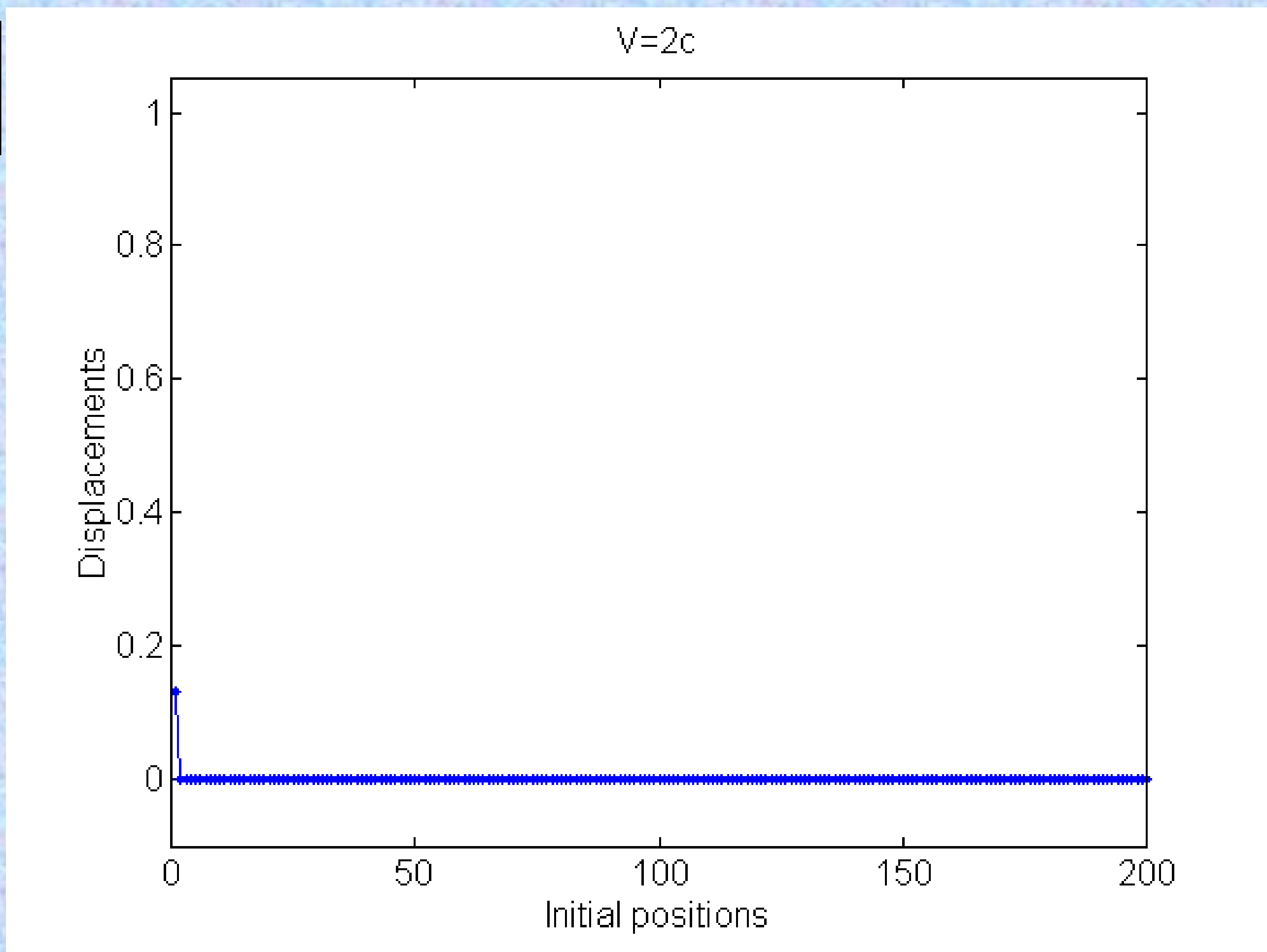
Single supersonic kink. Profile.

$$V = 2c$$



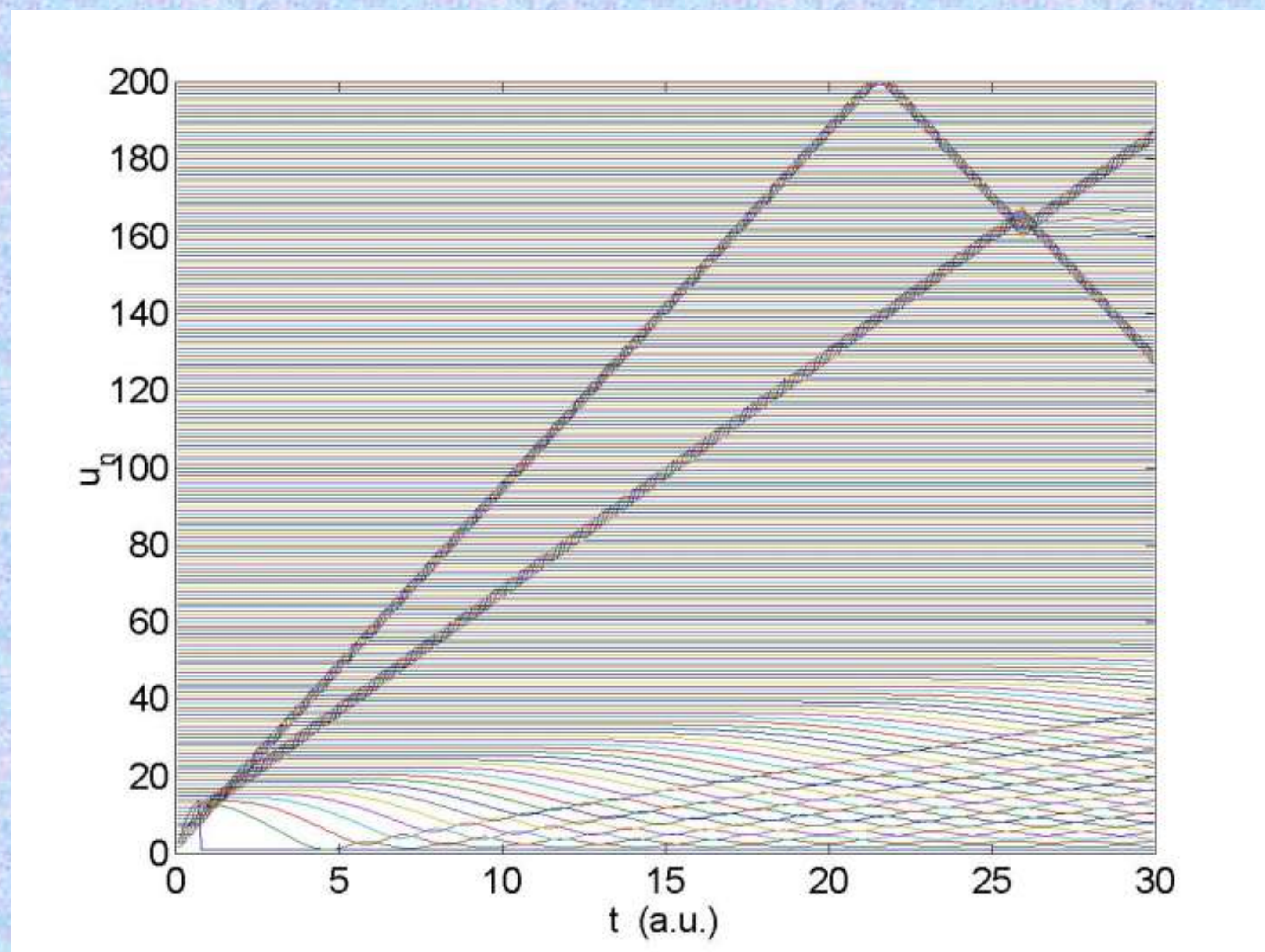
Single supersonic kink. Video.

$$\mathrm{V} = 2c$$



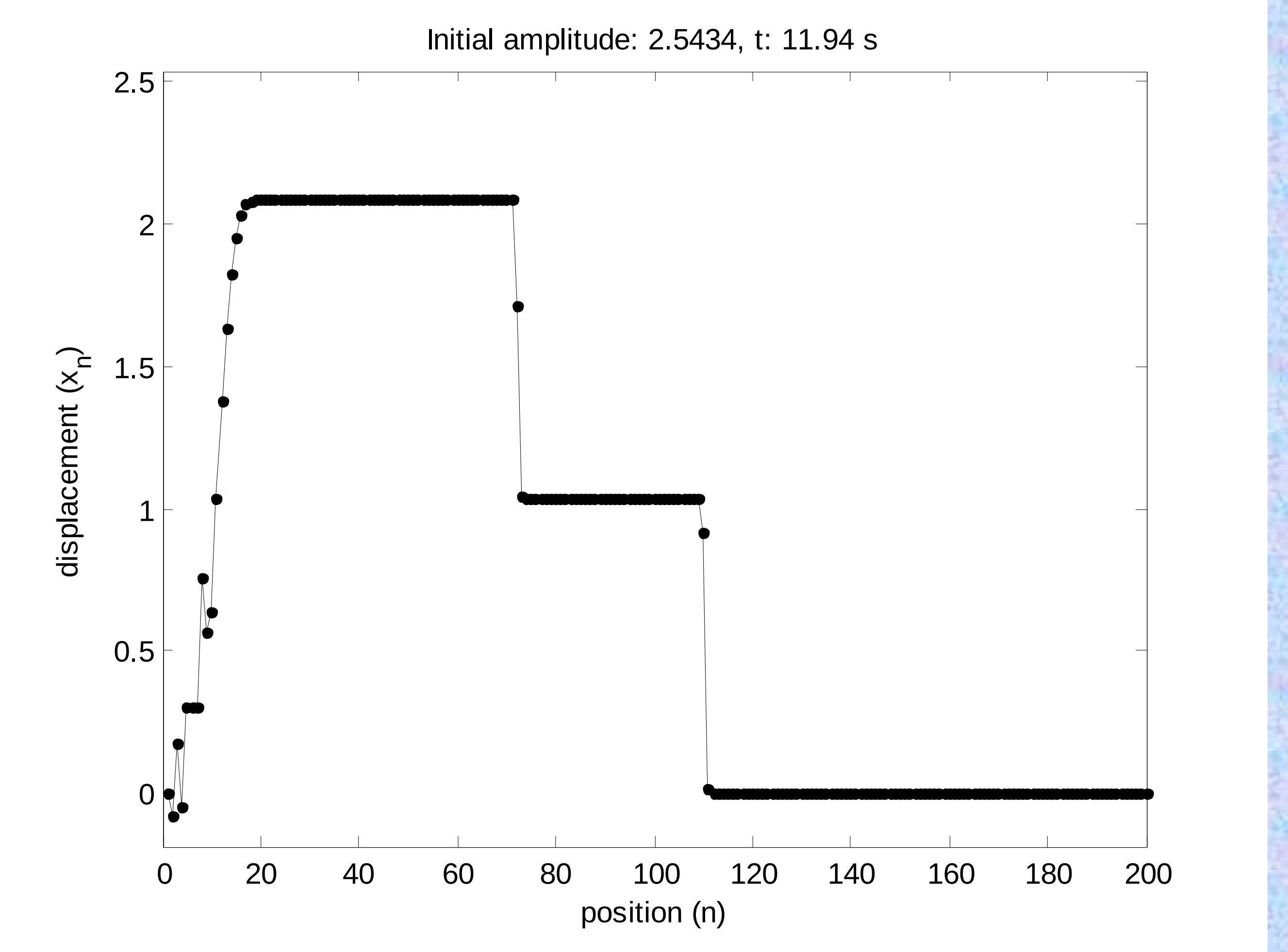
Double supersonic kink. Simulation

$$V = 4.1c$$



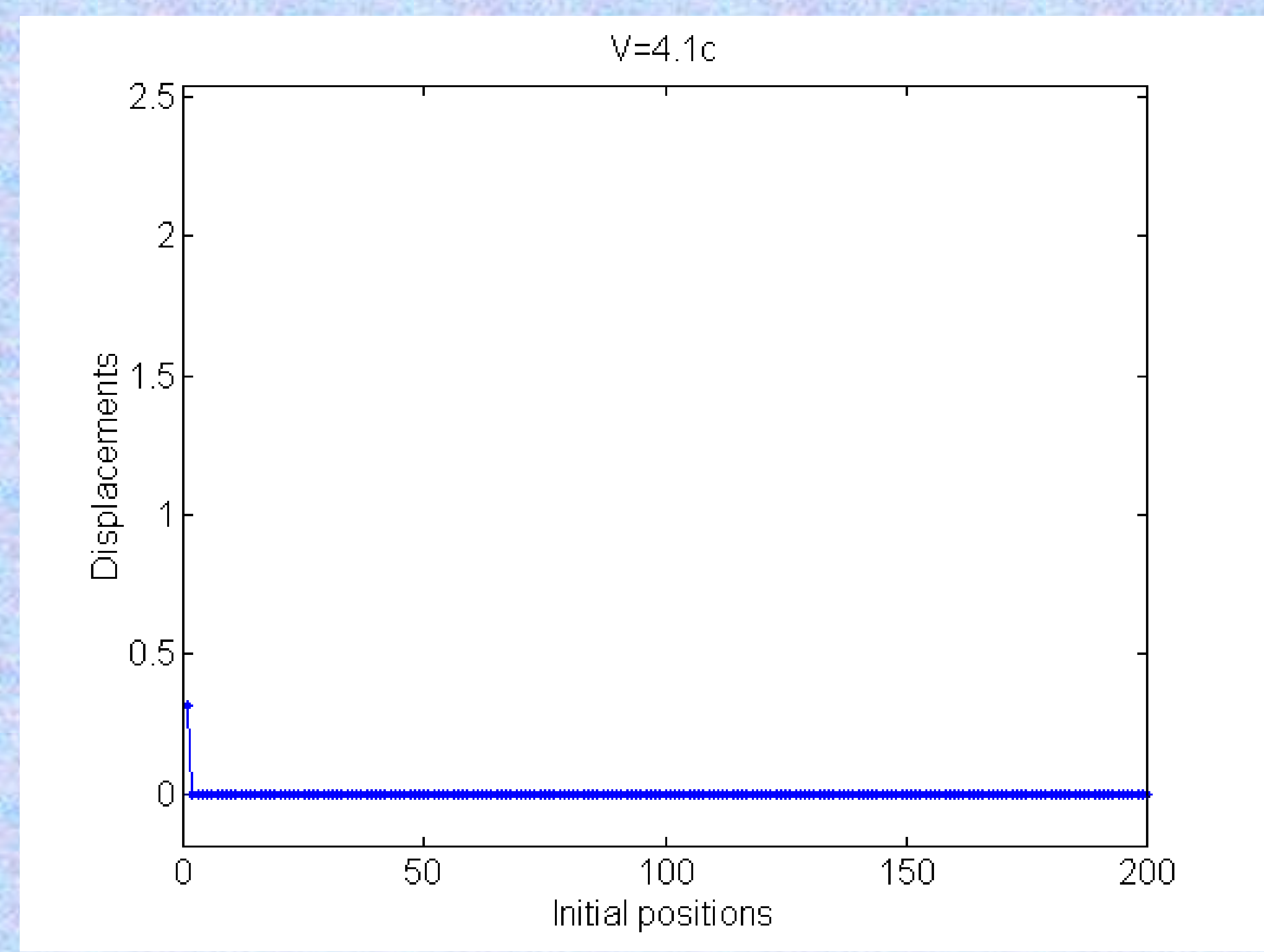
Double supersonic kink. Profile

$V = 4.1c$

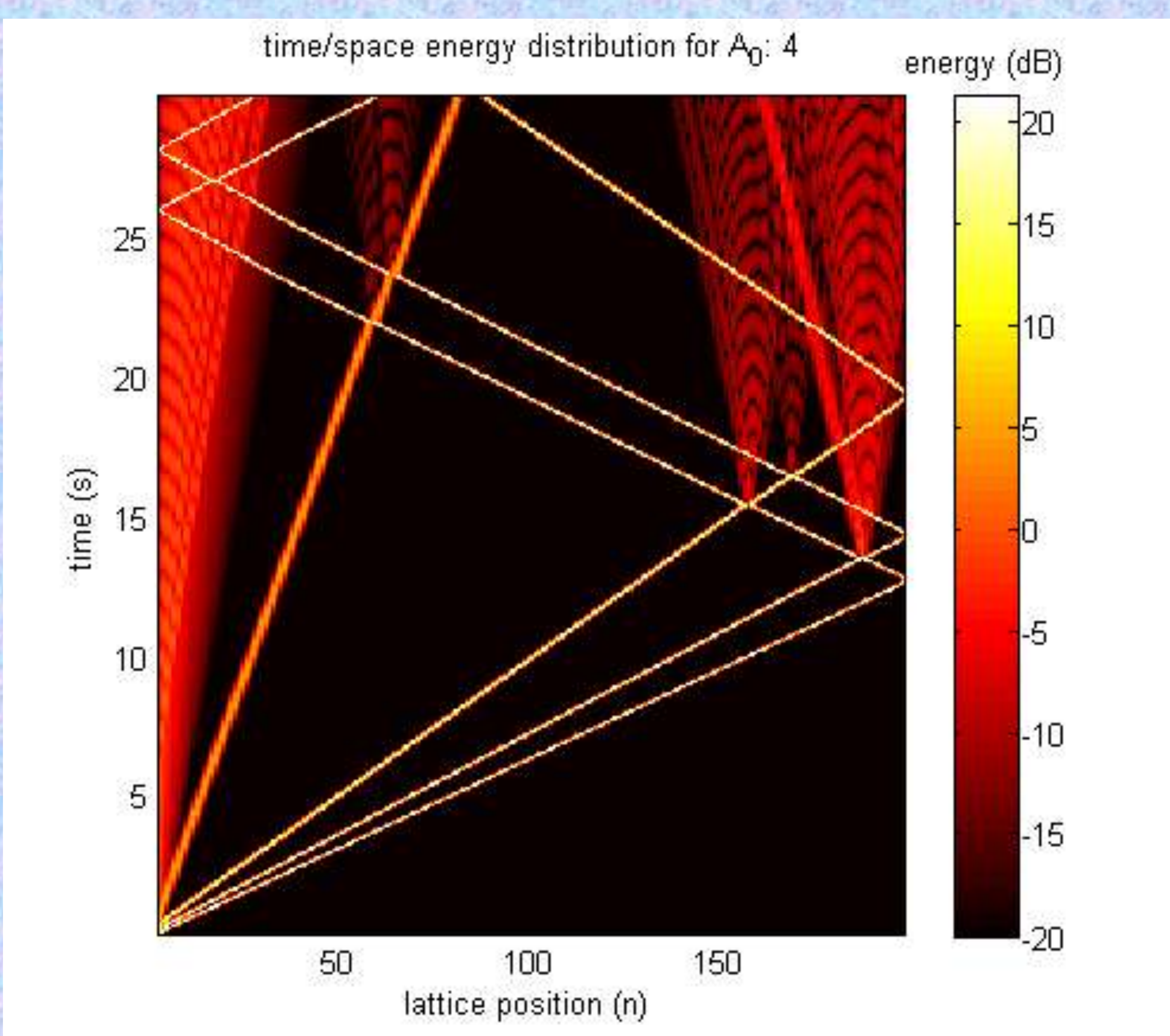


Double supersonic kink. Video

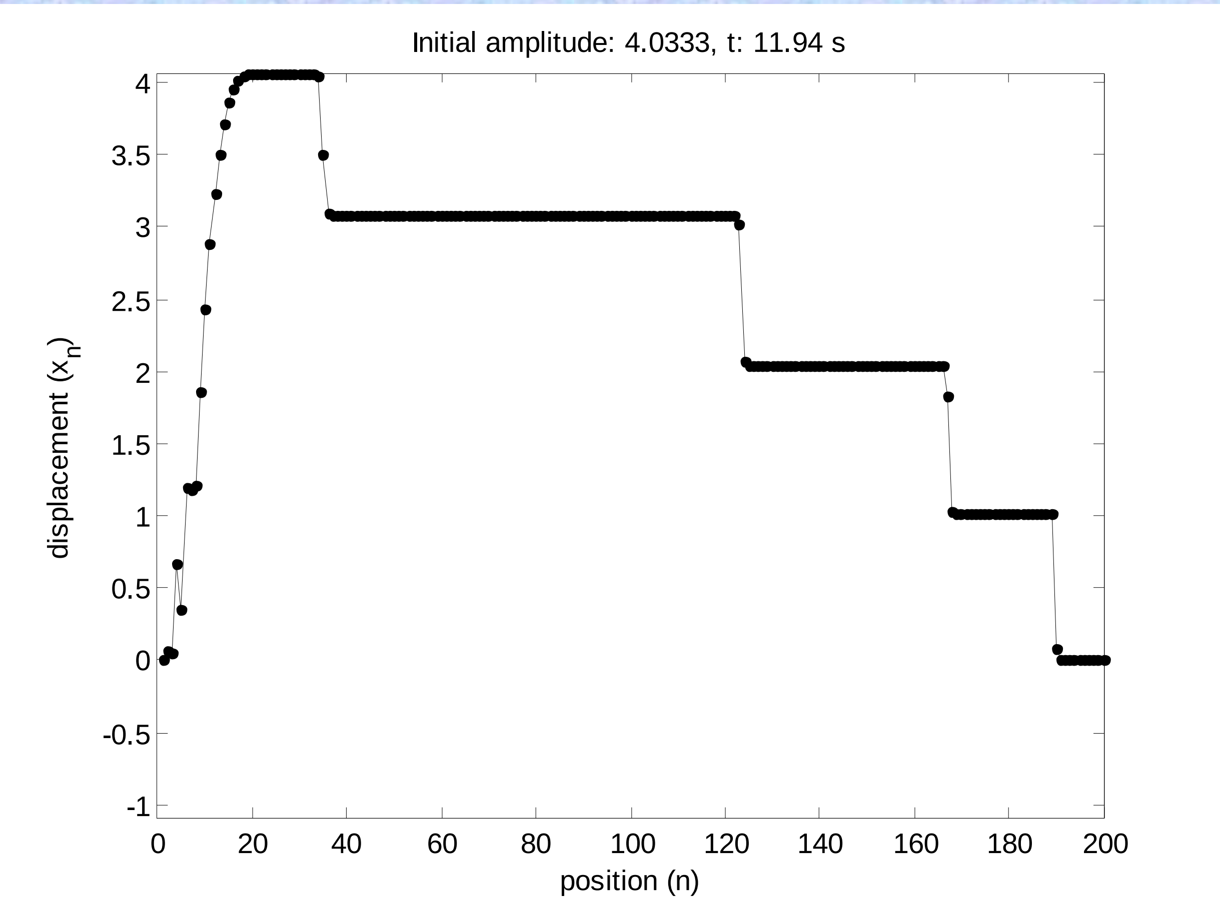
$$V = 4.1c$$



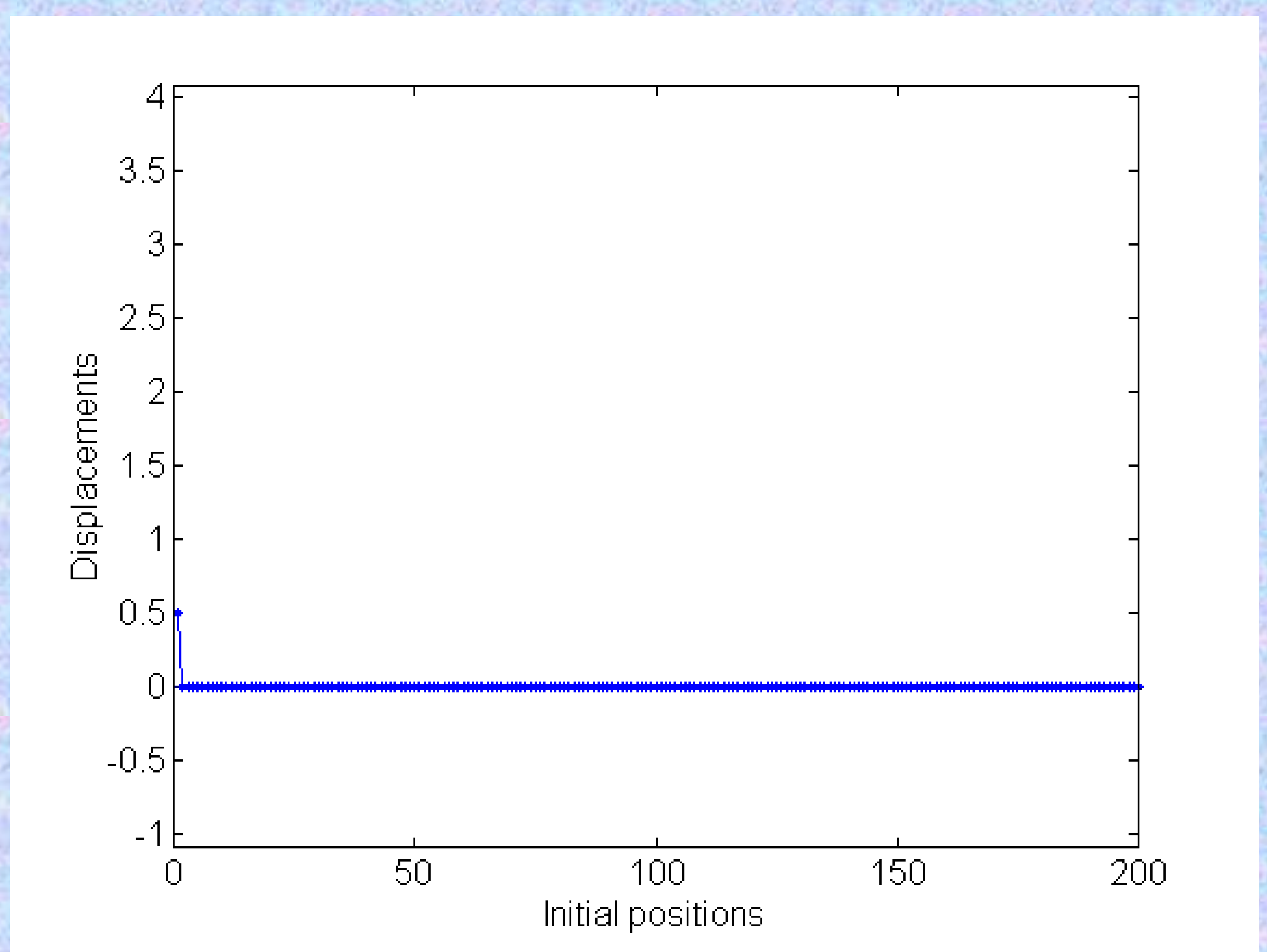
Three kinks. Energy-time



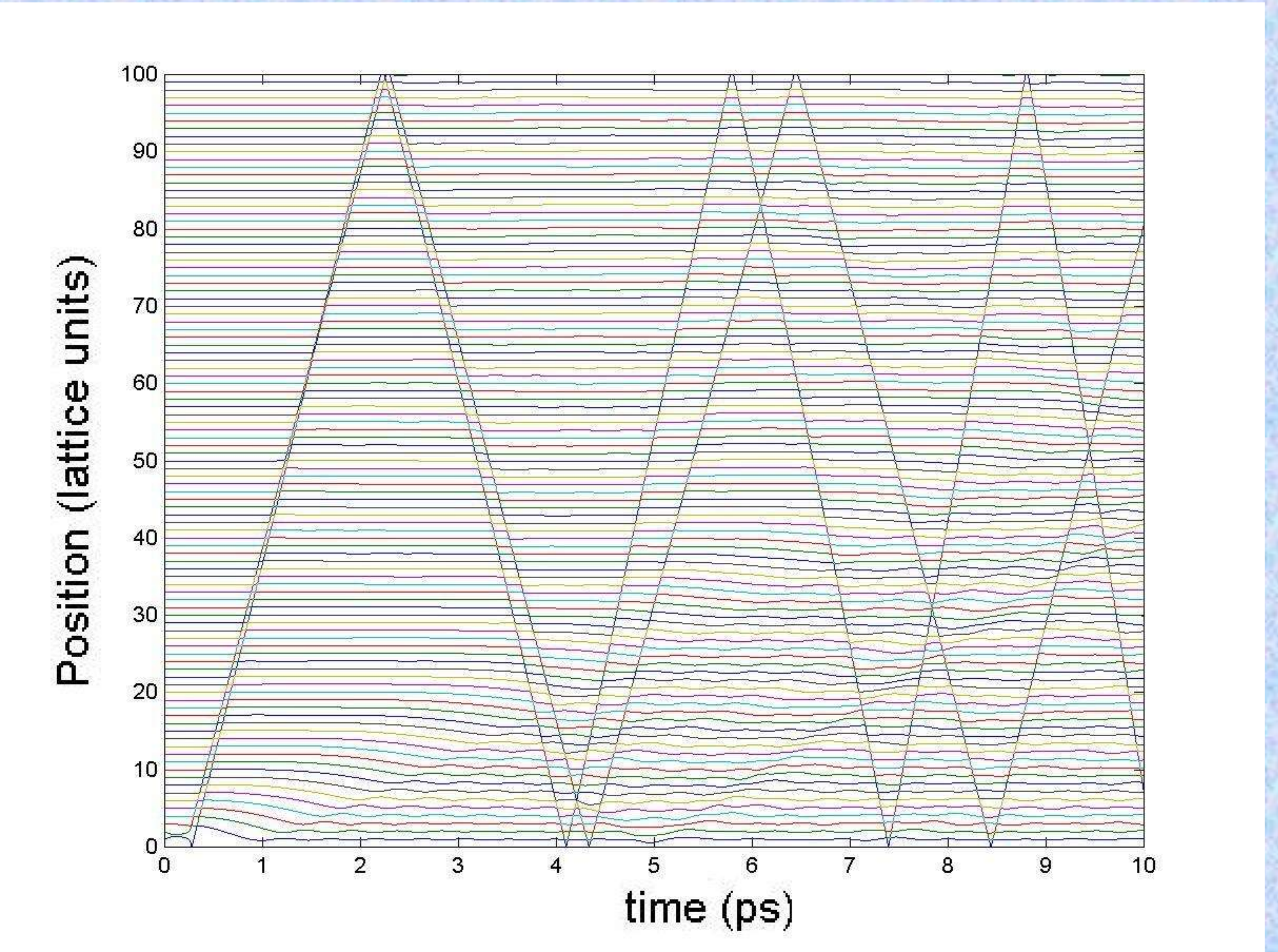
Four kinks. Profile



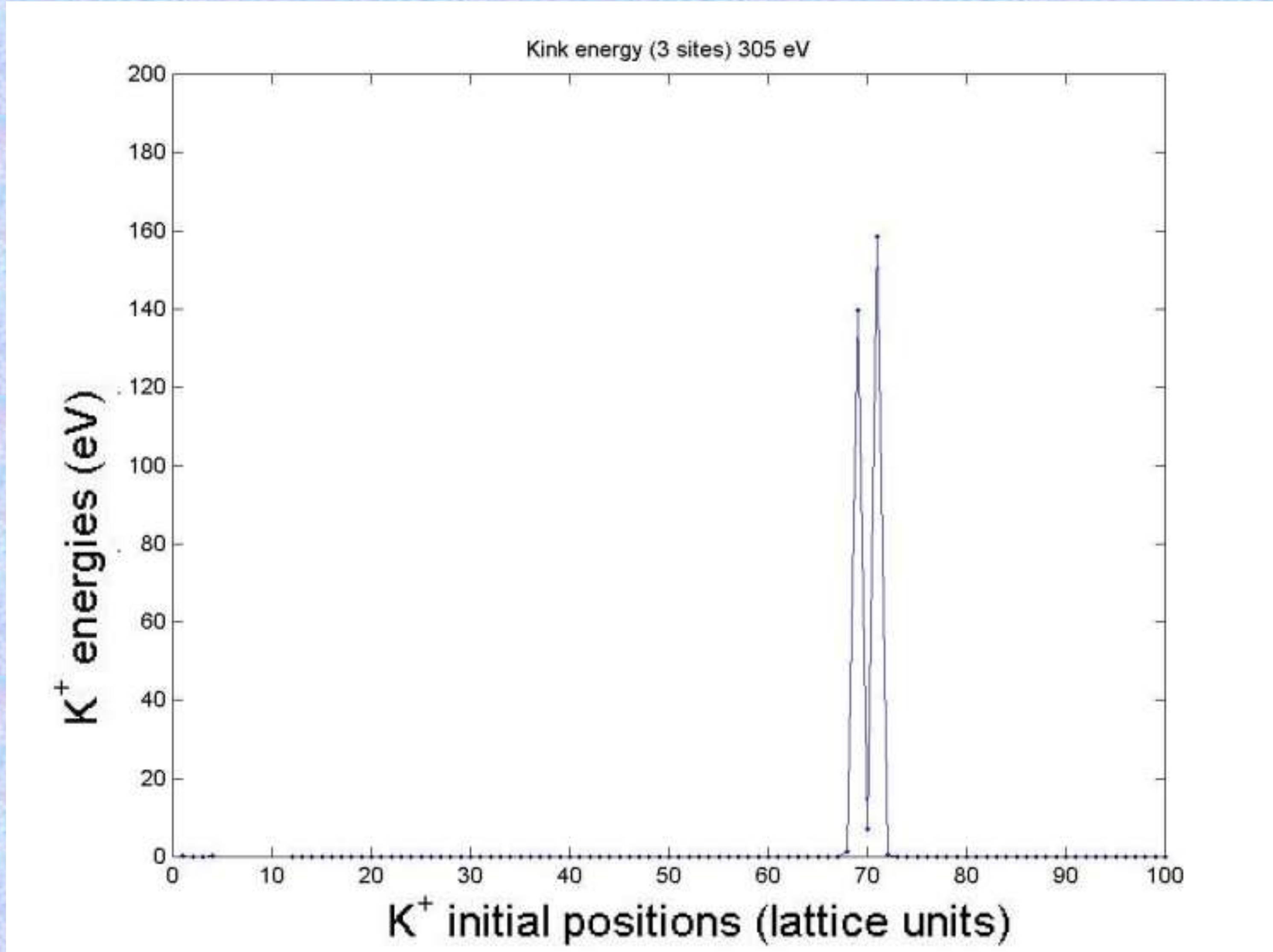
Four kinks. Video



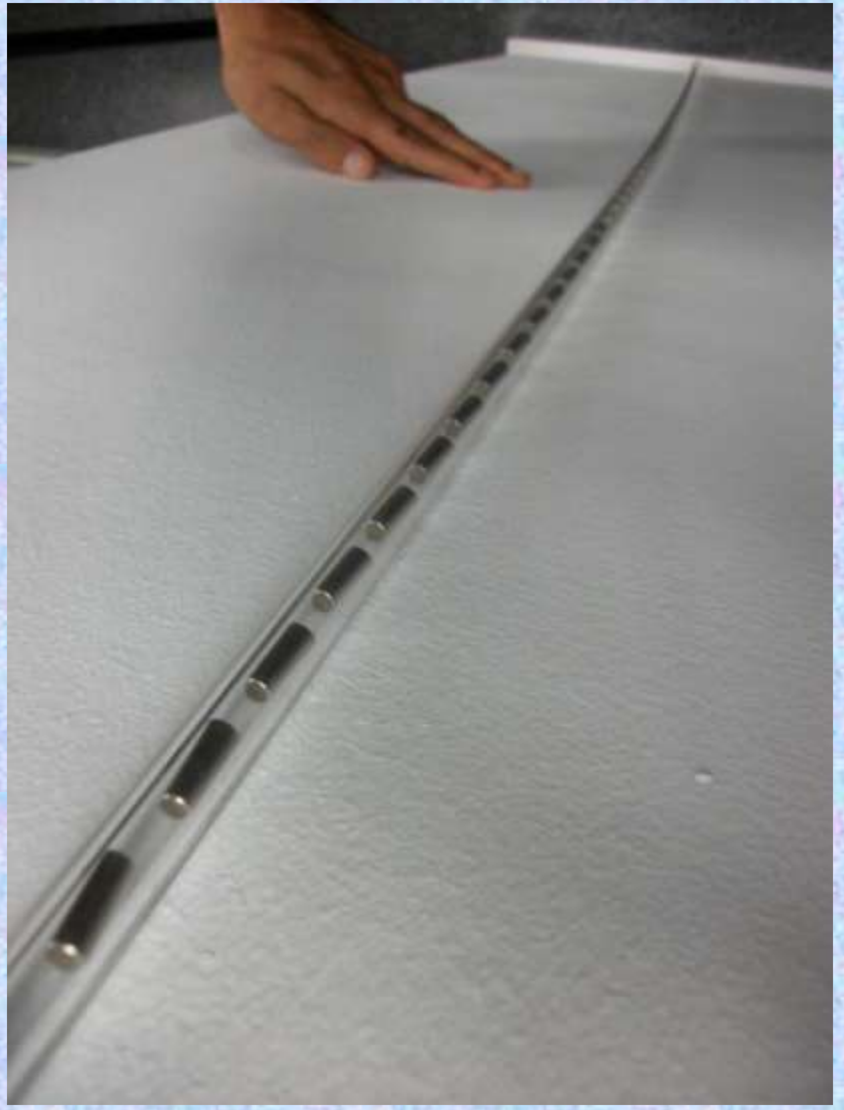
Physical units: kink: 26 km/s; phonons: 3.2 km/s



Physical units, energy profile



A magneto-mechanical model



Made out of magnets.
Potentials identical to Coulomb's

Moving and static excitations

Conclusions

- There is something energetic and localized propagating in the layers of muscovite
- A special characteristic of muscovite is that is has repulsive Coulomb's layers
- Potassium repulsion is probably the dominant interaction in the potassium layers
- Typical FPU polynomial coupling is most likely very unsuitable for muscovite layer modelling.
- There are very energetic and localized kinks travelling in Coulomb's chains with muscovite parameters, with properties well described by the theory
- Their energy can be fairly large
- Coulomb's kinks are good candidates for quodons

References

Kosevich, Yu. A., Khomeriki, R. & Ruffo, S. (2004).
Supersonic discrete kink-solitons and sinusoidal patterns with “magic” wave number in anharmonic lattices, *Europhys*, *Lett*. 66, 21-27.

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