MOVING EXCITATIONS IN CATION LATTICES

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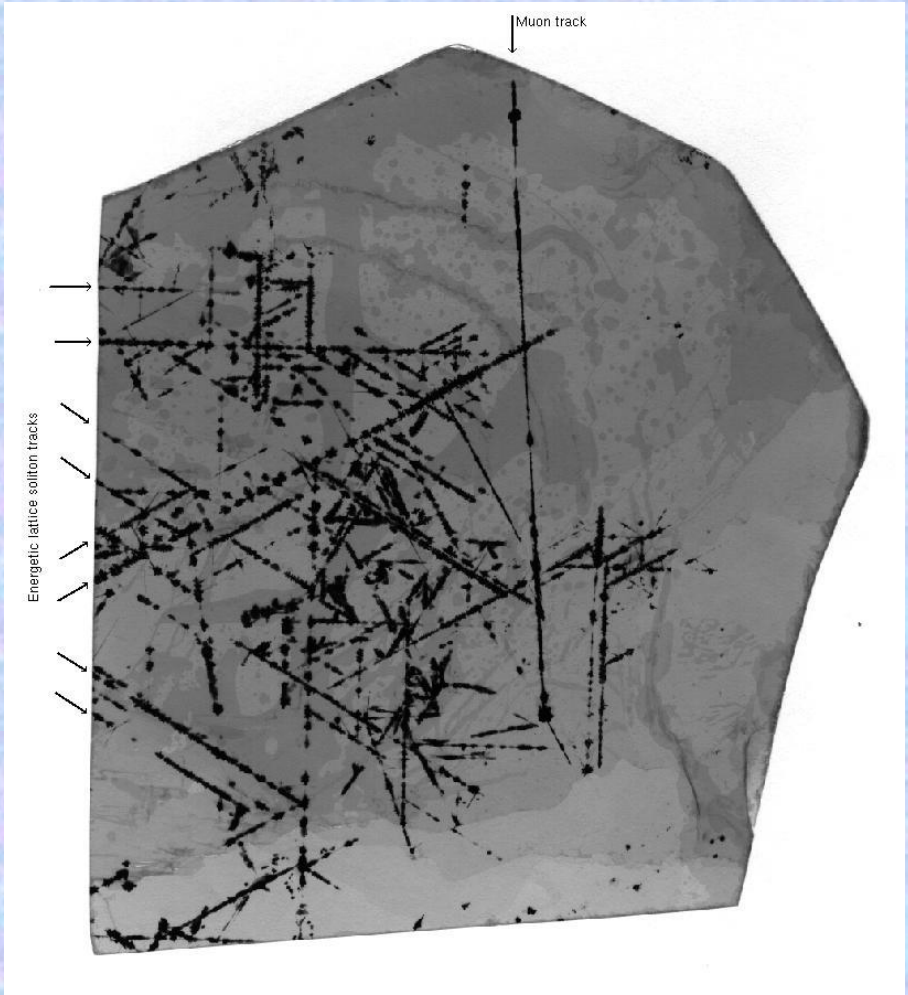


International Conference
PROBLEMS OF THEORETICAL PHYSICS
dedicated to Alexander Davydov 100th birthday
Kiev, Ucraine, October 8-11, 2012

Σκετχη οφτηε ταλκ

- 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

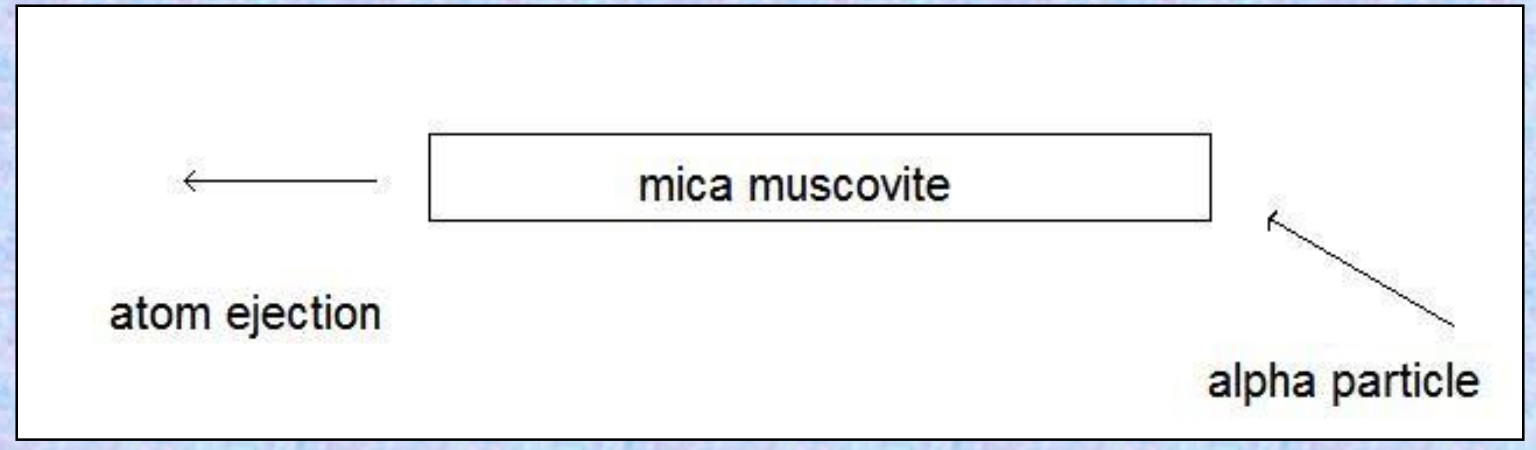
Record of muon excitations in muscovite: Quodons (Russell)



- 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.

Εξπεριμ εντα λε ωιδενχε οφ τραωελλινγ εξχιτατιονσ ιν μ ιχα μ υσχοωατε

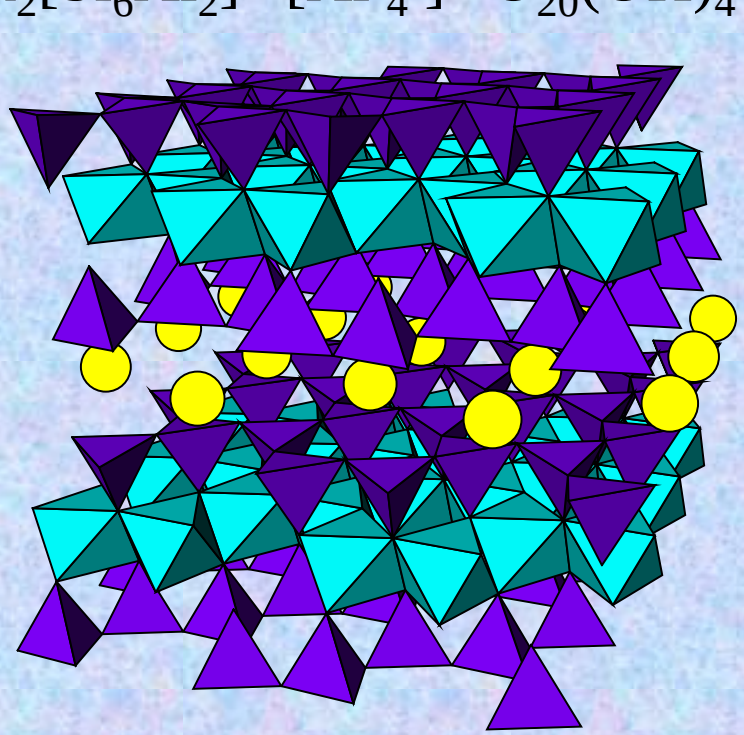


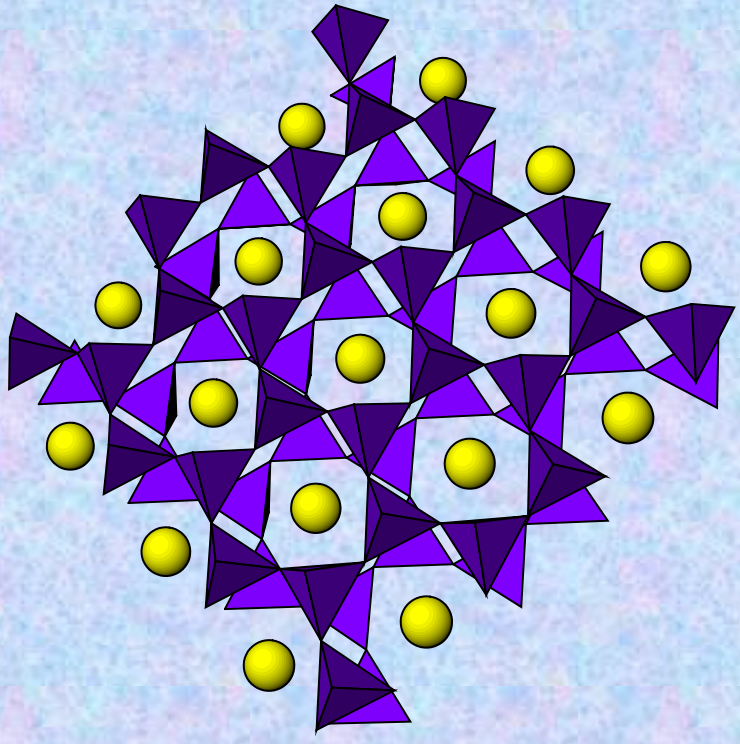
Trajectories along lattice directions within the K^+ layer

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

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



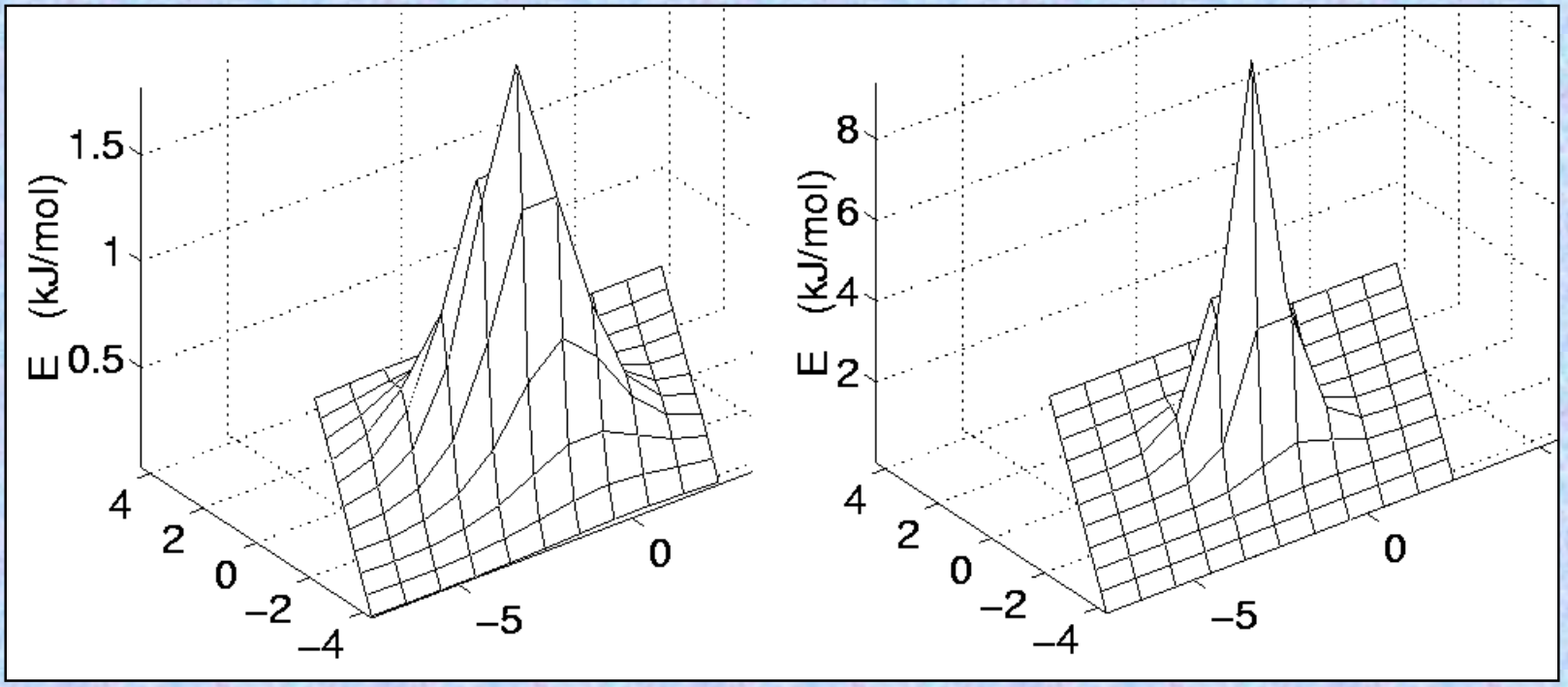


K^+

Transversal breathers have low energies and move slowly

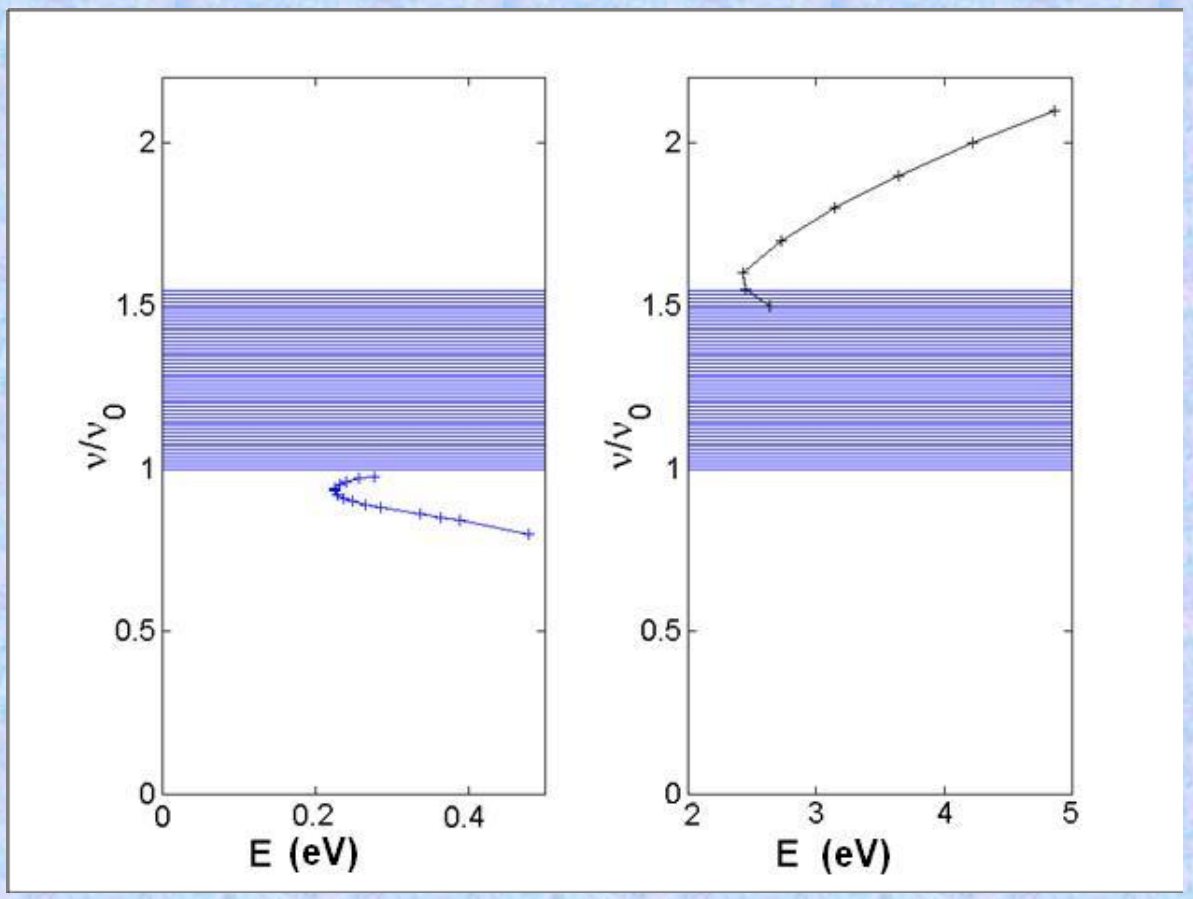
Soft breather, E=0.2~0.4 eV $\nu \sim 5 \bullet 10^{12}$ Hζ

Hard breather. E ~0.36eV



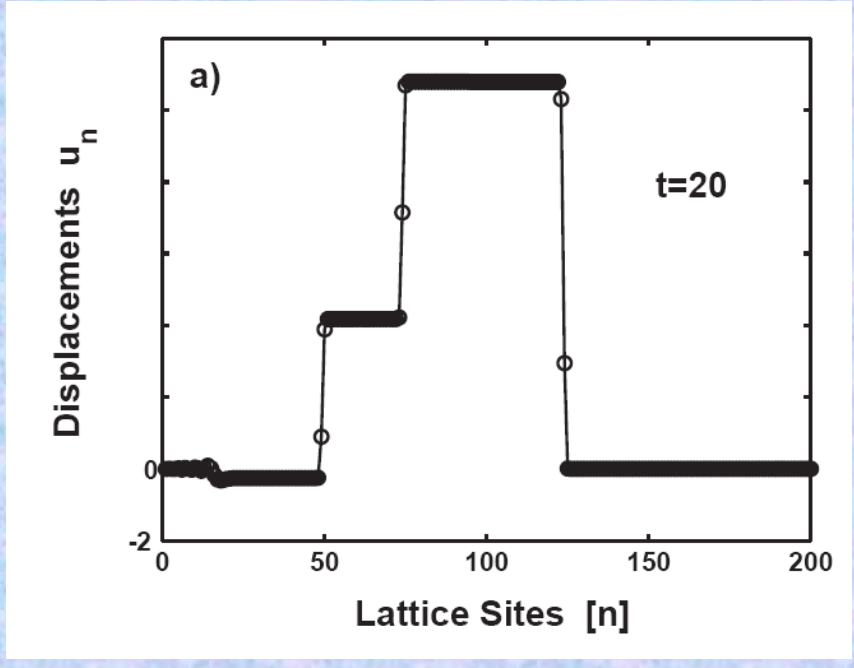
Dubinko, V.I., Selyshchev, P.A. & Archilla, J.F.R. (2011). Reaction-rate theory with account of the crystal anharmonicity. *Phys. Rev.* E 83, 041124, 1-13

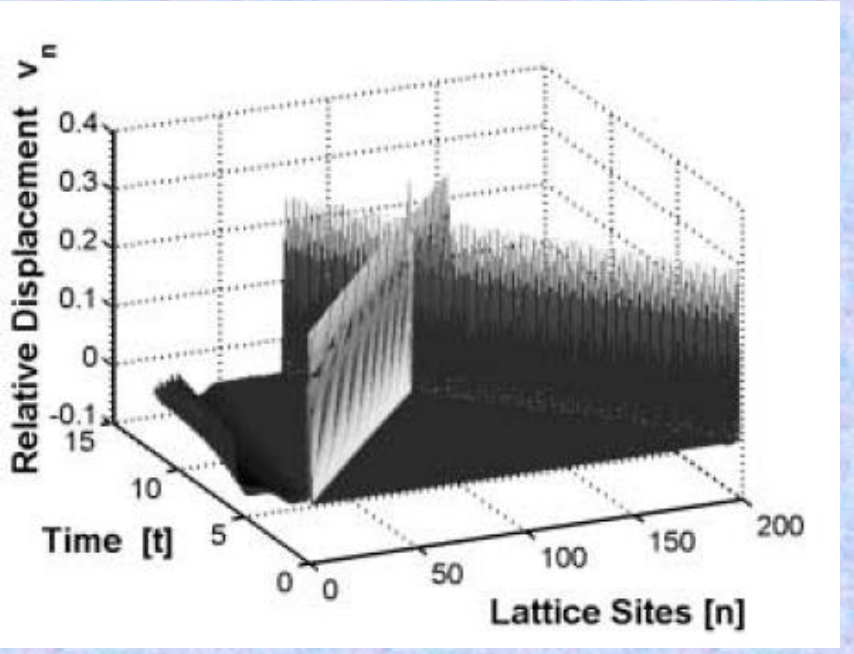
Transversal soft and hard breather spectra



$\nu_0 = 167.5 \chi \mu^{-1}$
$\sim 5 \bullet 10^{12}$ Hζ
~20 μ ες

Supersonic kinks move very fast and have large energies.

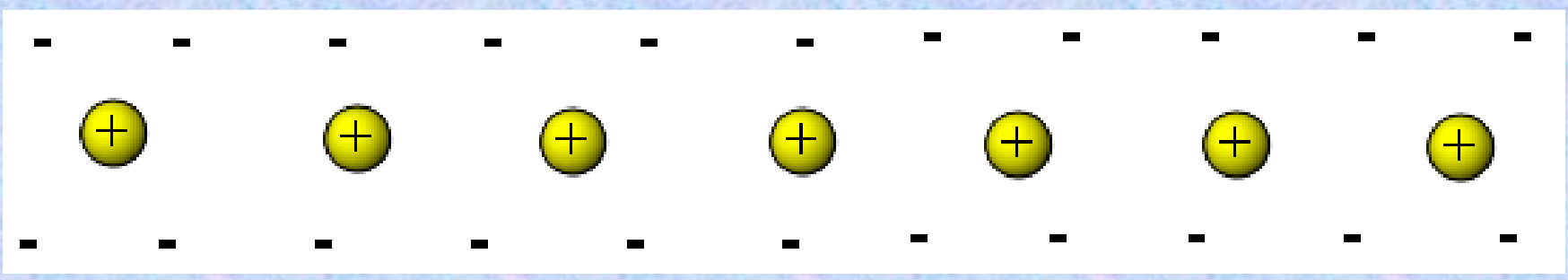




Transversal kinks in a beta FPU lattice

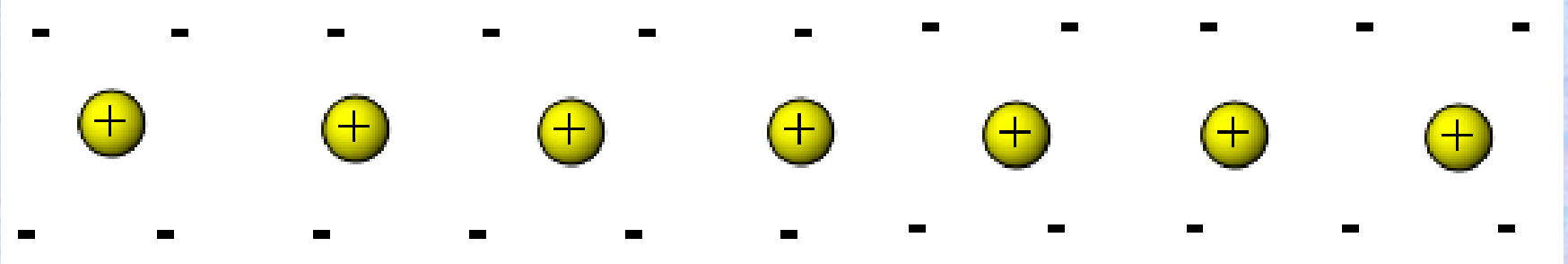
Yu A Kosevich, c, R & Ruffo, S. (2004). Supersonic discrete kink-solitons and sinusoidal patterns with "magic" wave number in anharmonic lattices. *Europhys. Lett.*, 66, 21–27.

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

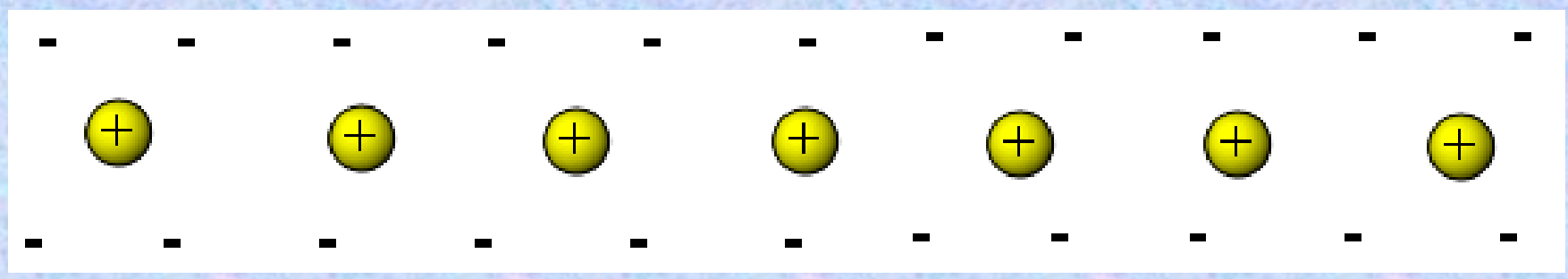


$$m_K \frac{\mathrm{d}^2 x_n}{\mathrm{d}t^2} = -\frac{Ke^2}{(x_{n+1} - x_n)^2} + \frac{Ke^2}{(x_n - x_{n-1})^2}$$

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

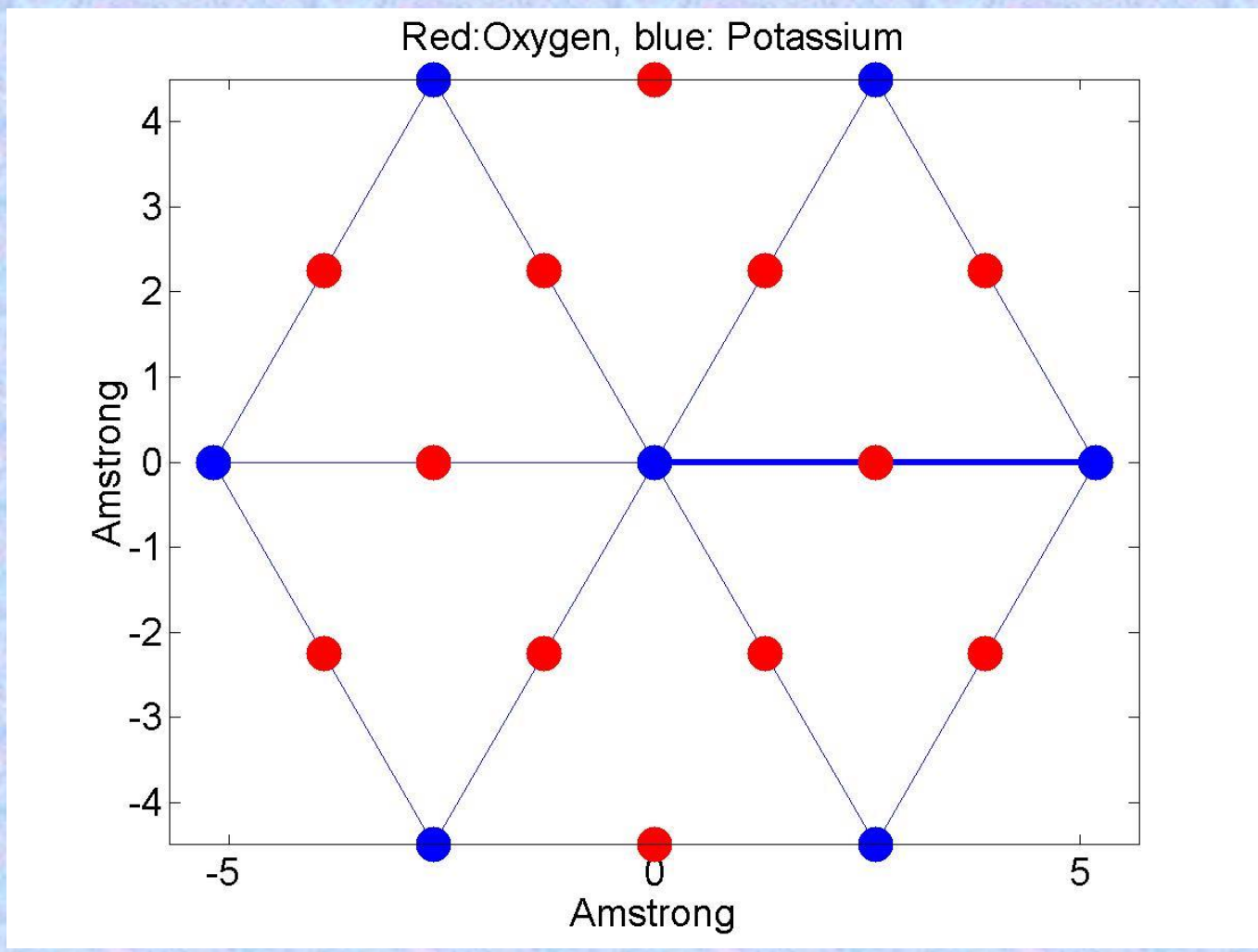
$$\text{Units:} \quad \text{a} = 5.19\,\text{A}, \quad \tau = \frac{1}{\omega_0} = \sqrt{\frac{m_K a^3}{2Ke^2}} \cong 0.2\,\text{ps}$$

What's spetial about Coulomb's repulsión?



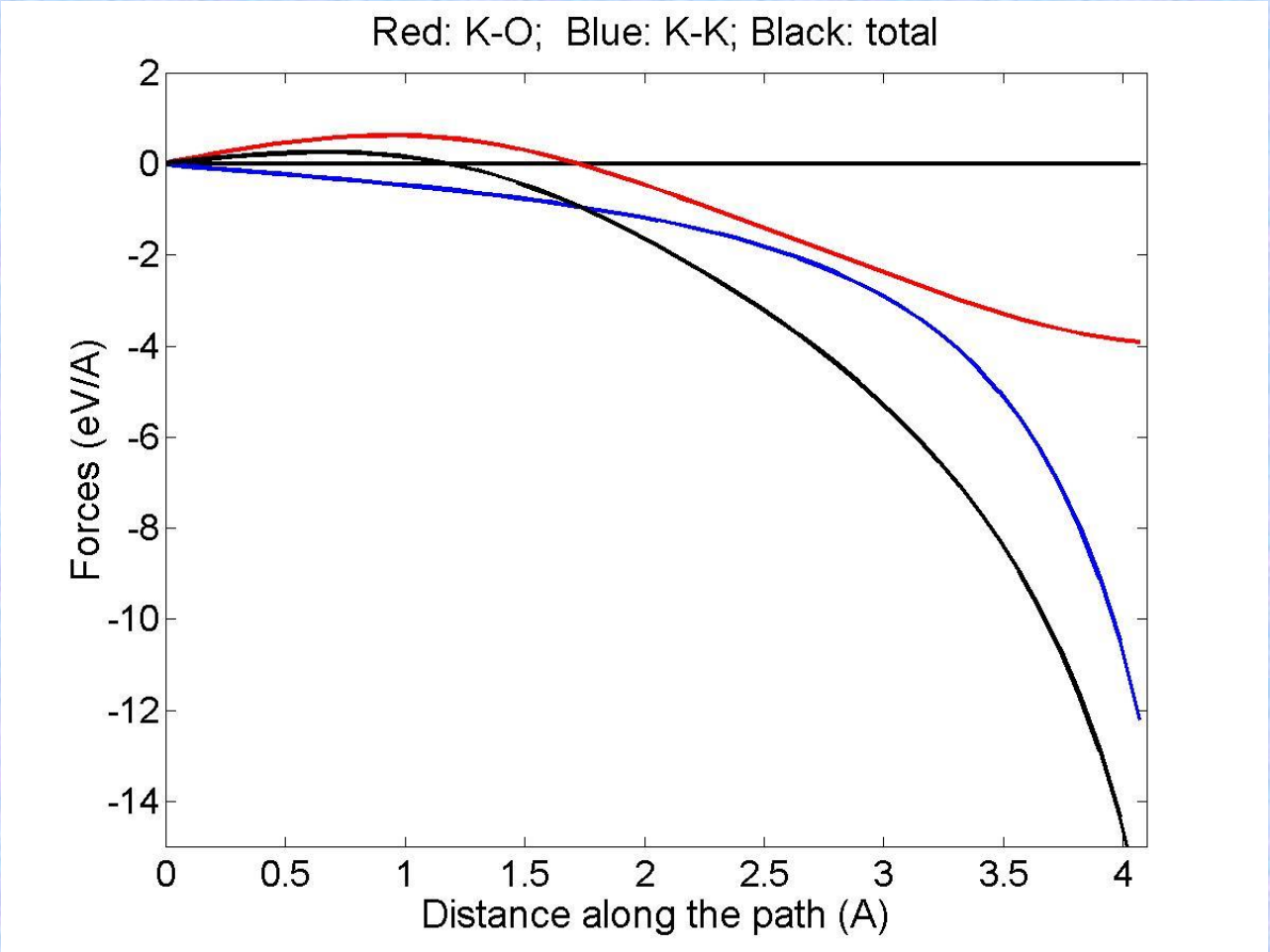
- Forces decay, fewer phonons as compared with harmonics.
- We now that it is there
- There is not a potential well
- Forces that increase with the distance are not a good physical description for this system with large perturbations.

Is the model absurd?



Muscovite empirical potentials

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



Coulomb interaction

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

Phonon spectrum

Linearized equation:

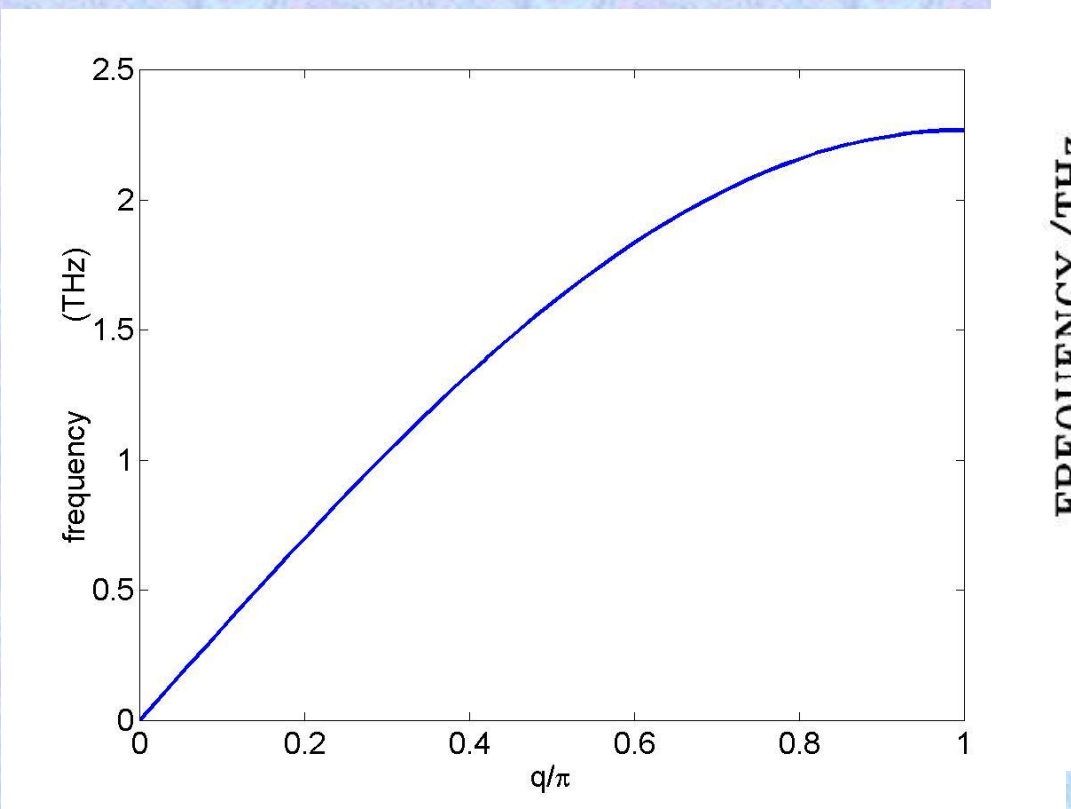
$$\ddot{u}_n = c^2(u_{n+1} + u_{n-1} - 2u_n) \qquad c = \sqrt{2} \ \text{speed of sound}$$

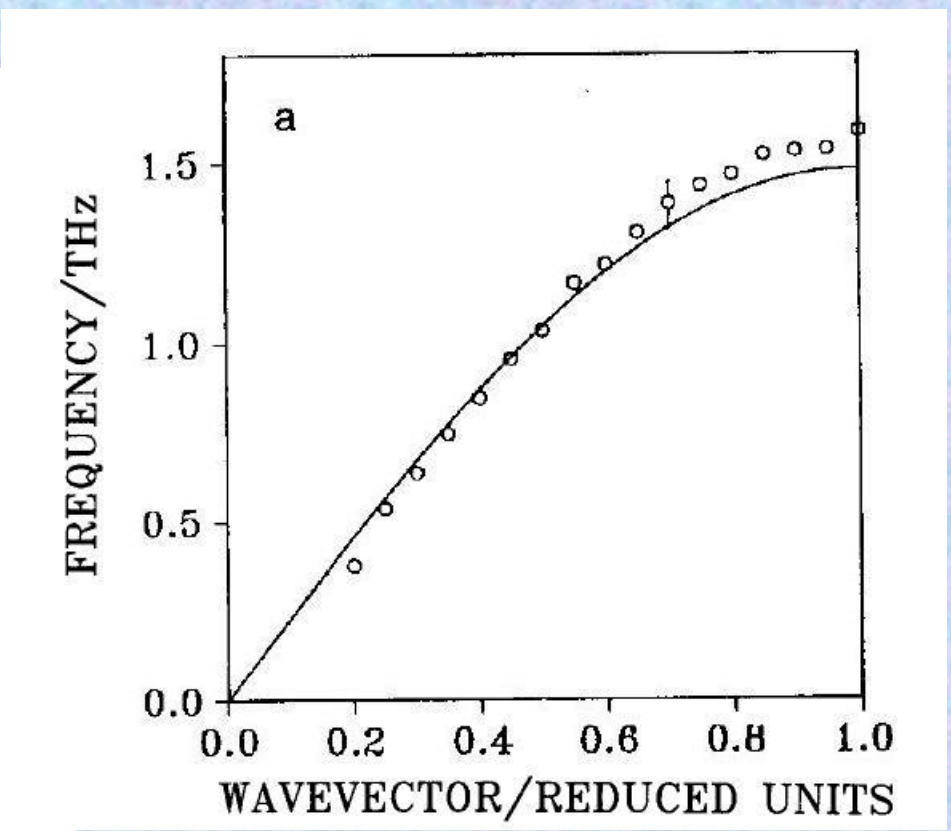
$$\omega_{\text{ph}} = \omega_{\text{M}} \sin(\frac{q}{2}) \qquad \text{Maximum phonon frequency } \omega_{\text{M}} = 2c$$

$$V_{\text{ph}} = \frac{2c\sin(\frac{q}{2})}{q} \ ; \ V_{\text{group}} = c\cos(\frac{q}{2}) \qquad V_{\text{ph,max}} = V_{\text{group,max}} = c$$

How they compare with experiments?

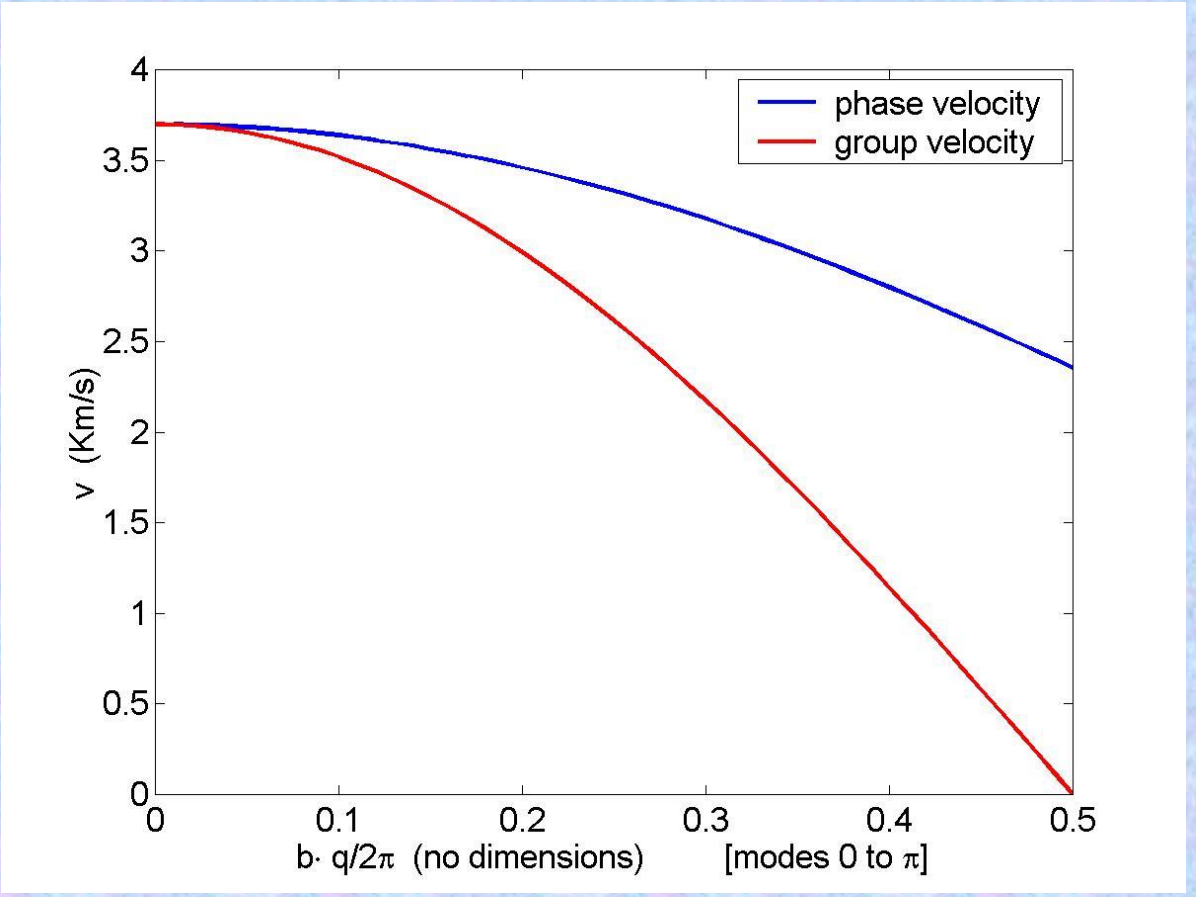
Phonon spectrum





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

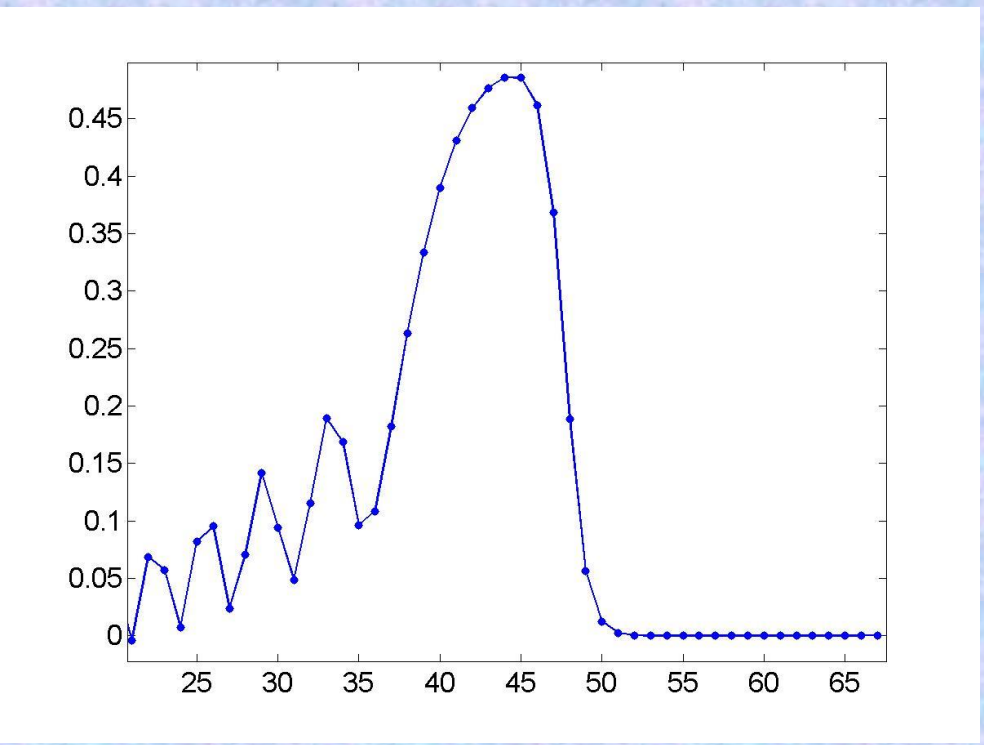
G. Brudeylins, D. Schmicker, Elastic and inelastic helium atom scattering at a cleaved mica sheet. *Surface Science*, 333: 237-242 (1995).

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

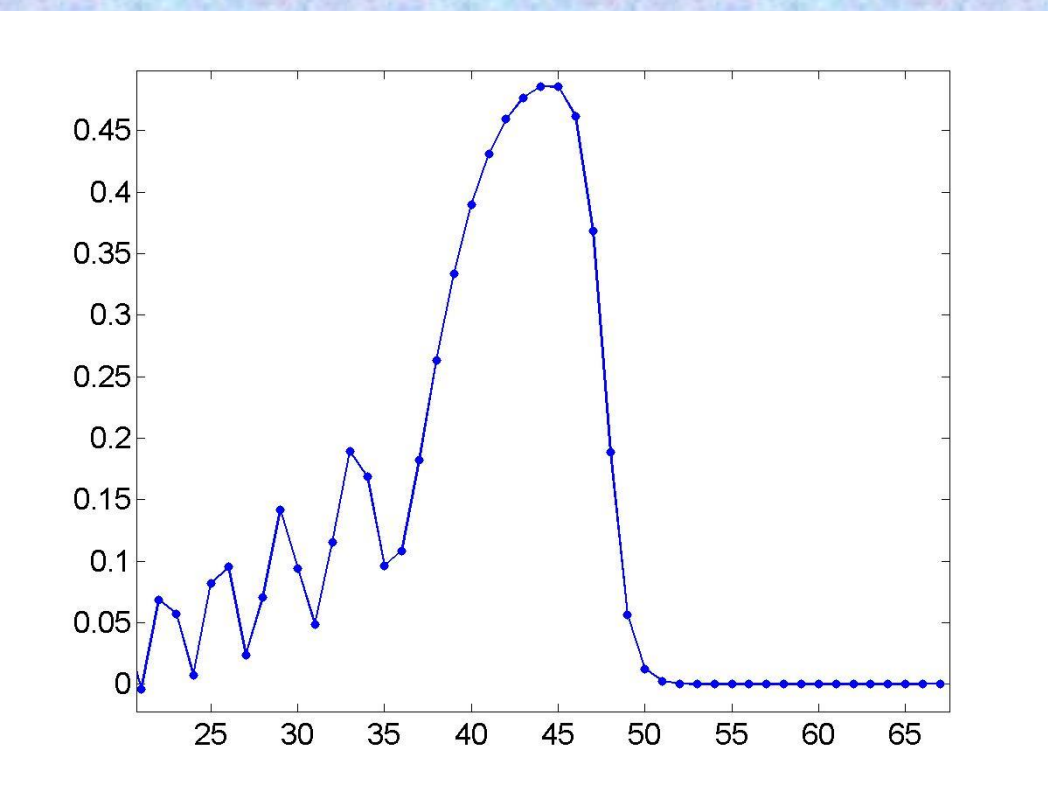
Supersonic solitons: moving, localized, non-oscillating solutions

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

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

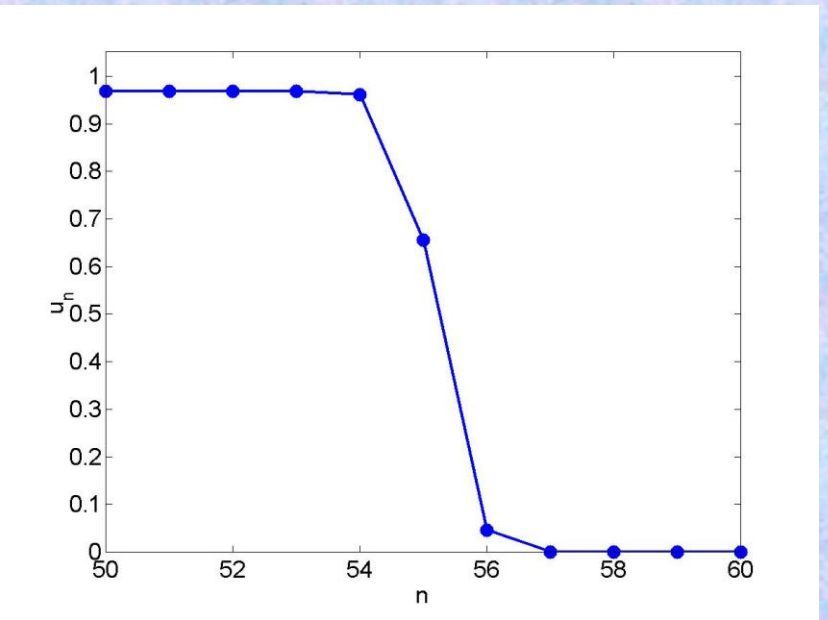
v is alway larger than the sound velocity.

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: $q = \frac{2\pi}{3}$, 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 $\theta = qn - \omega t$

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

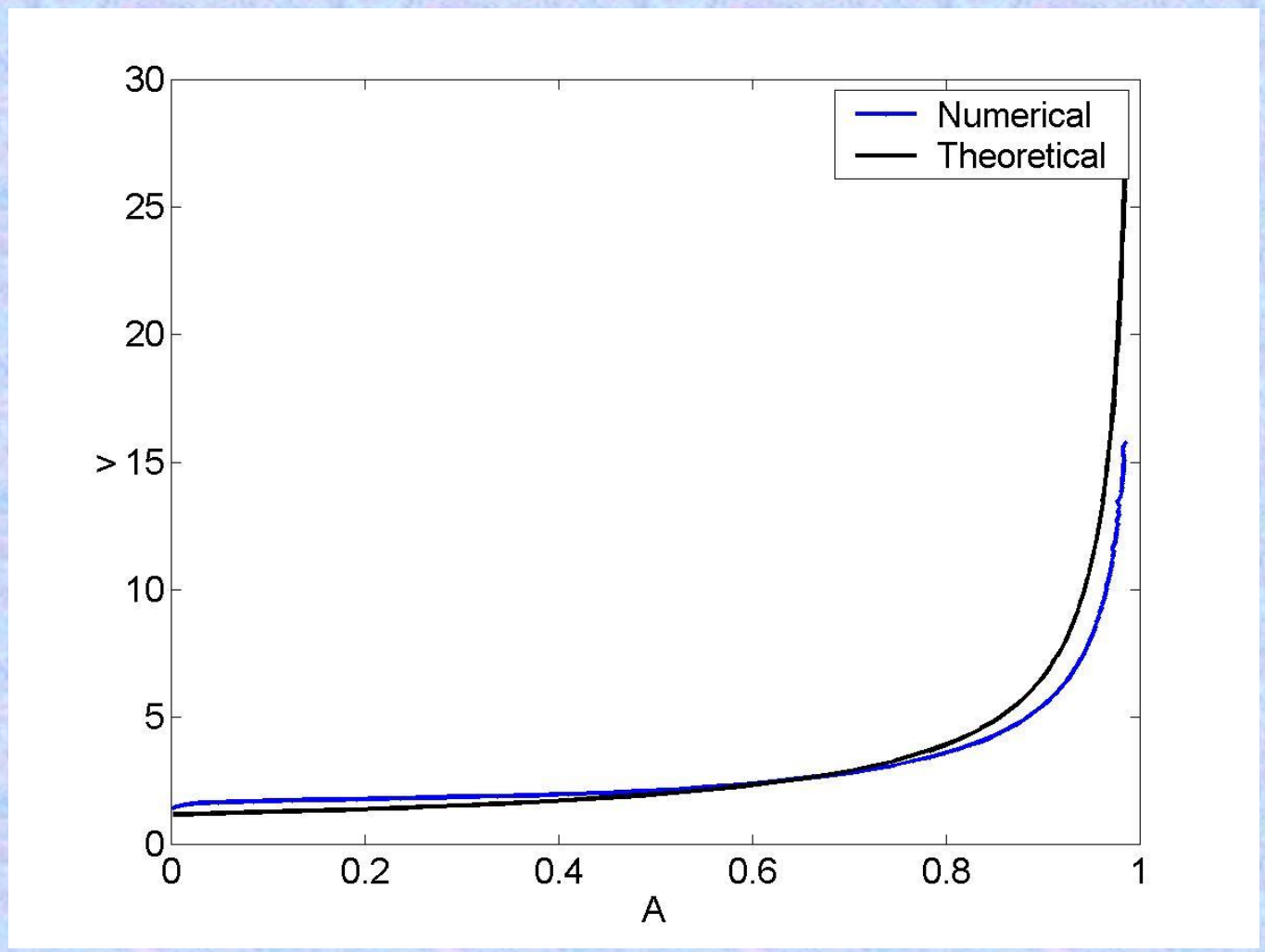
$$a_1 = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2}(F_n - F_{n+1} - F_{n-1})\cos(\theta)\,\mathrm{d}\theta$$

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

Kinks are also supersonic

Kinks RWA, velocity versus amplitude

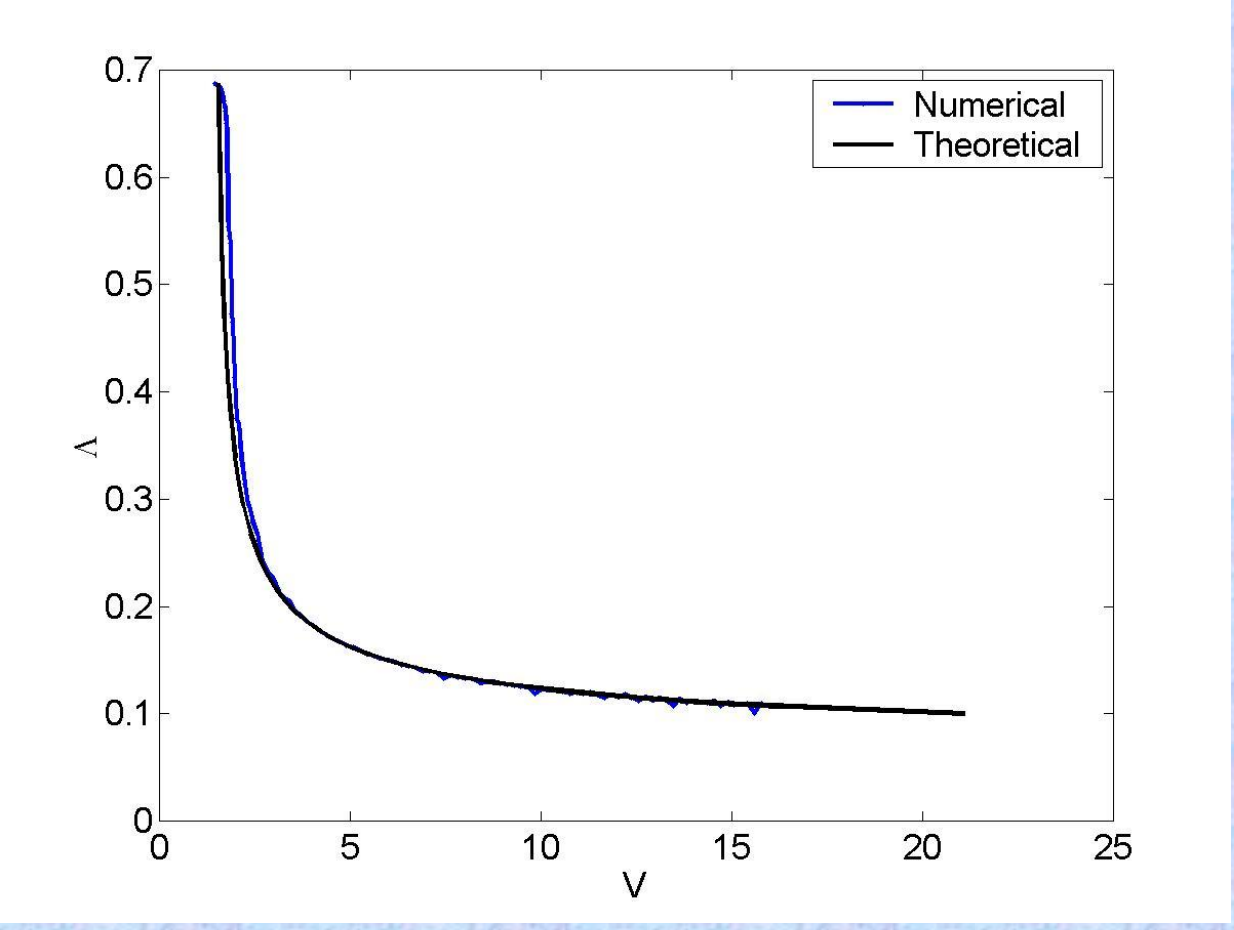
$$V = \frac{3\sqrt{3}c}{2\pi(1-A)^{3/4}}$$



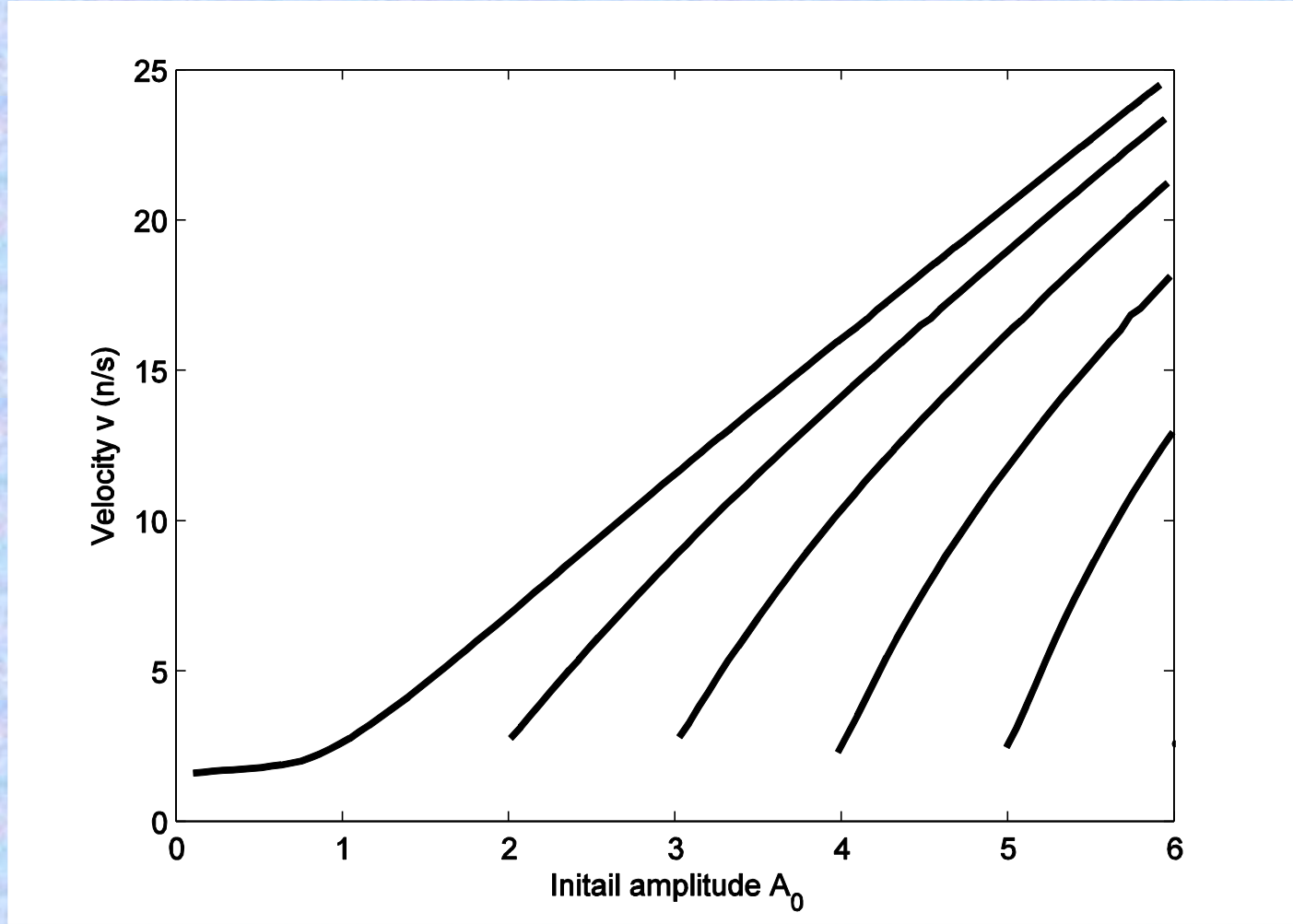
Kinks tails, decay lenght versus velocity

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

$$\text{with } \Lambda = \frac{1}{\xi}$$

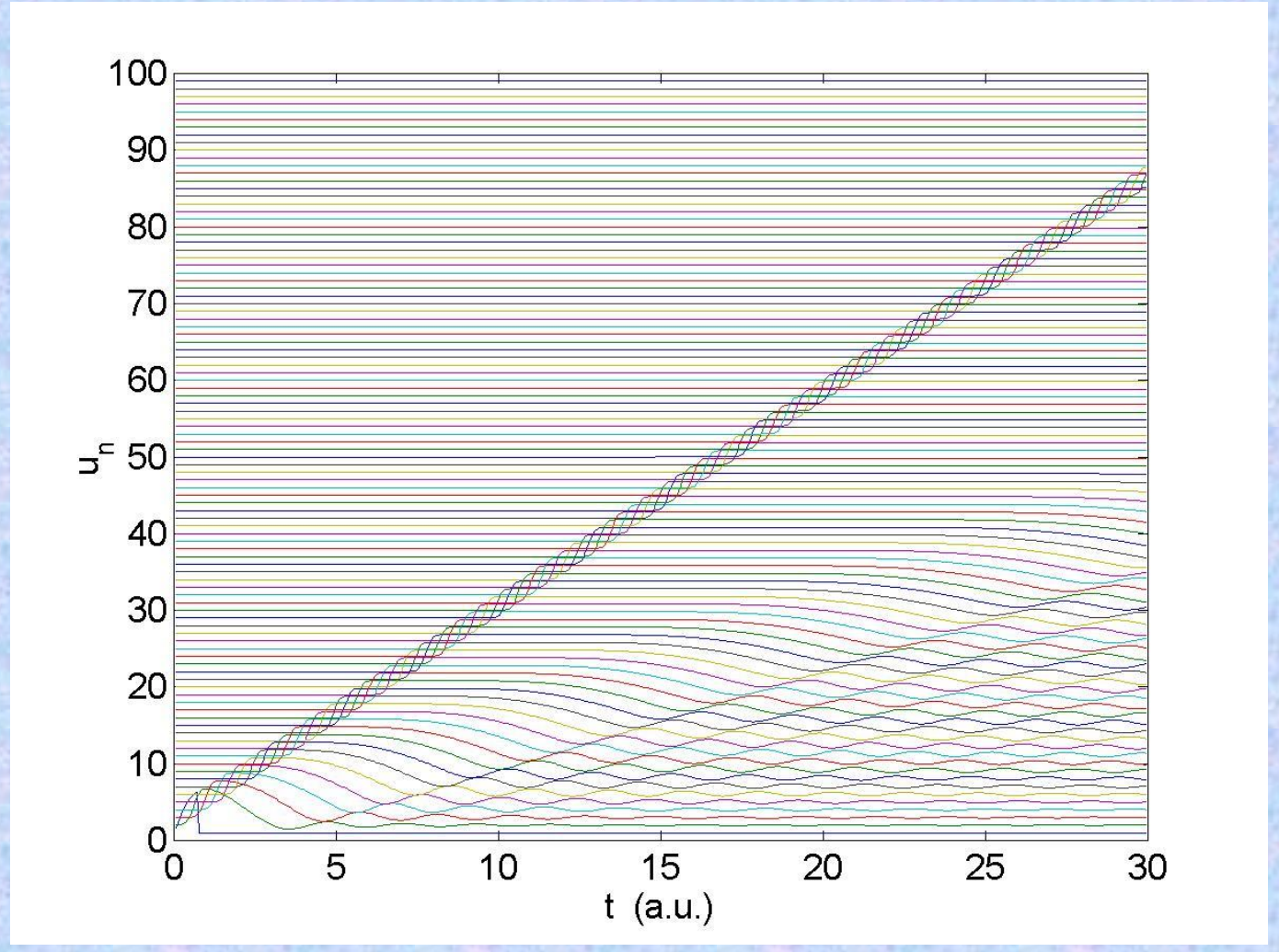


Kink simulation, Velocity-Initial amplitude



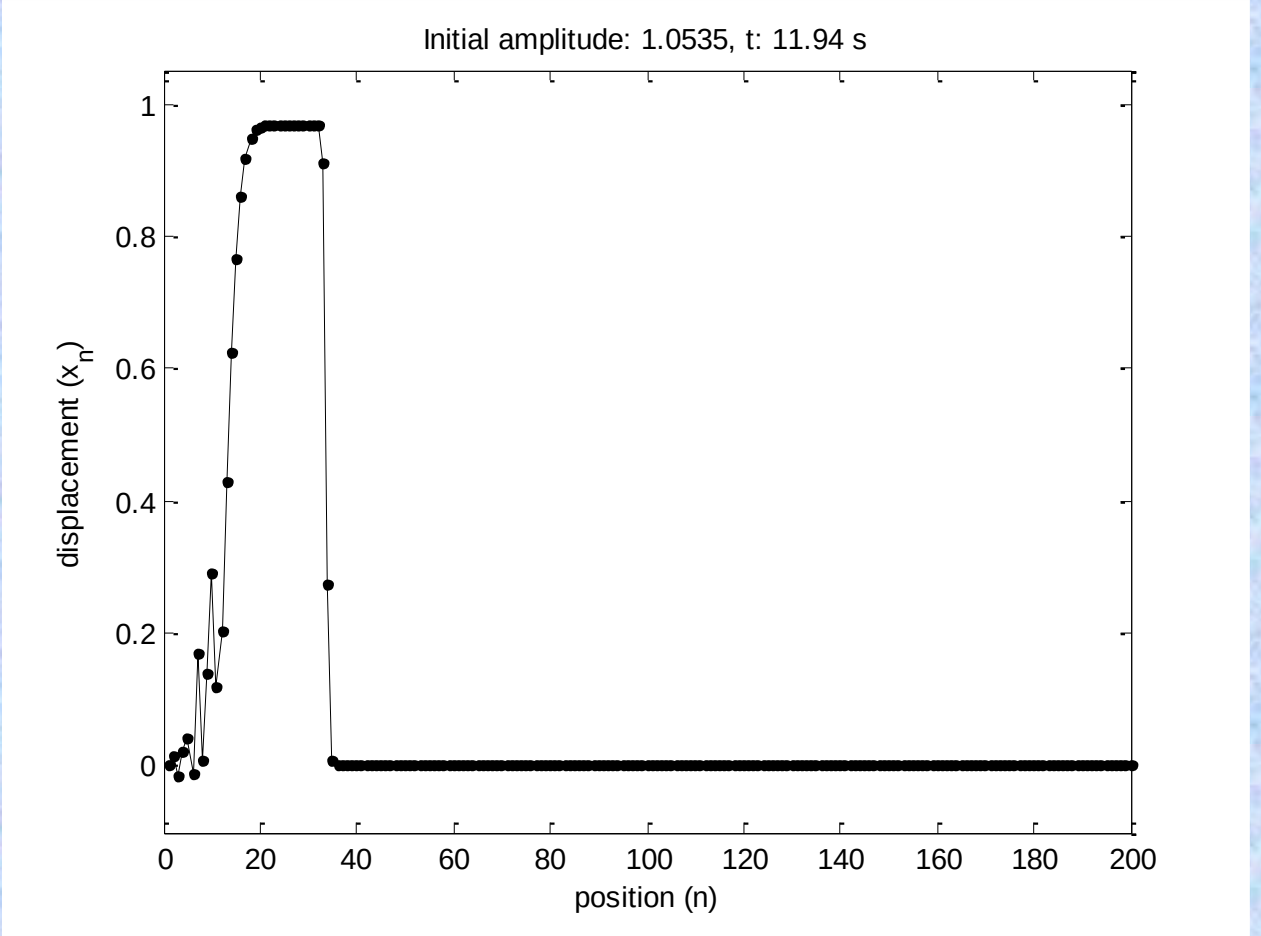
Single supersonic kink. Simulation

$$V = 2c$$



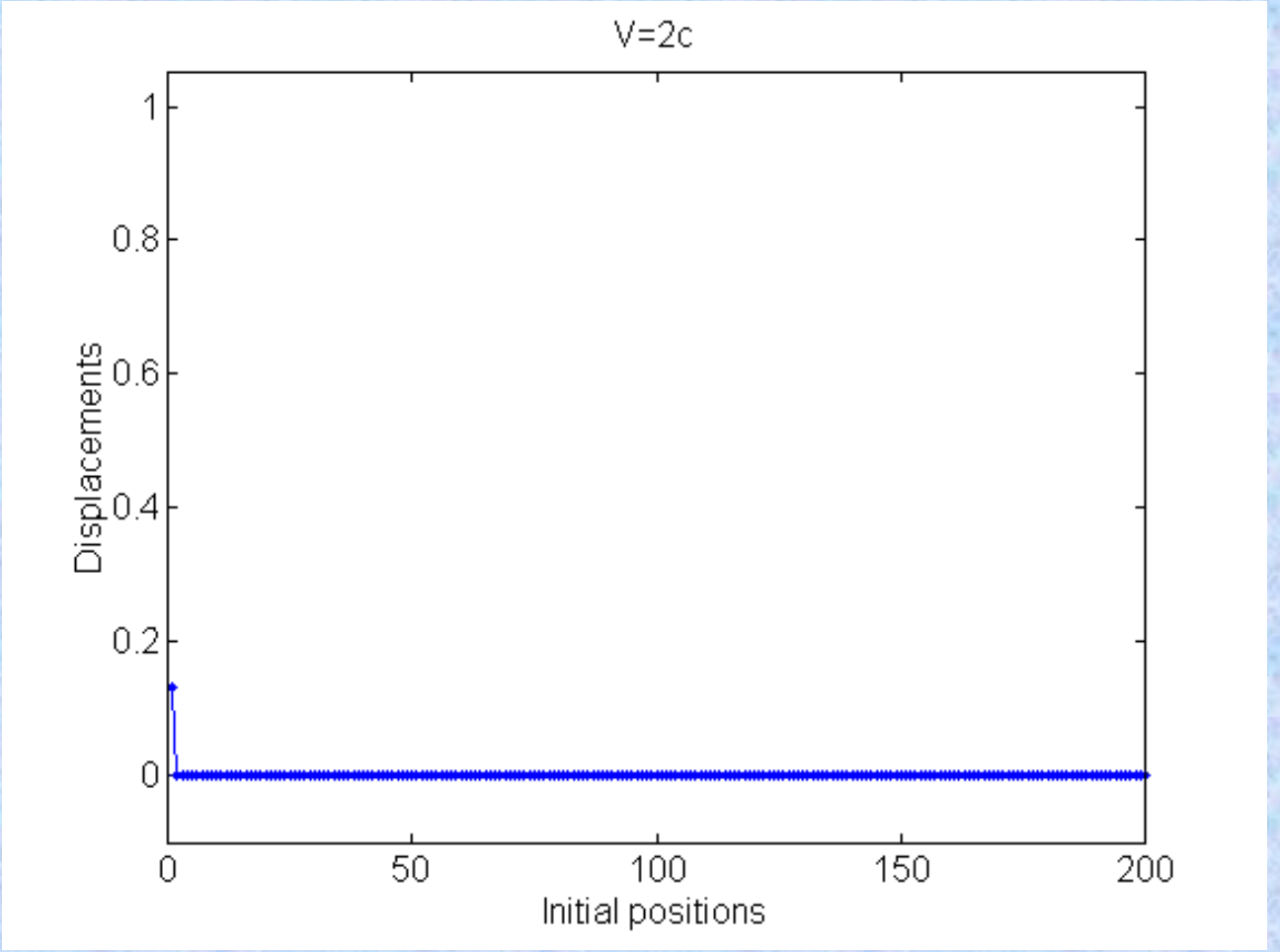
Single supersonic kink. Profile.

$$V = 2c$$



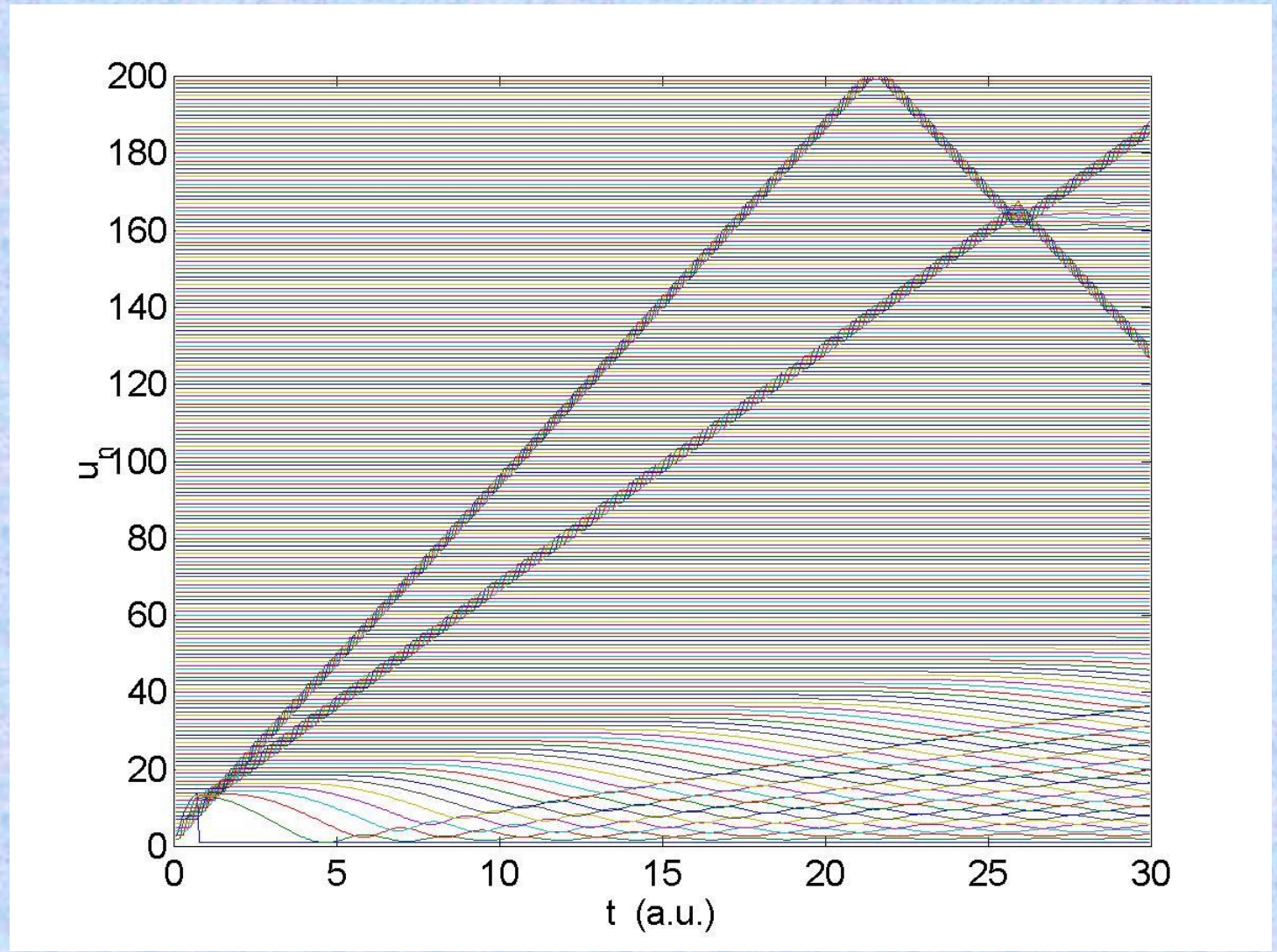
Single supersonic kink. Video.

$$V = 2c$$



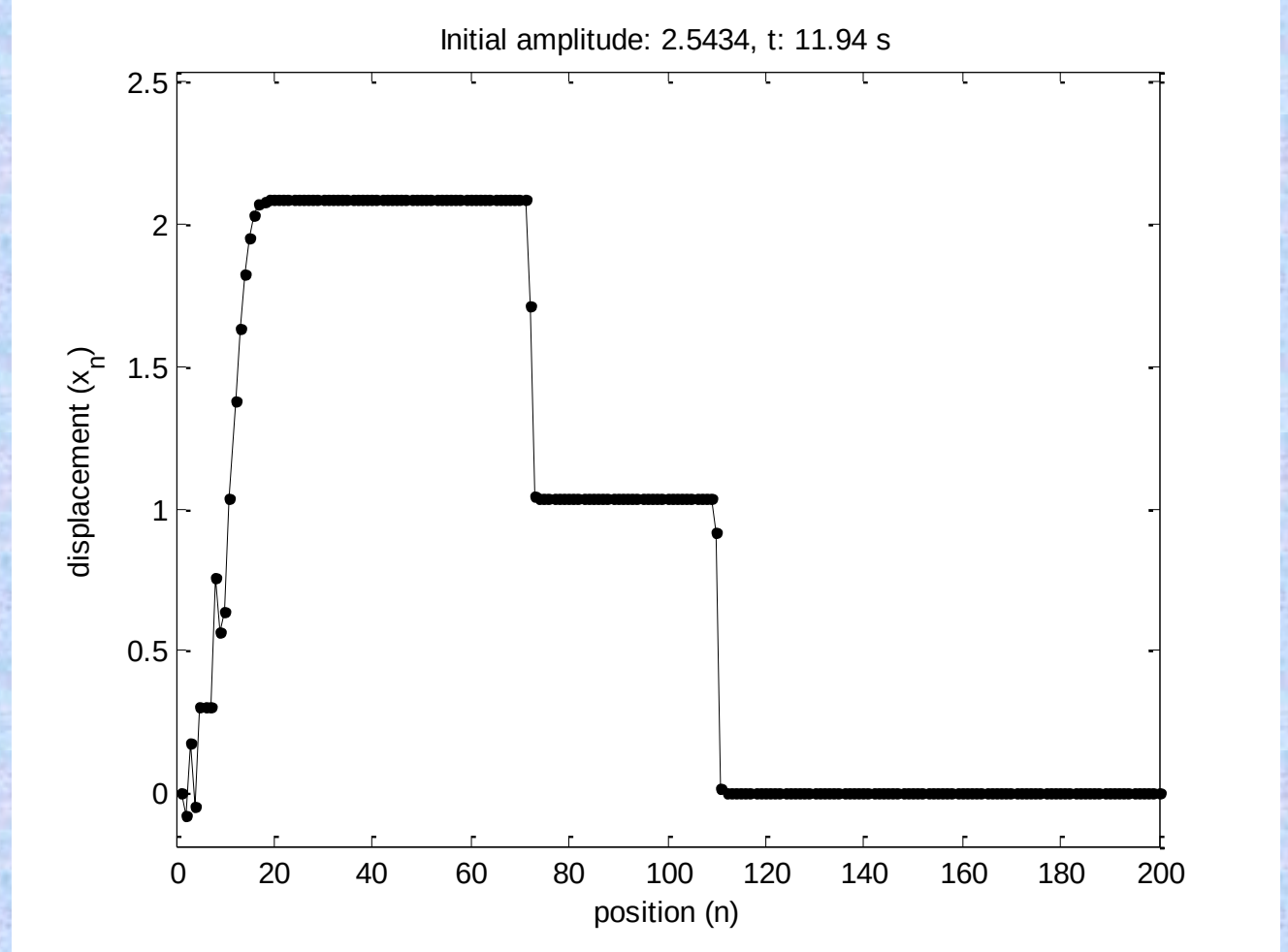
Double supersonic kink. Simulation

$$V = 4.1c$$



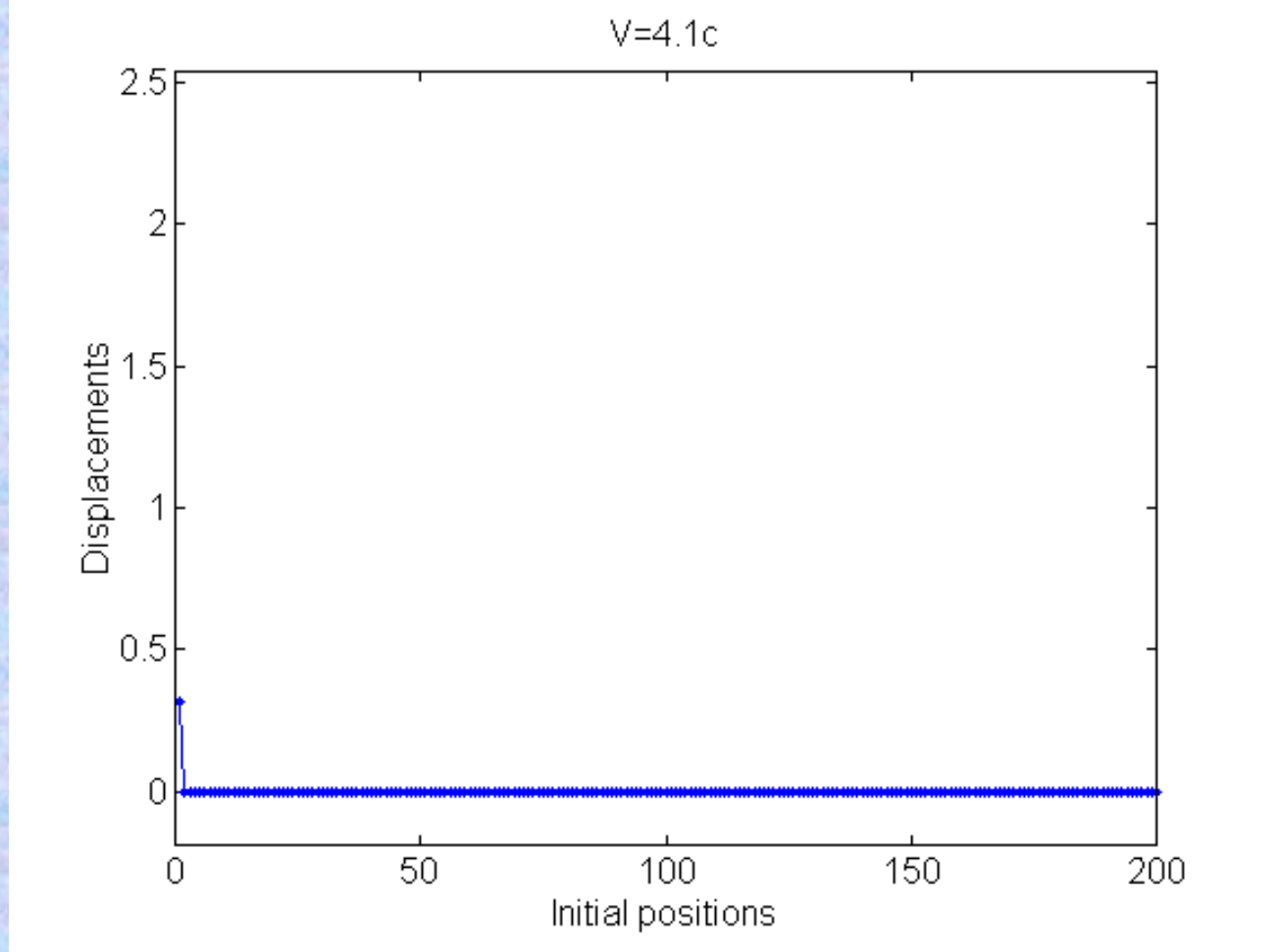
Double supersonic kink. Profile

$$V = 4.1c$$

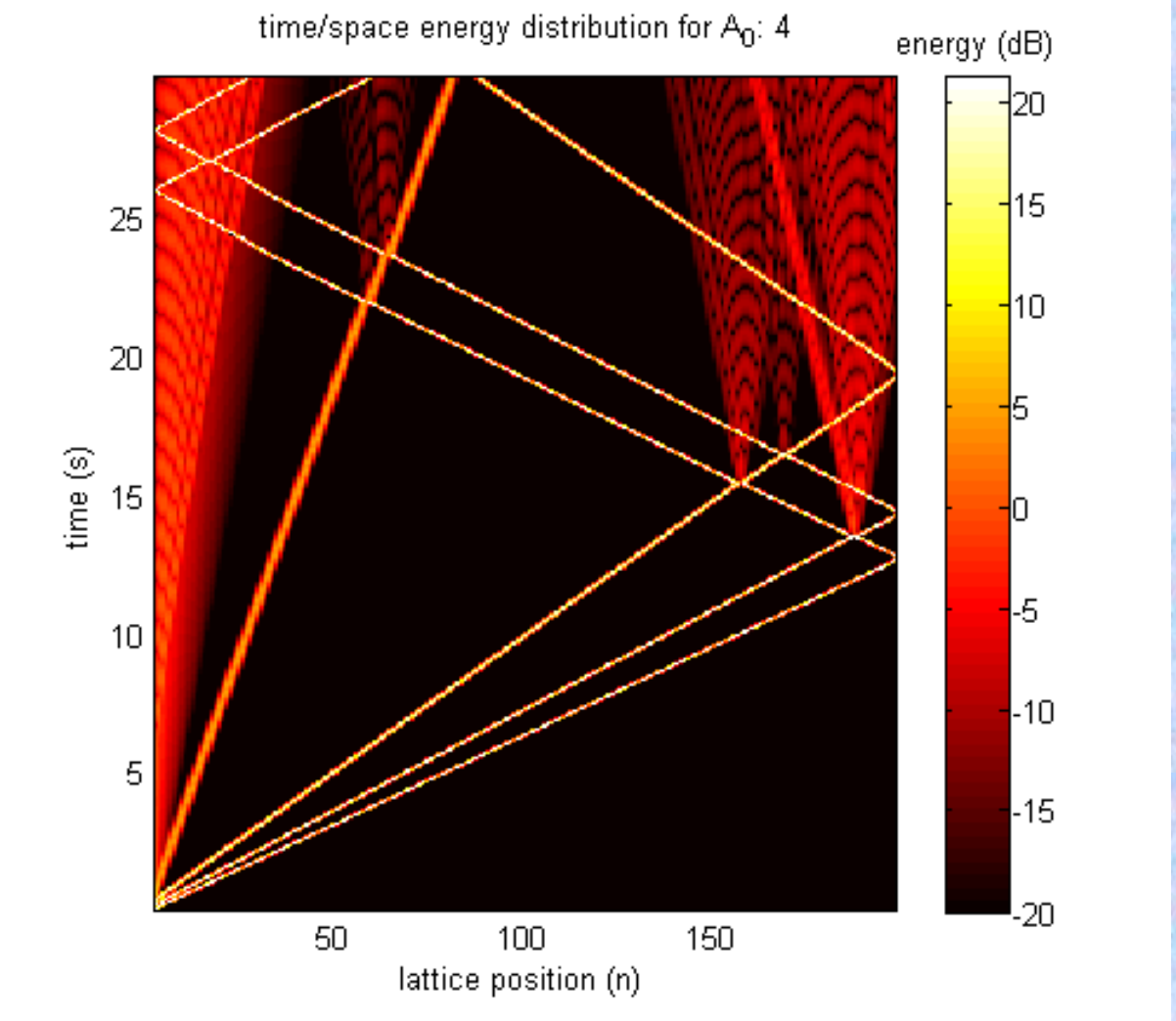


Double supersonic kink. Video

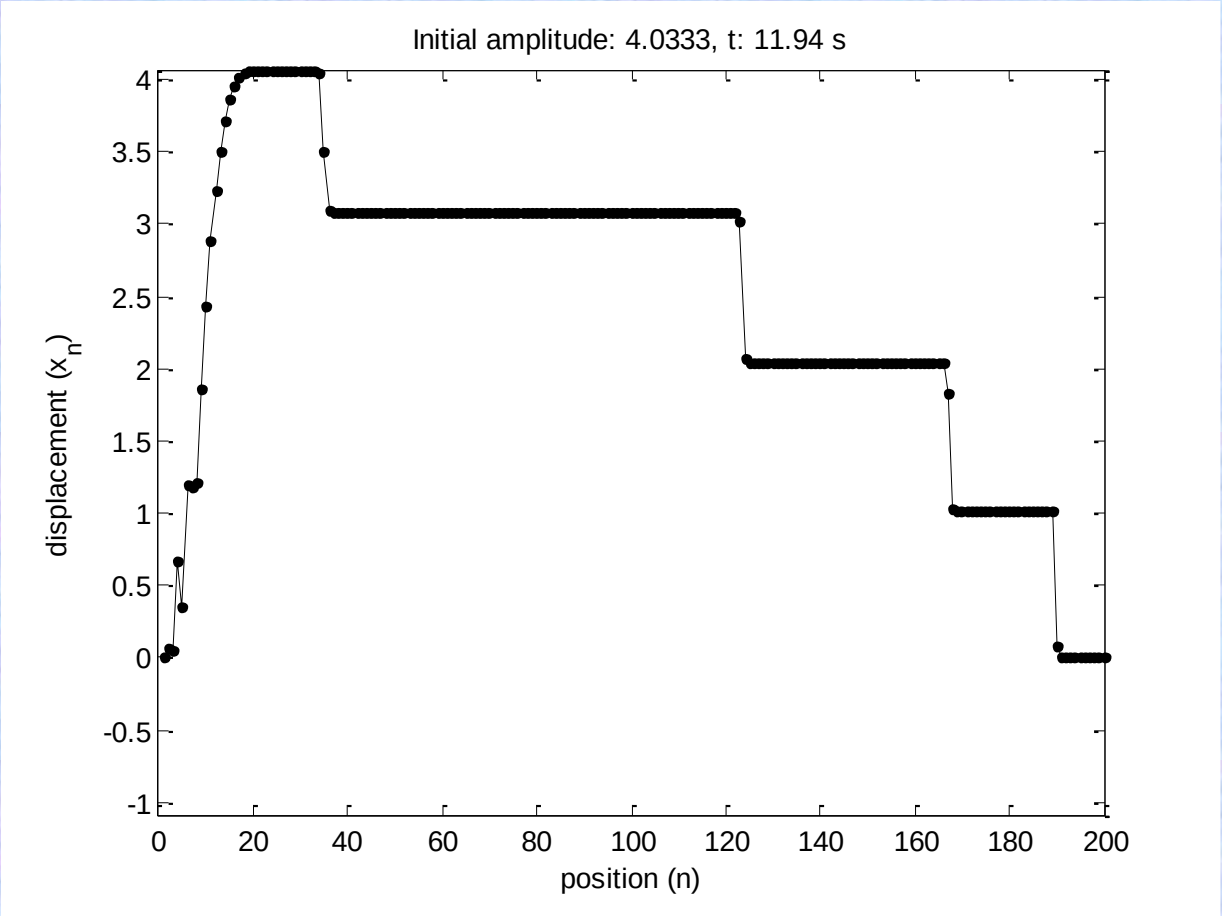
$$V = 4.1c$$



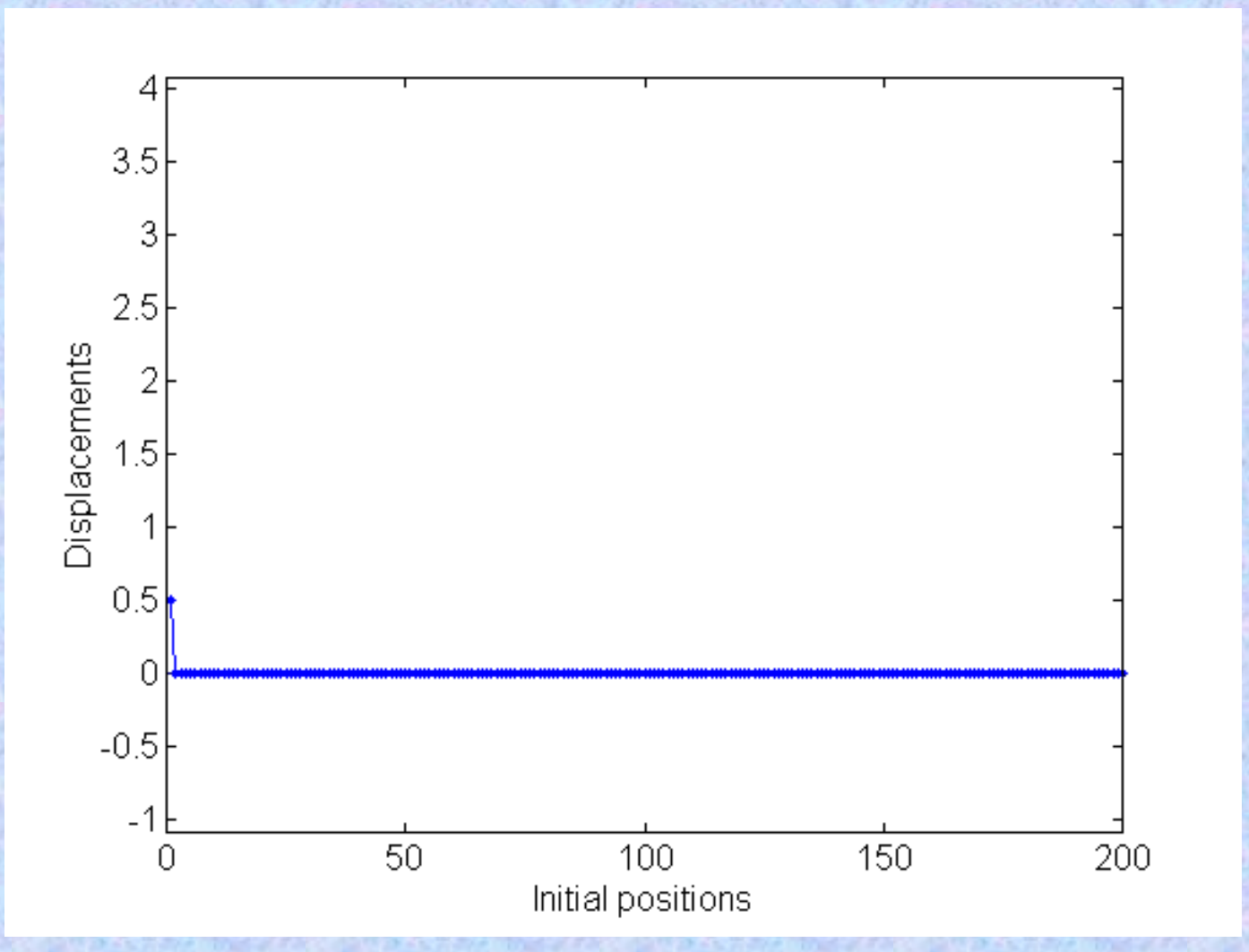
Three kinks. Energy-time



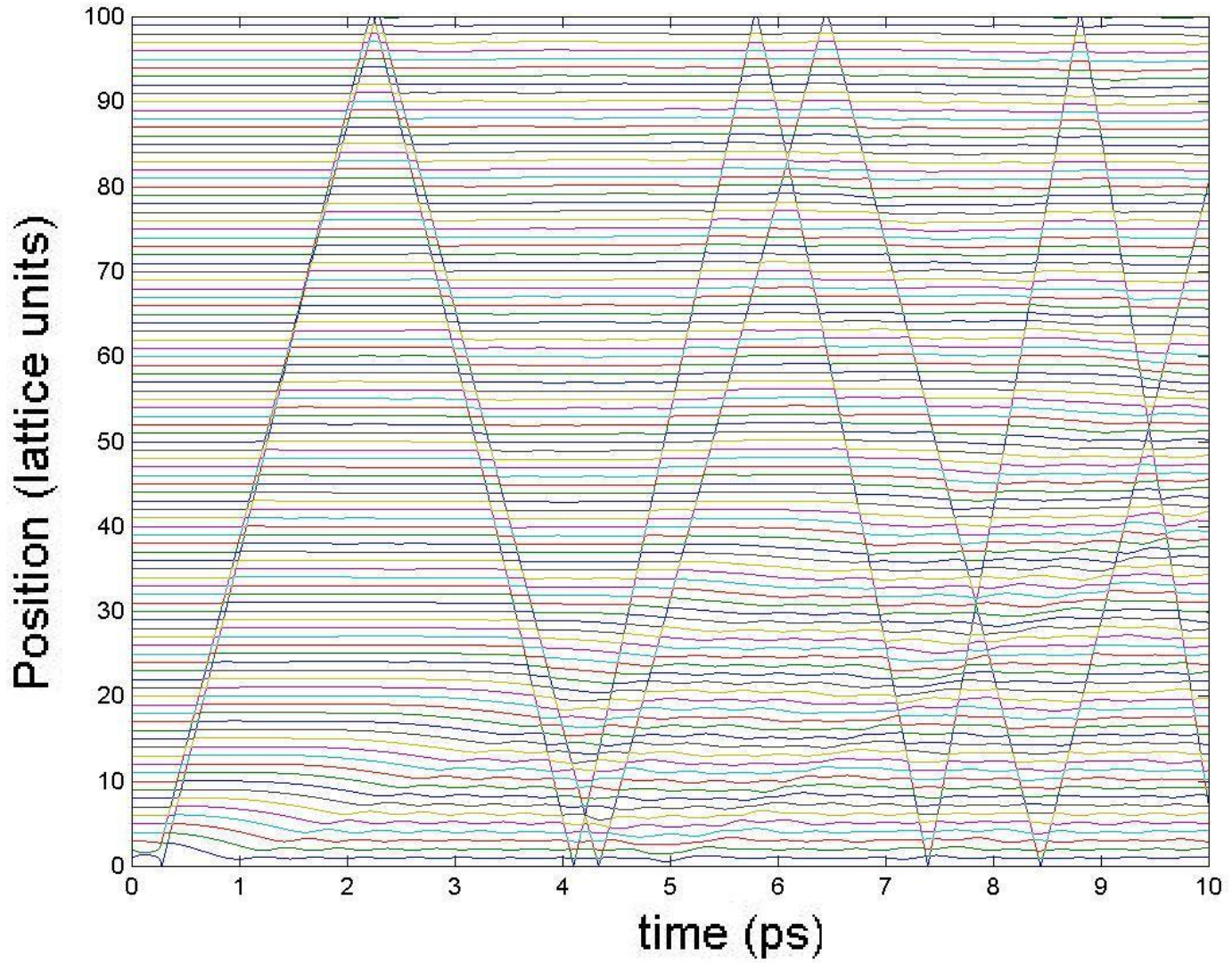
Four kinks. Profile



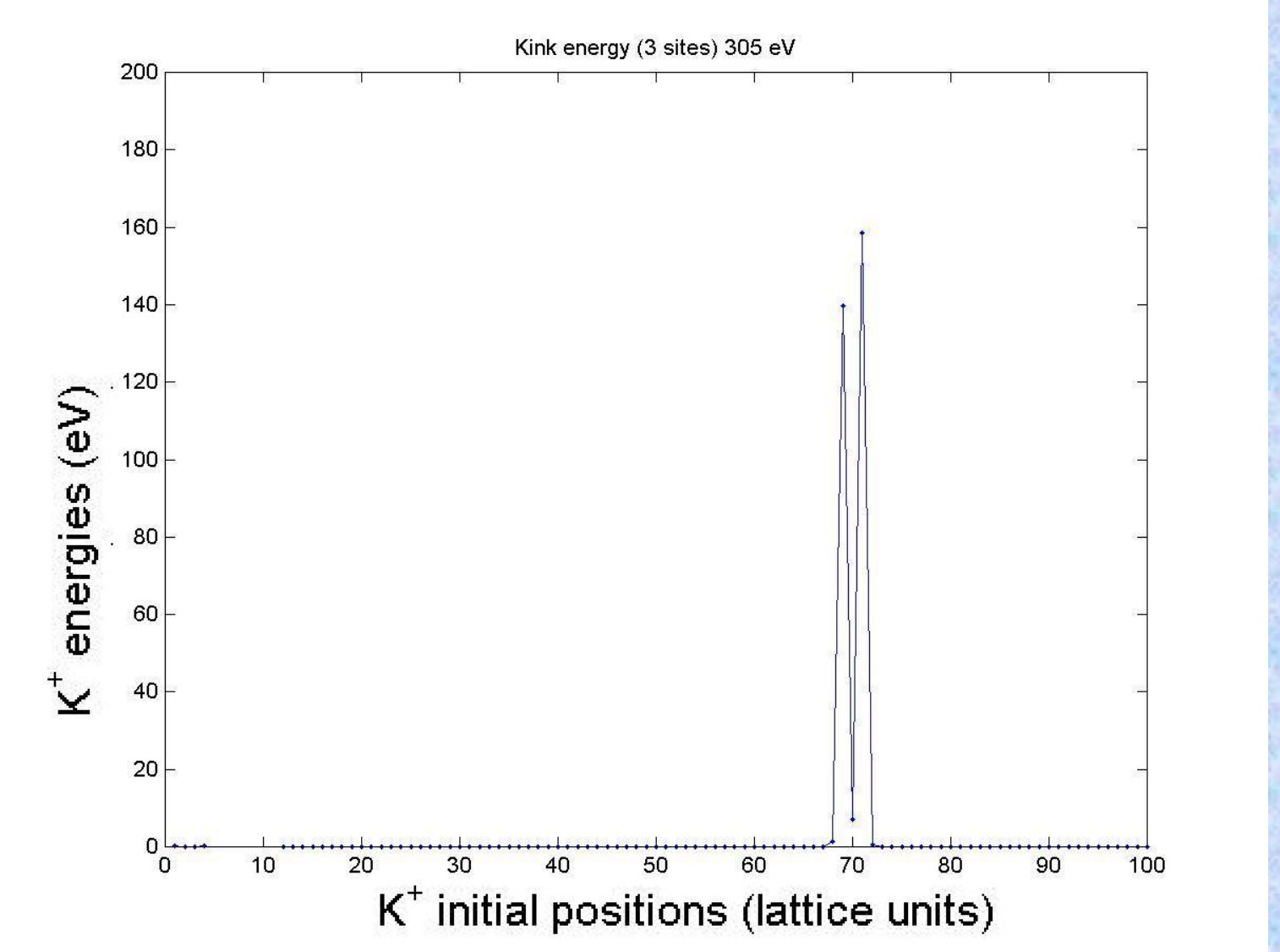
Four kinks. Video



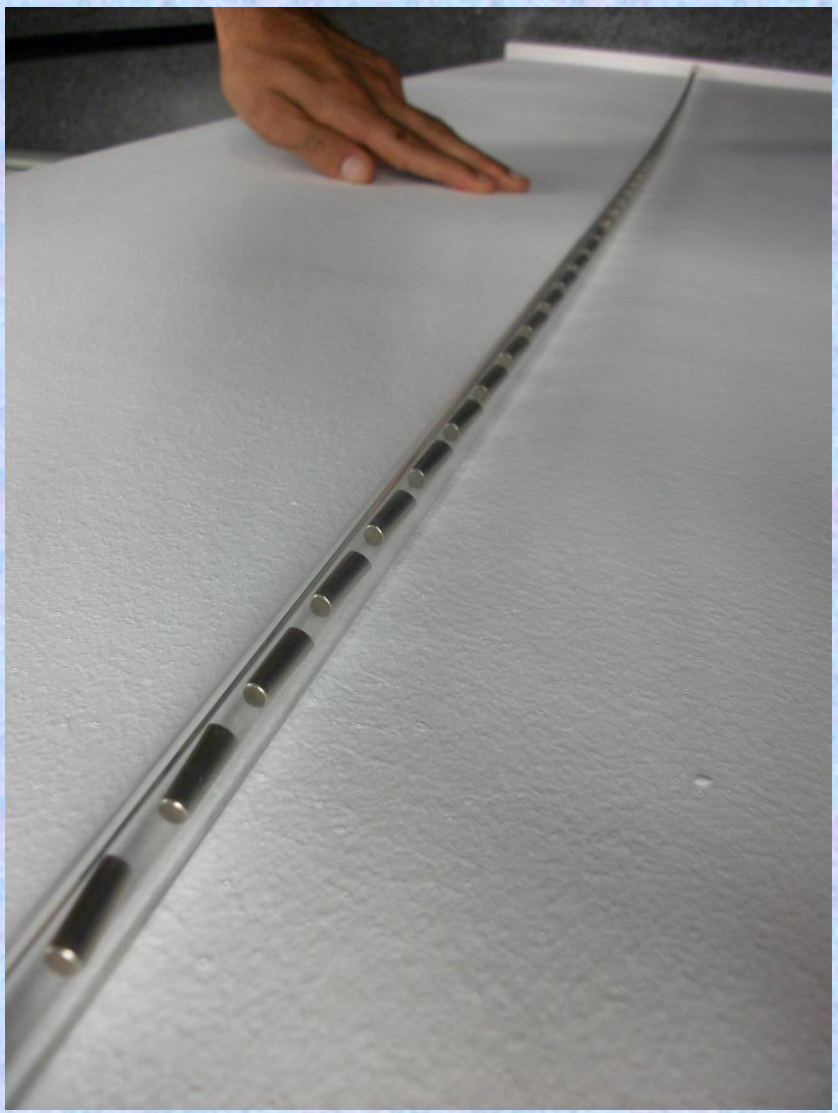
Physical units: kink: 26 km/s; phonons: 3.2 km/s



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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Phys Rev E 83, 041124,1-13.

Russell, F. M. & Eilbeck, J. C. (2007).
Evidence for moving breathers in a layered crystal insulator at 300K.
Europhys, Lett., 78, 10004,1-5.