EFFECT OF ZBL POTENTIAL ON KINKS IN REPULSIVE LATTICES

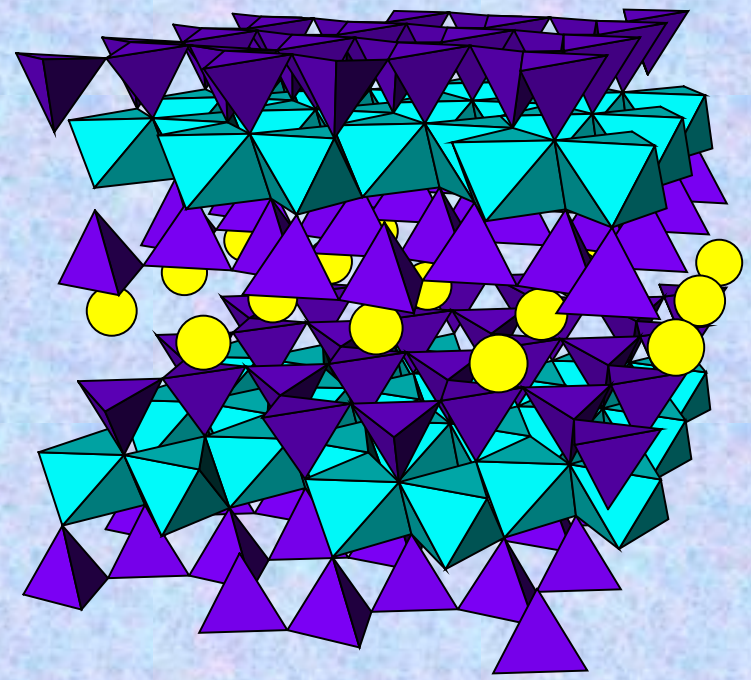
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Sevilla, Spain
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Semenov Institute of Chemical Physics,
Moscow, Russia
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Institute of Pure and Applied Mathematics, Valencia, Spain
Inspiration by **Mike Russell**, Heriot-Watt University, Edinburgh, UK



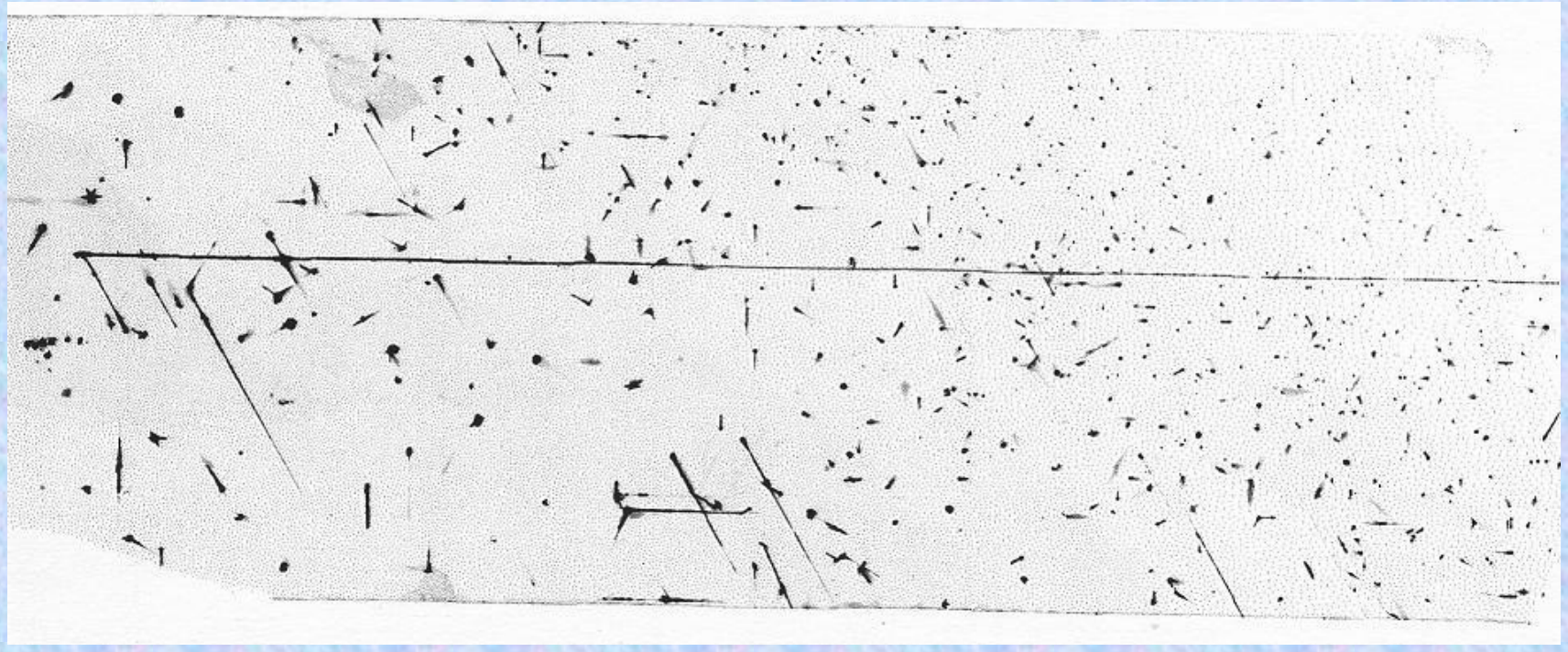
IV international Symposium on Strong Nonlinear Vibronic and Electronic Interactions in Solids
Tartu, Estonia, May 1-3-3, 2013

Σκετχη οφτηε ταλκ

- Mica as a tracks recording material
- Kinks in a minimal model of a cation lattice
- Kinks with ZBL potential
- Lattice kinks or crowdions
- Conclusions



Positron track in muscovite

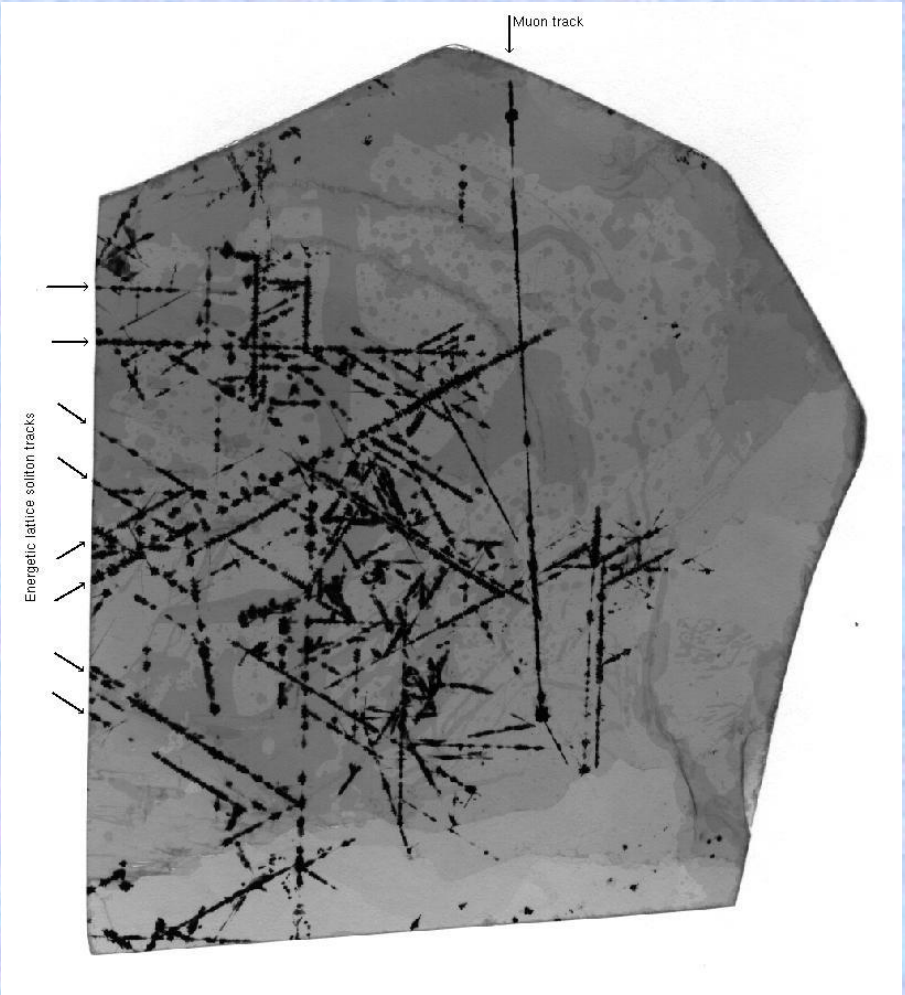


- Produced in the decay of K^{40} with 1.4Mev
- 3 per second per cm^3
- Tracks are Fe oxides, magnetite

Φοσσιλσολιδ σταται νυχλεαρ τραχκσ δετεχτορσ

- Young (1958) in Li F
- Silk and Barnes (1959), tracks from fission fragments in natural mica
- Price and Walker (1962): fossil particle tracks in natural mica
- Fossil SSNTD integrate events during geological times
- Sensitive period: specific values of pression, temperature, during the cooling process
- Identification of tracks in mica:
  F. M. Russell, PLA (1967), Nature (1968) , Nature (1969) , PLA (1988)

Θυοδονα: θυαα ονε-διμ ενααοναλεξχιτατιονσ (ΦΜ Ρυσσελλ)



- 0.1% of the tracks are explained because of charged particles, like muons, positrons, electron cascades.
- 99.9% of the tracks are within the lattice closed packed lines in the (001) plane.
- Mica's interior can be observed!

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

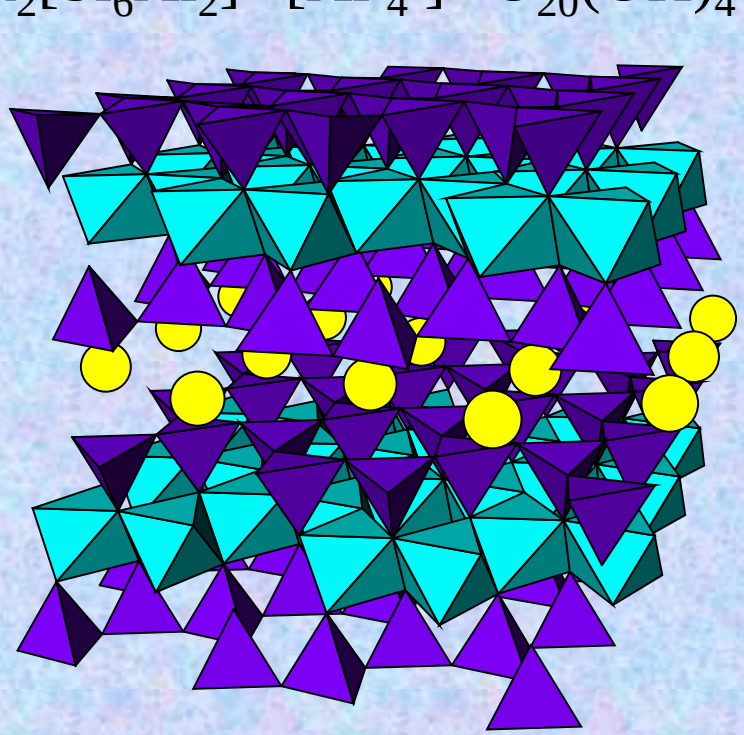


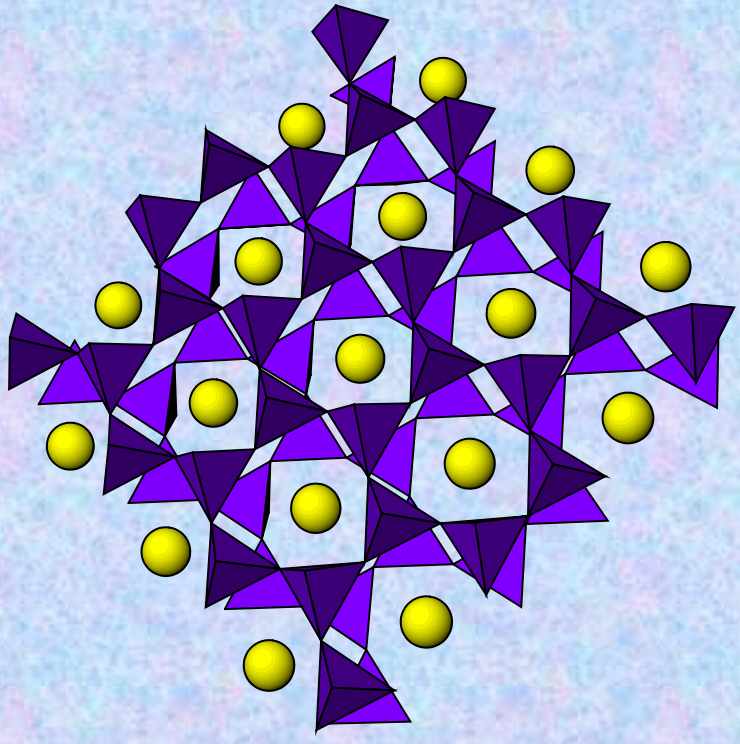
Trajectories along lattice directions within the K^+ layer .
Surface binding energy of ejected atoms unknown:
typical values 3-8 eV

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

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

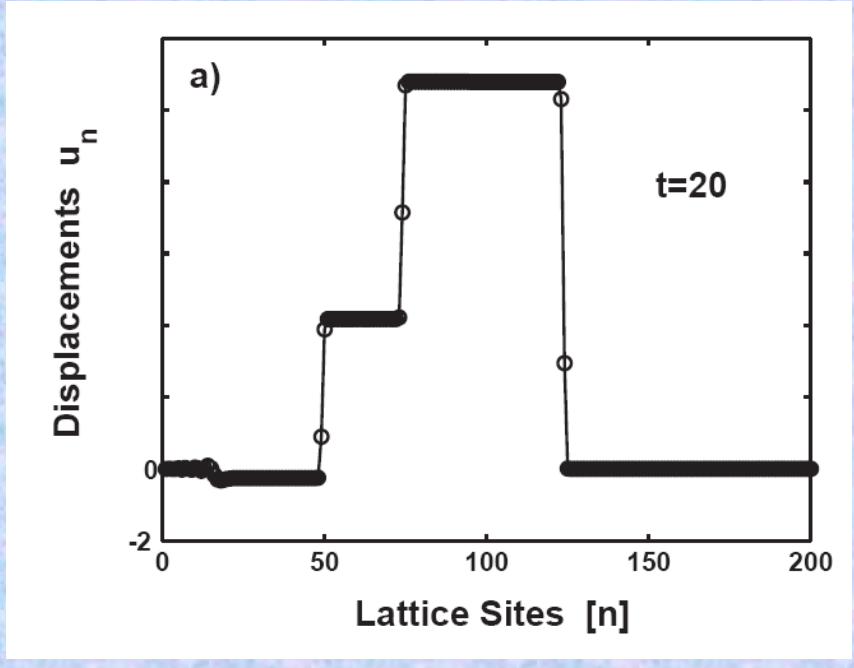


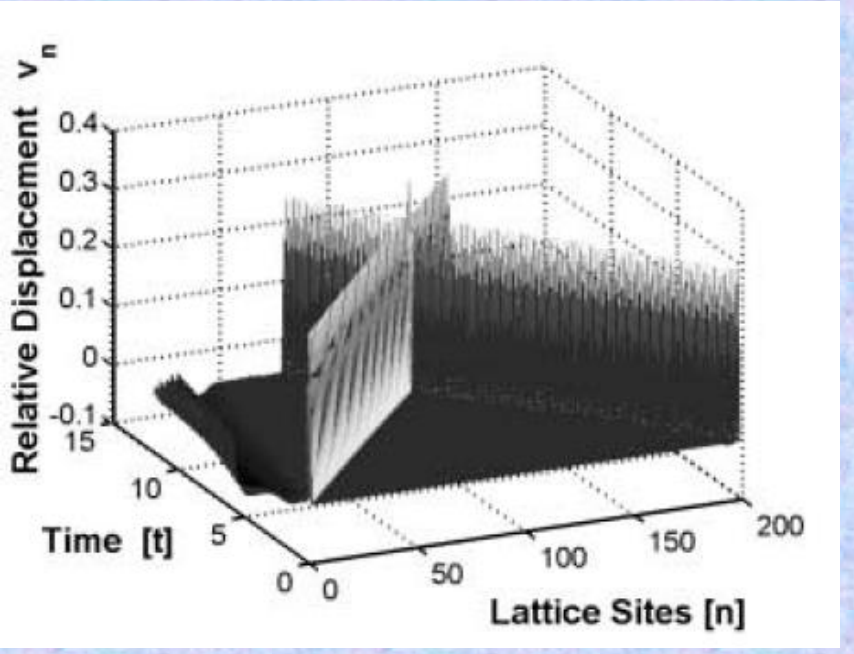


K^+ : 2D lattice of repulsive particles

K^+

Supersonic kinks move very fast and have large energies.

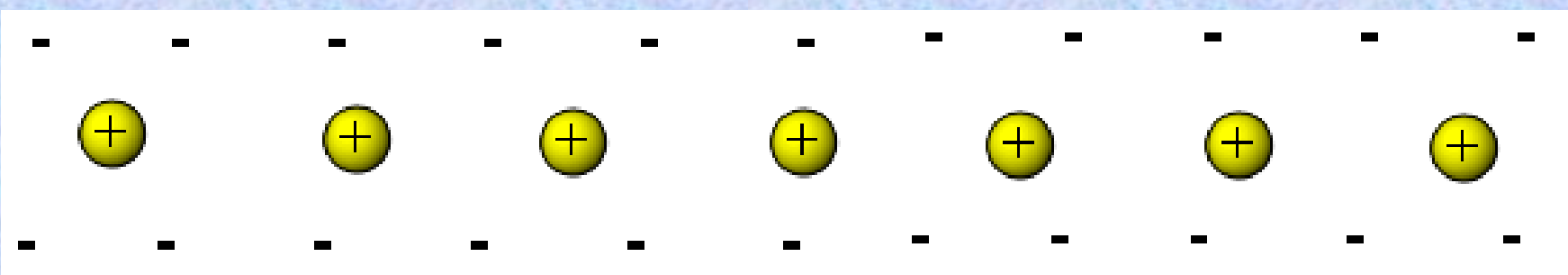




Transversal kinks in a beta FPU lattice

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.

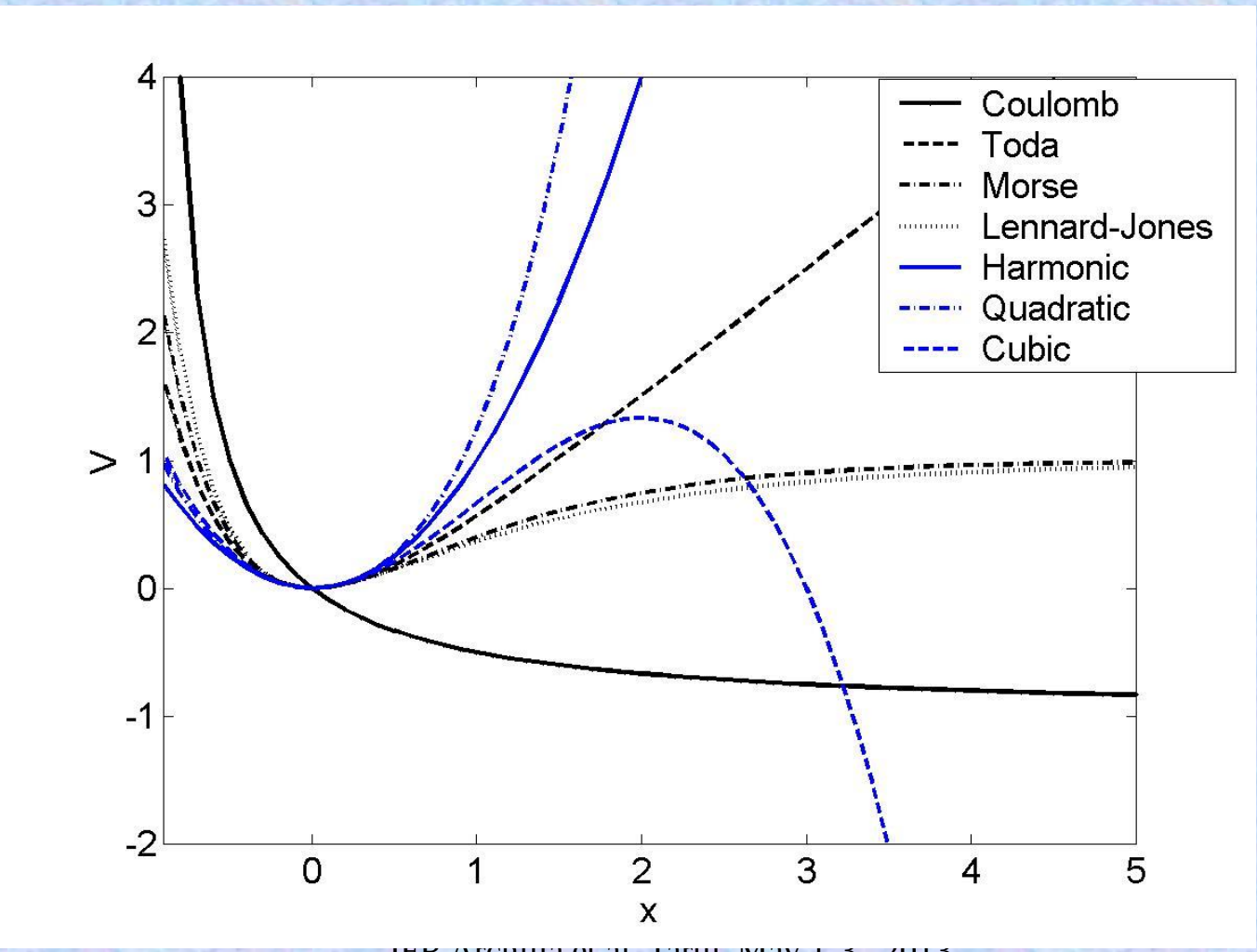
Minimal model of a Coulomb repulsive lattice



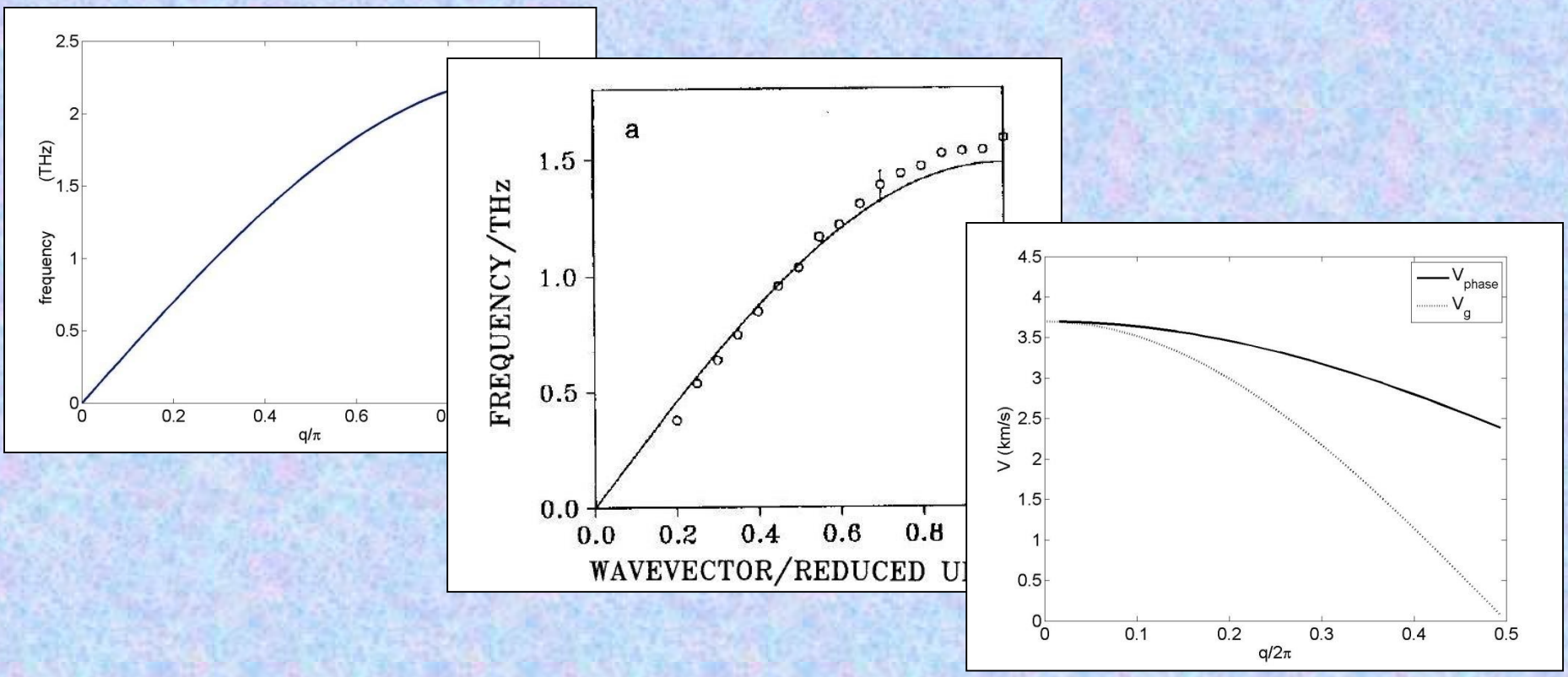
- Longitudinal perturbations
- Cations are in a negative medium so:
  - Coulomb's repulsion is rapidly screened
  - The system does not explode
  - We limit initially long to nearest neighbours
- Negative charge at the borders keep cations inside

Minimal model

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



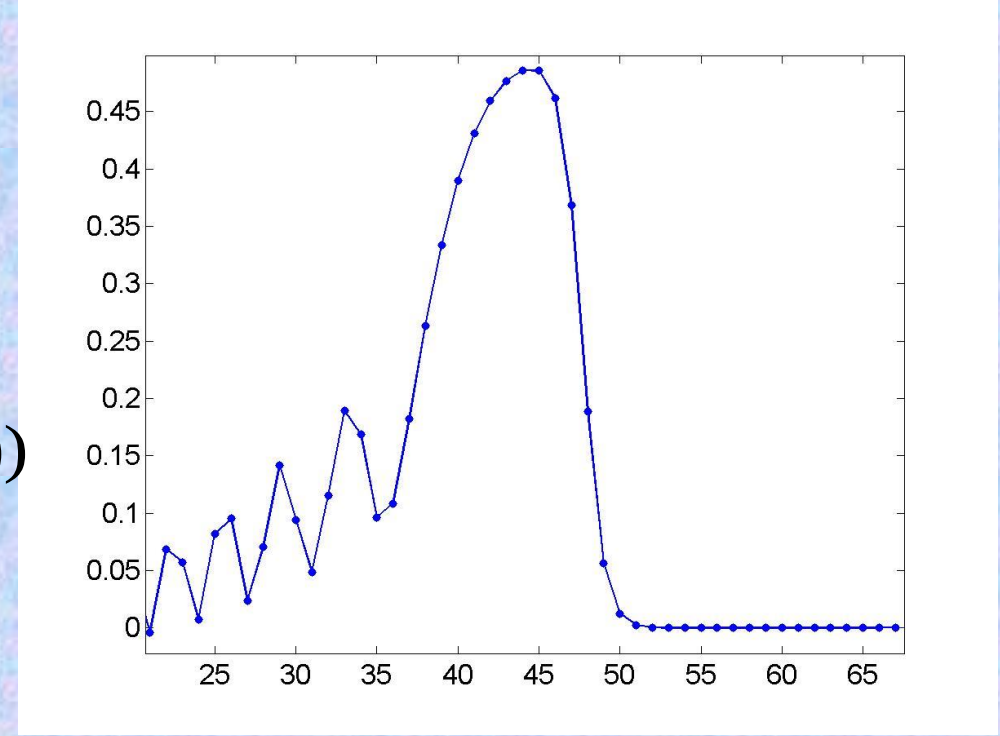
Phonon spectrum and speed of sound



D.R. Collins et all, *Phys. Chem. Minerals.* 19: 520-527 (1993)
G. Brudeylins, D. Schmicker,. *Surface Science*, 333: 237-242 (1995).

Tail analysis. What kind of excitation we can expect?

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



Proposed tail solution:

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

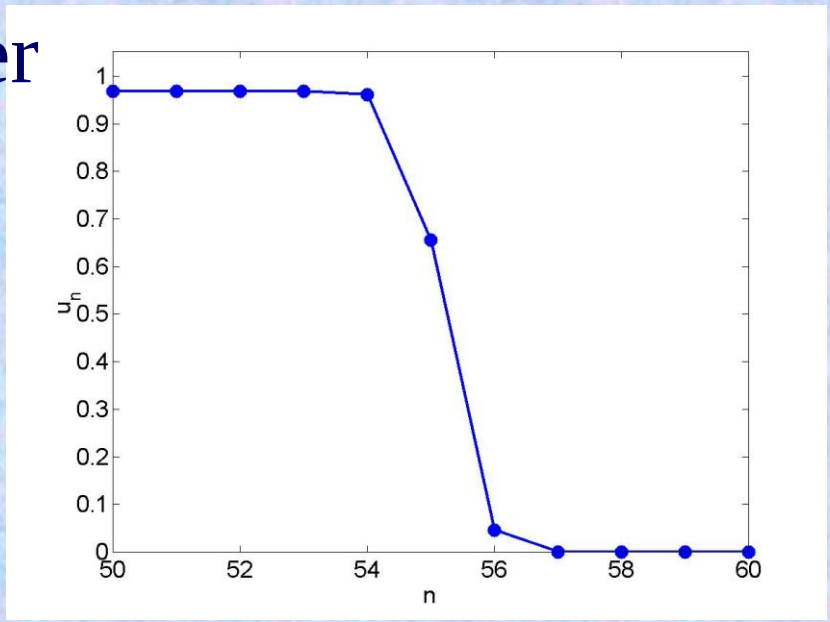
Solitons are supersonic:

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

Moving oscillating tails are subsonic, but kinks are supersonic

Kinks with magic wave number

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: $q = \frac{2\pi}{3}$, Only three bonds and two particles are 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 $\theta = qn - \omega t$

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

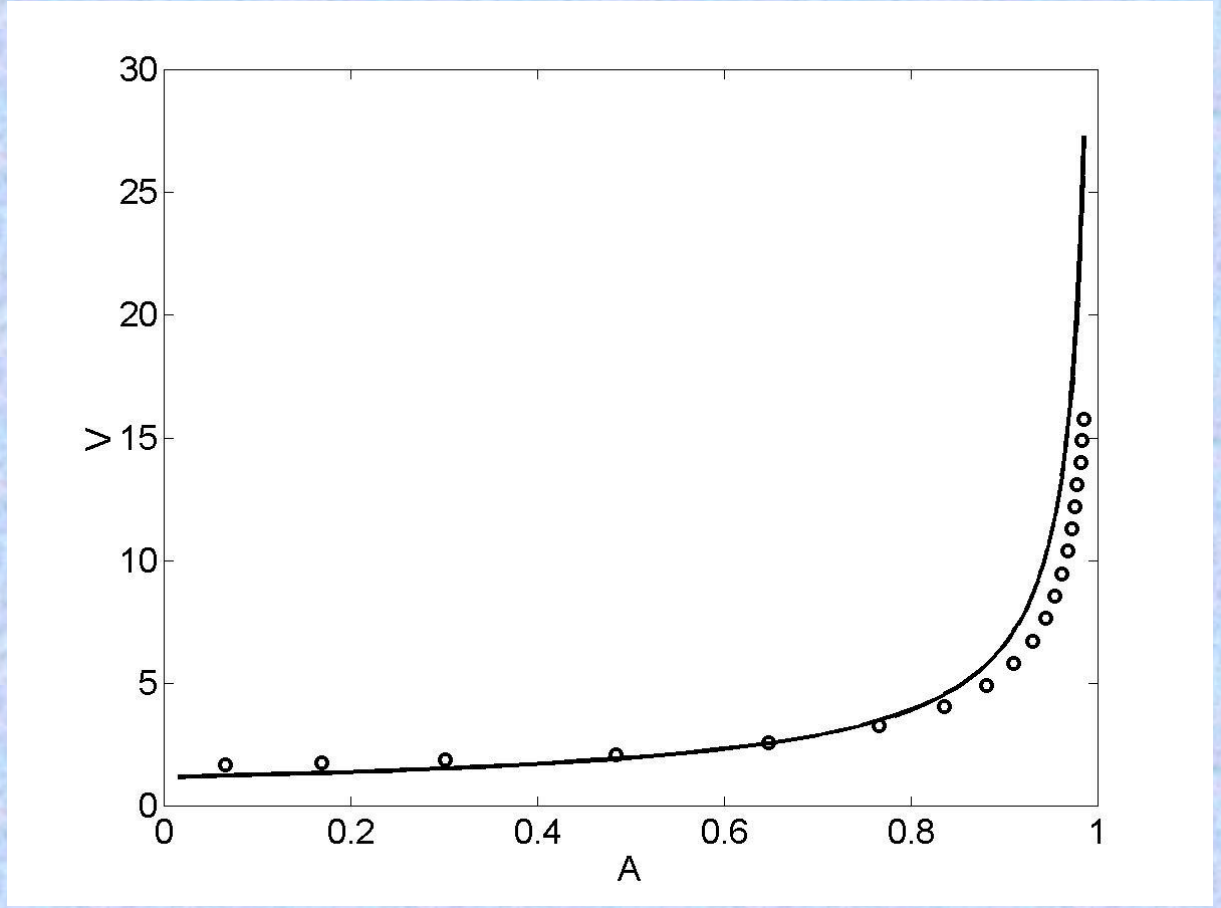
$$a_1 = \frac{1}{\pi}\int_{-\pi/2}^{\pi/2}(F_n - F_{n+1} - F_{n-1})\cos(\theta)\,\mathrm{d}\theta$$

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

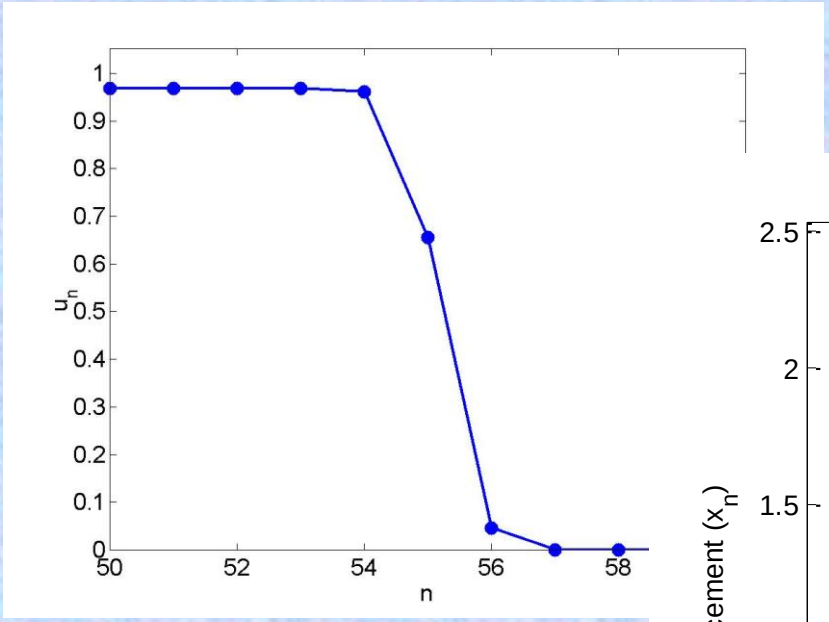
Kinks are supersonic

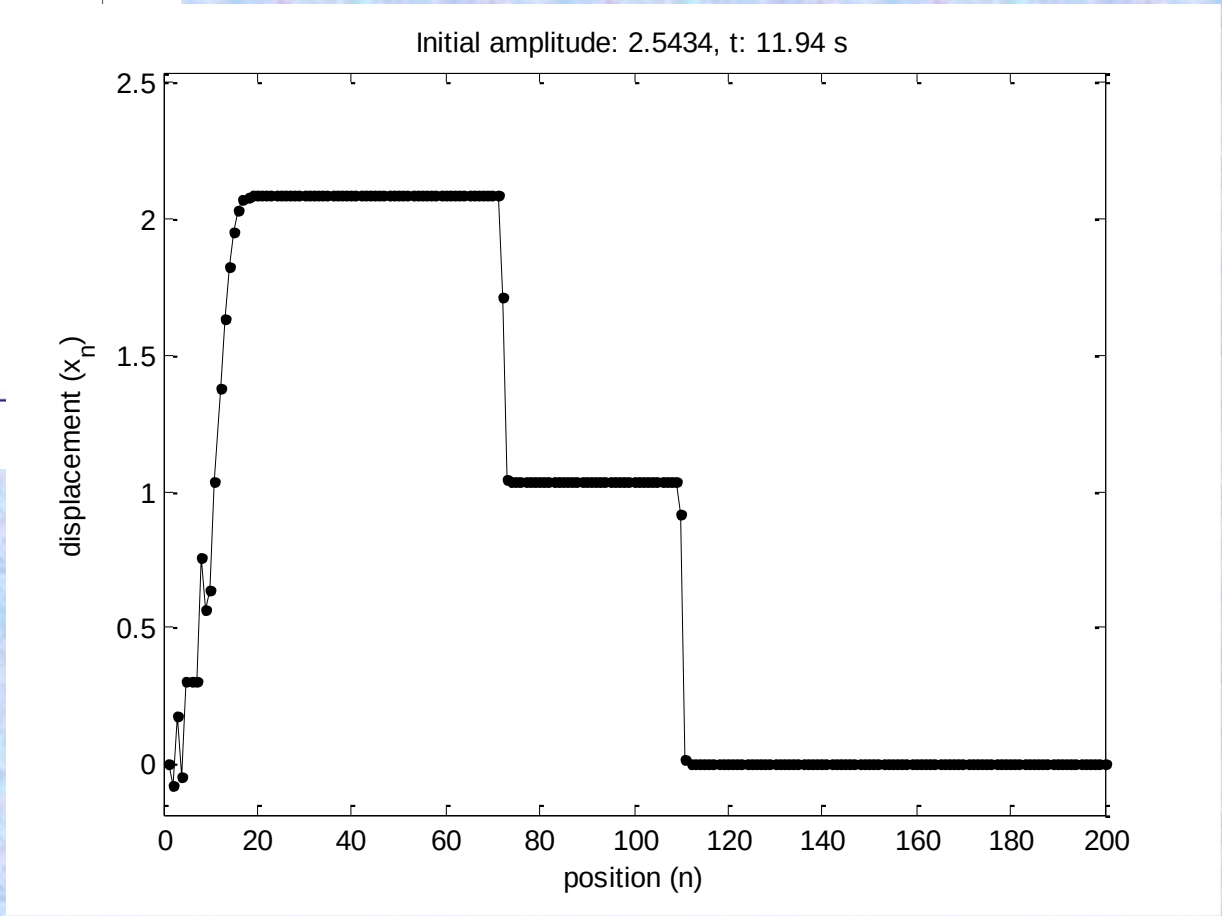
Kinks RWA, velocity versus amplitude

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



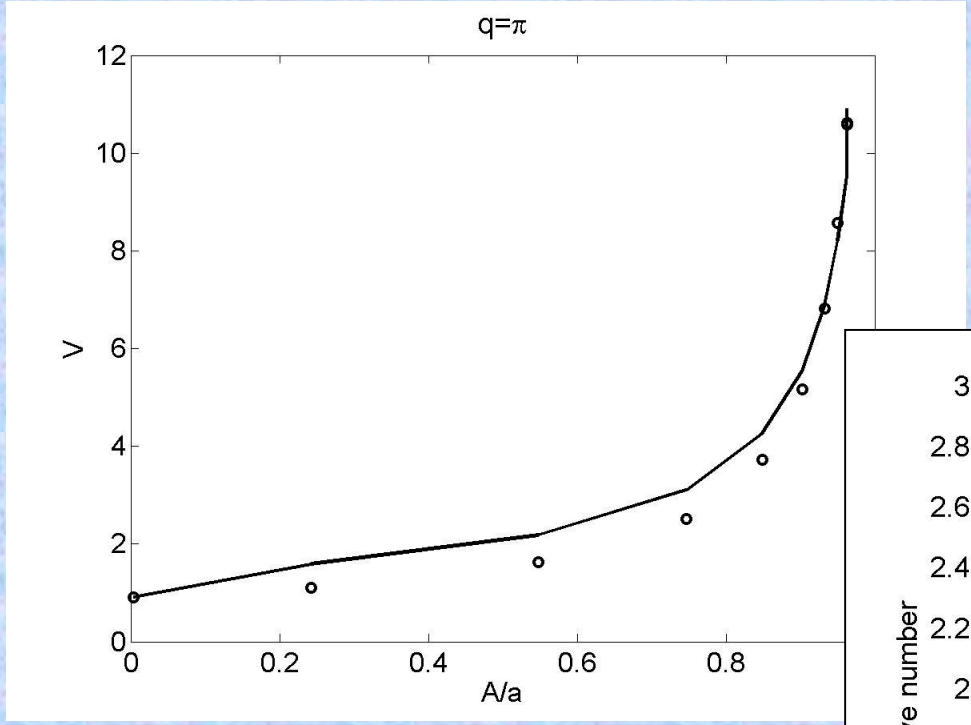
The not so magic wave number q=2π/3 (2)



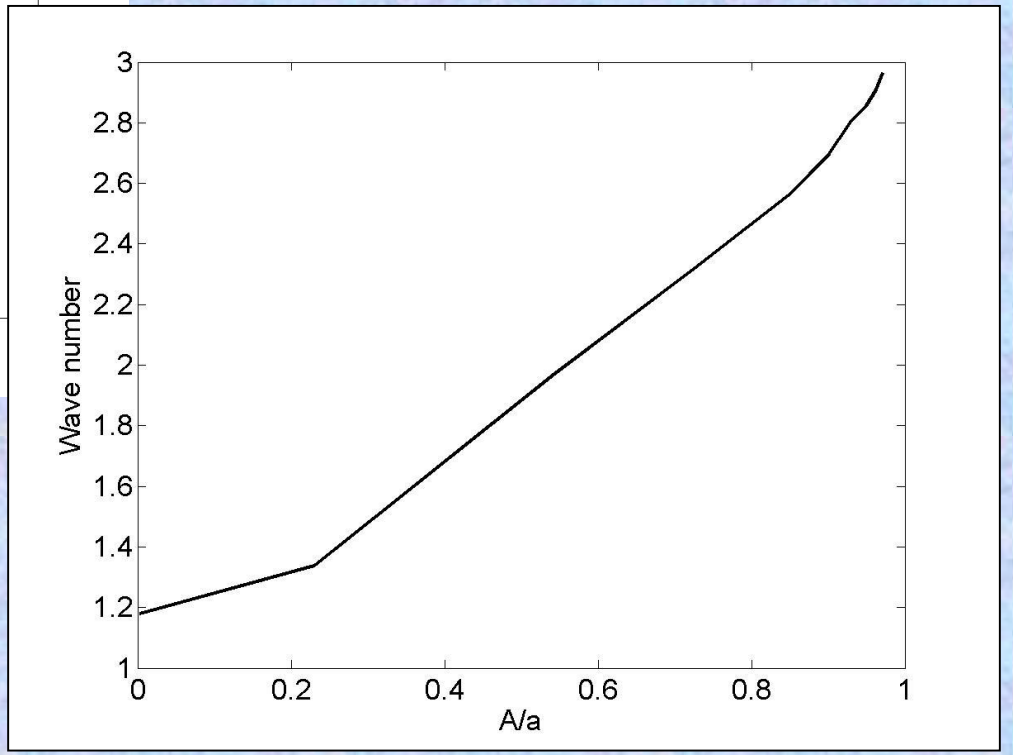


q=π means that there are 2 bonds and 1 particle changing

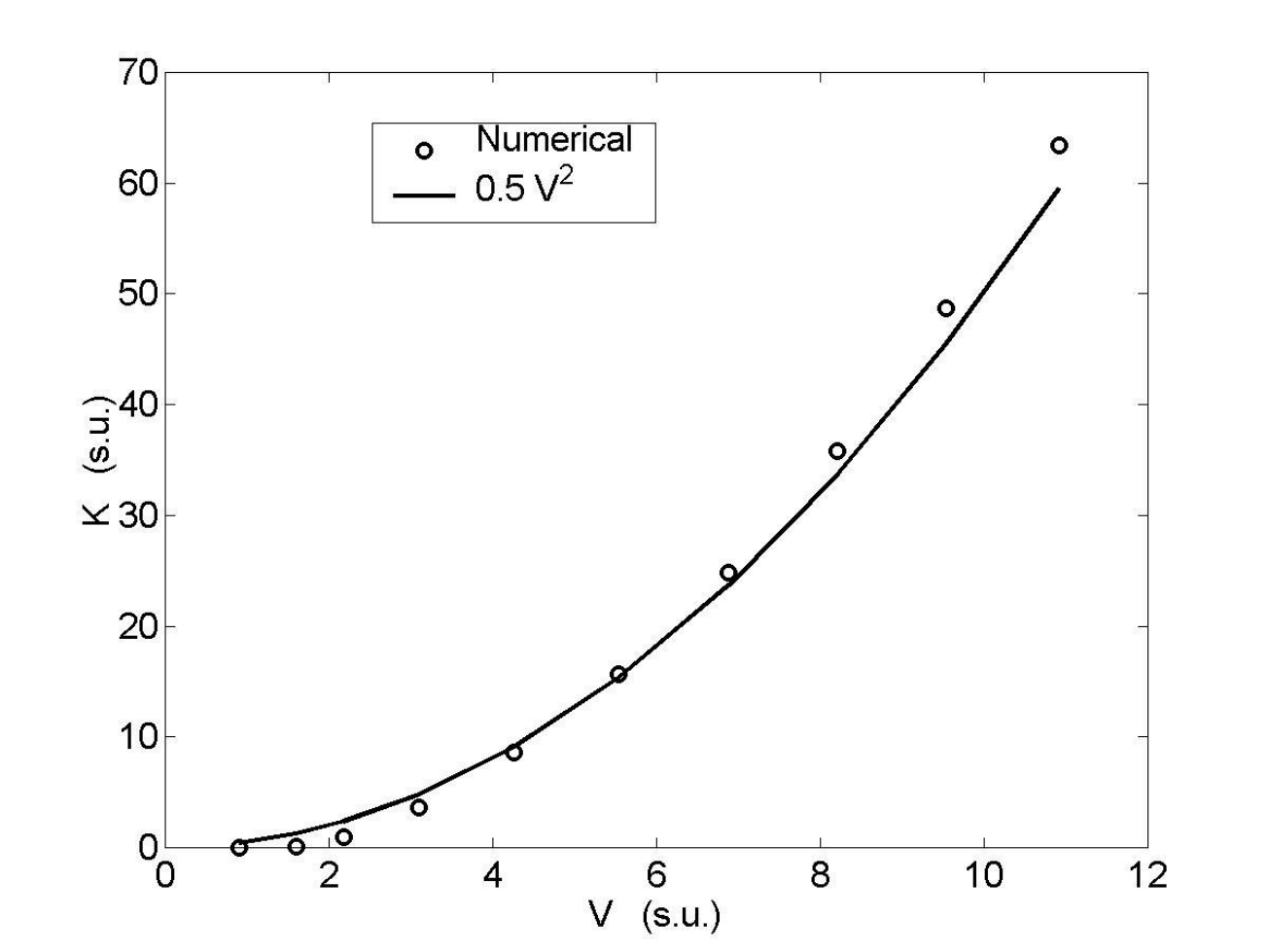
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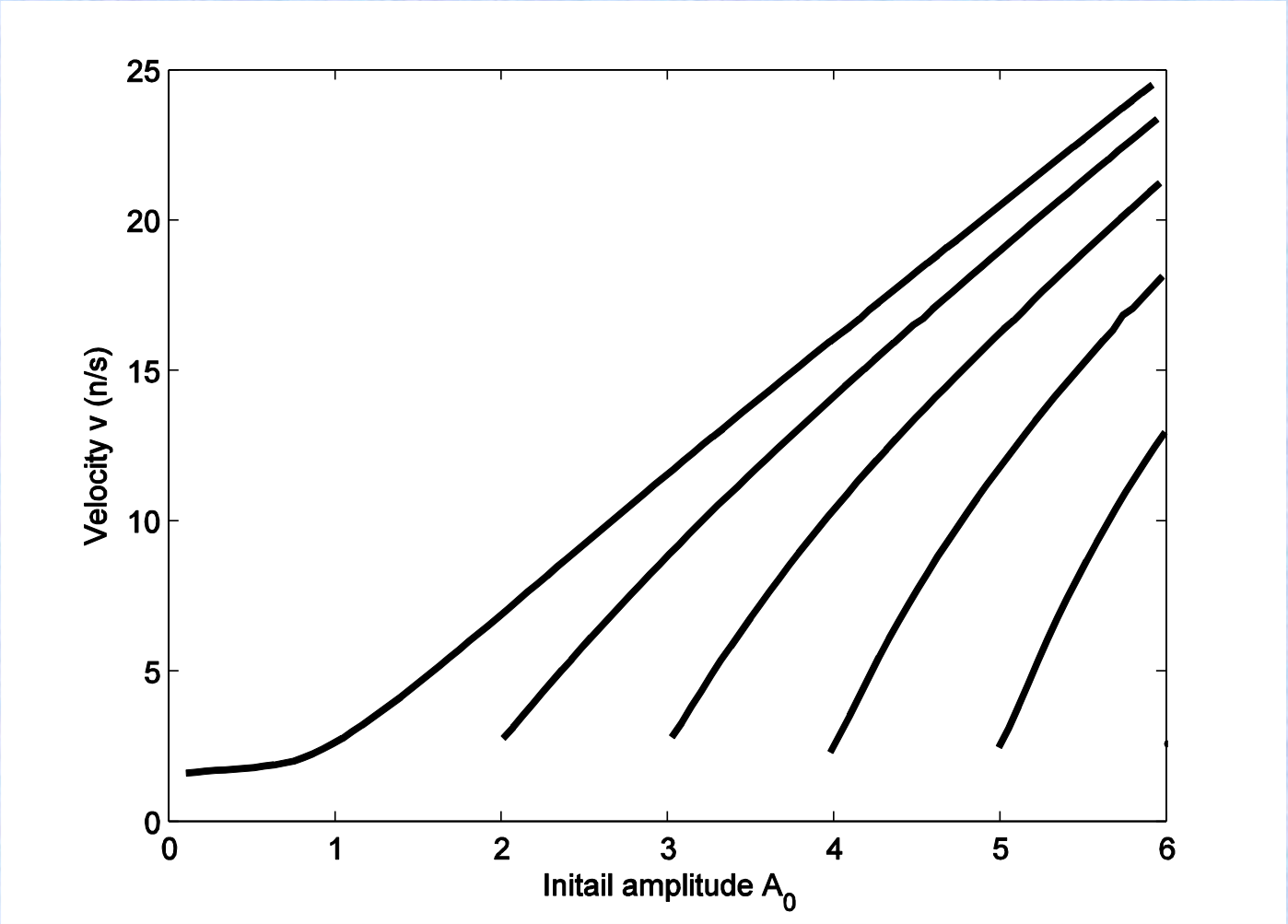


Kinetic energy versus velocity



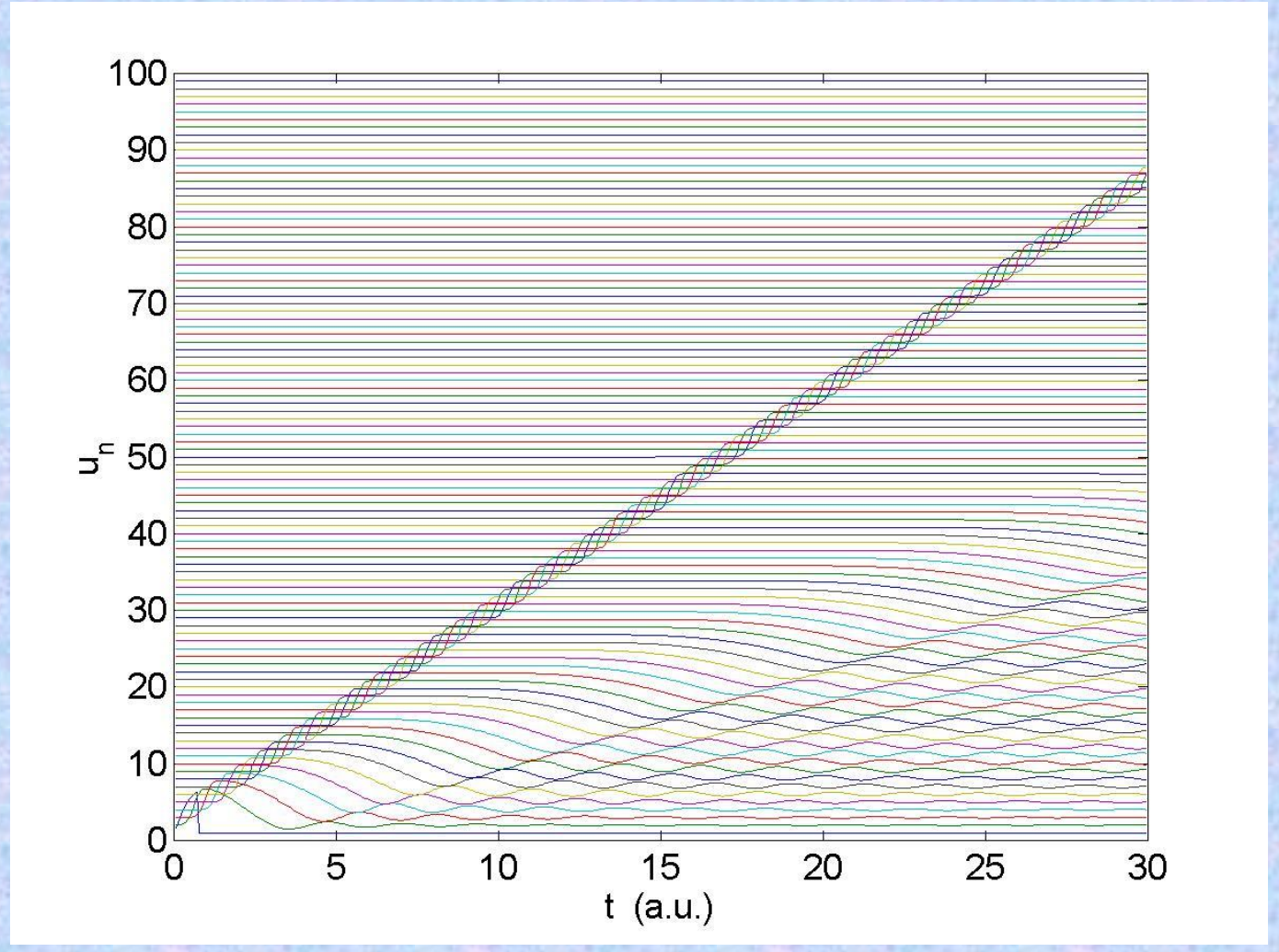
Kinks behave as particles with unit mass

Kink simulations, Velocity-Initial amplitude



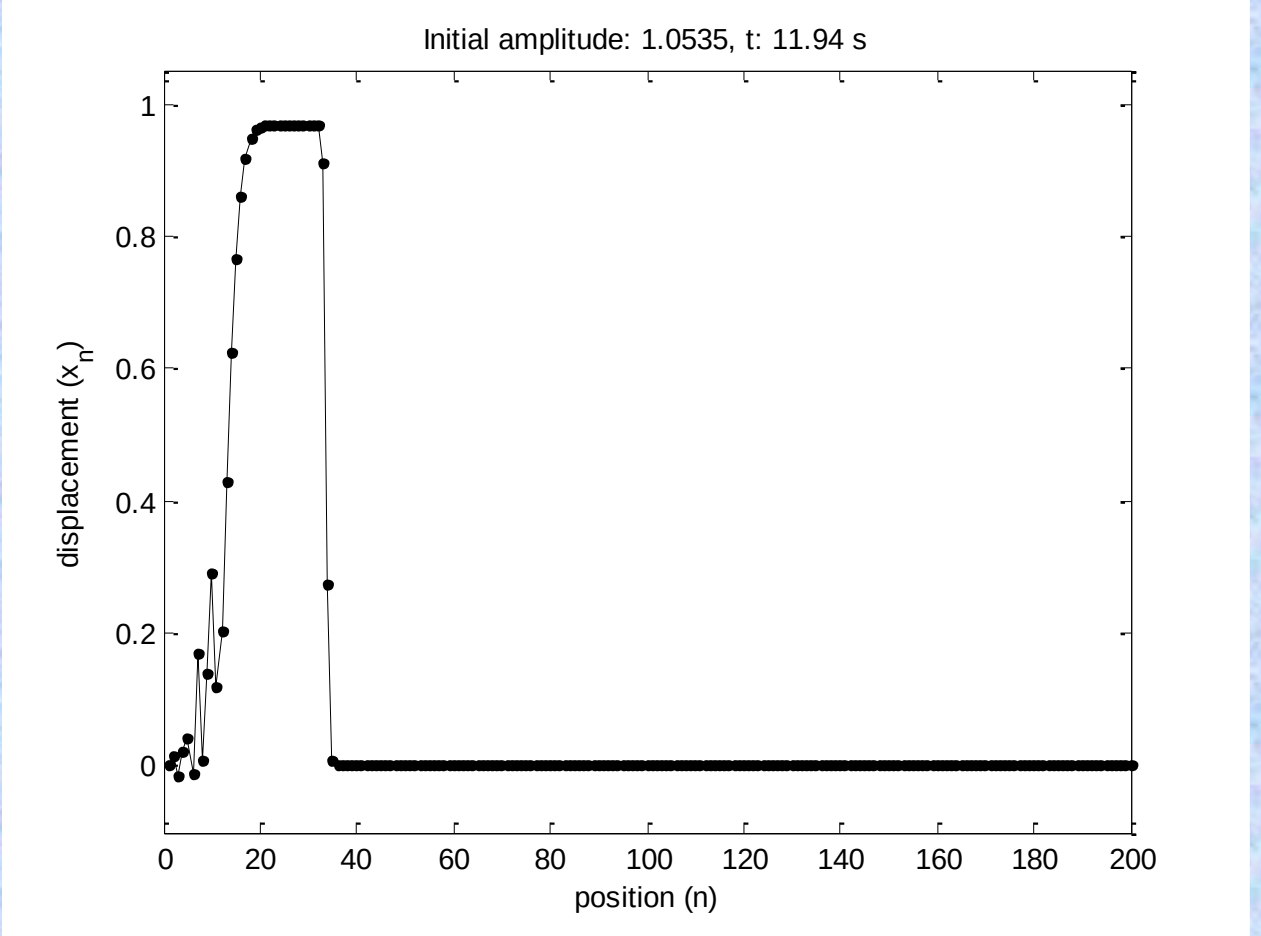
Single supersonic kink. Simulation

$$V = 2c$$



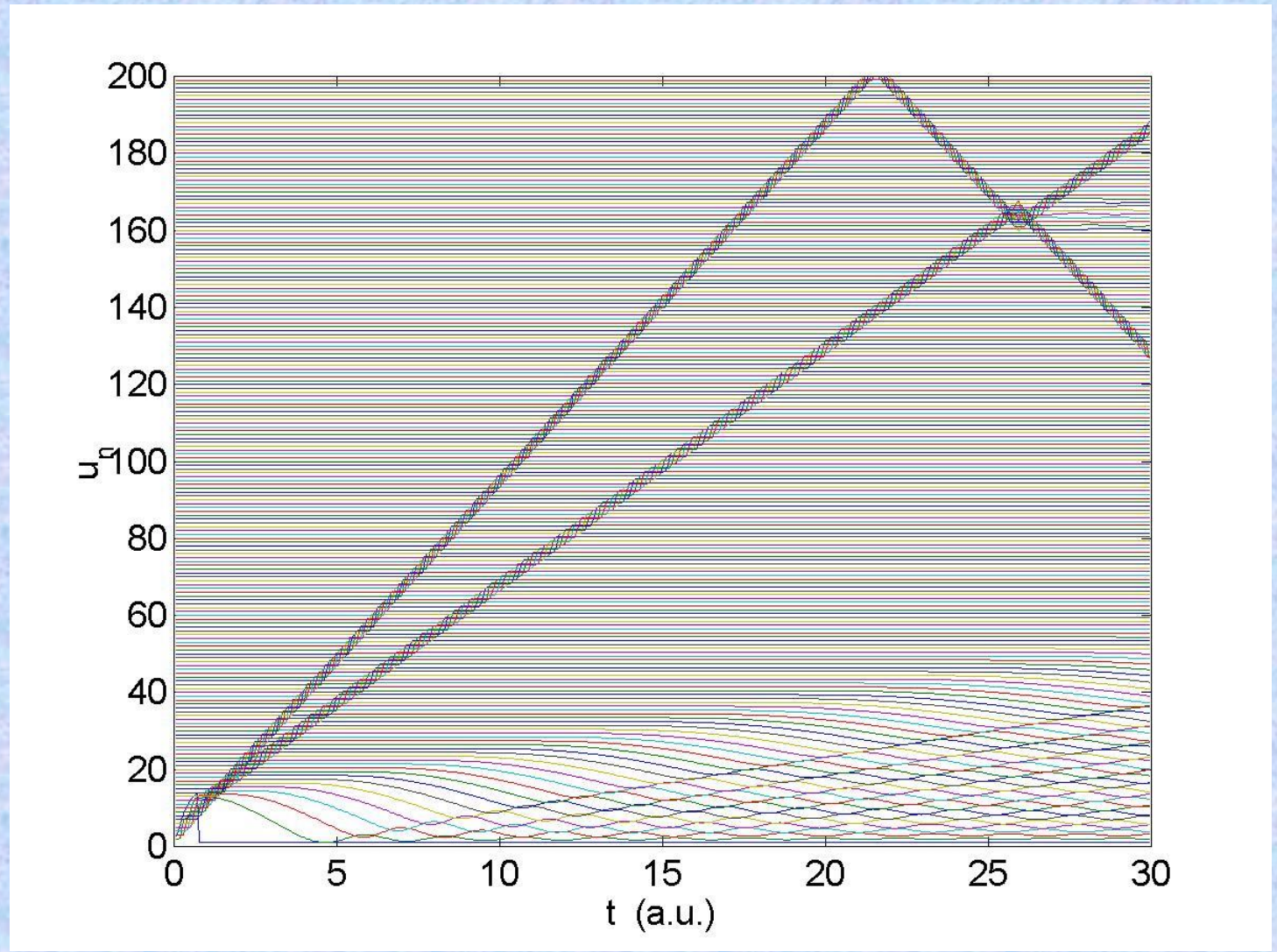
Single supersonic kink. Profile.

$$V = 2c$$

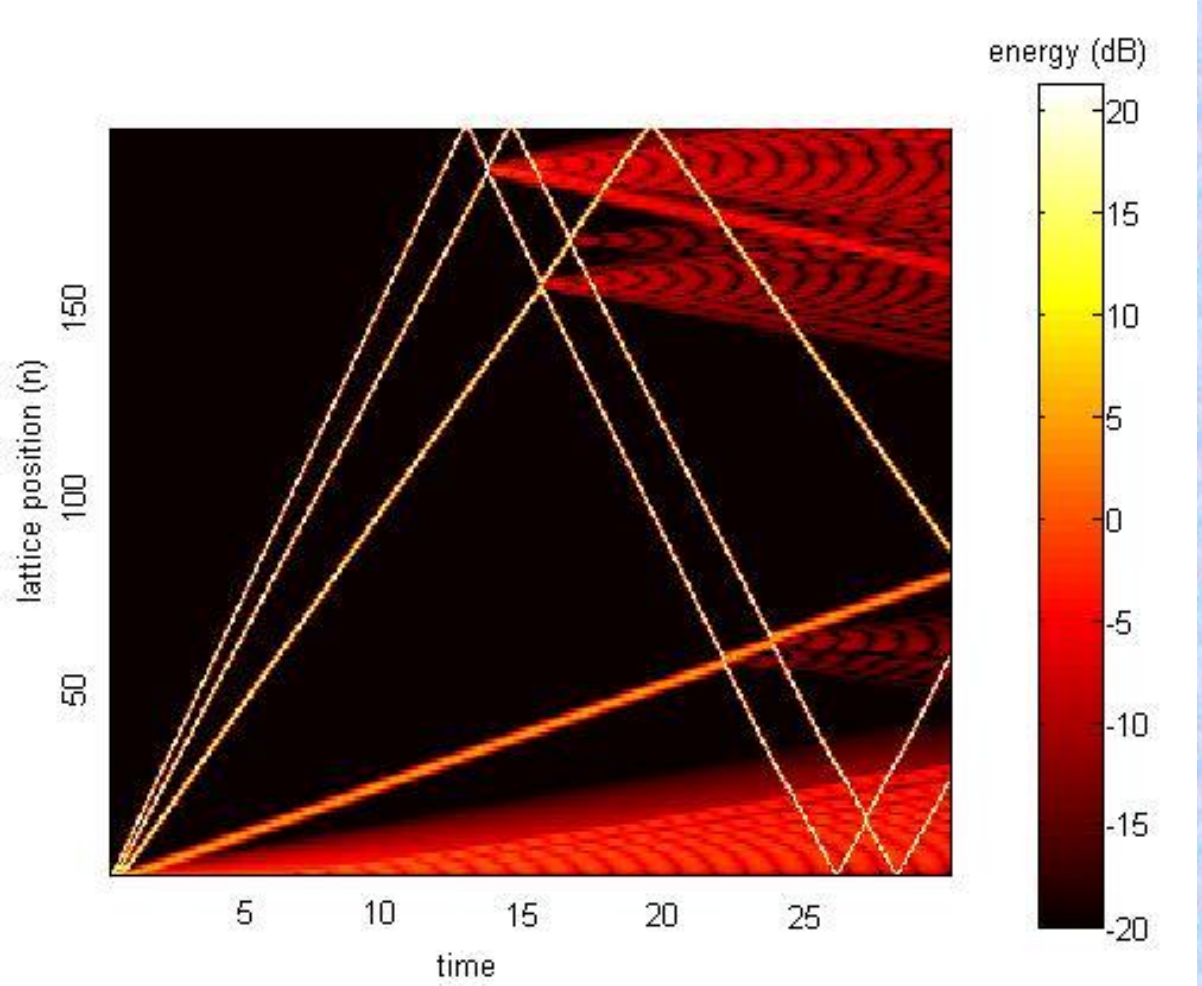


Double supersonic kink. Simulation

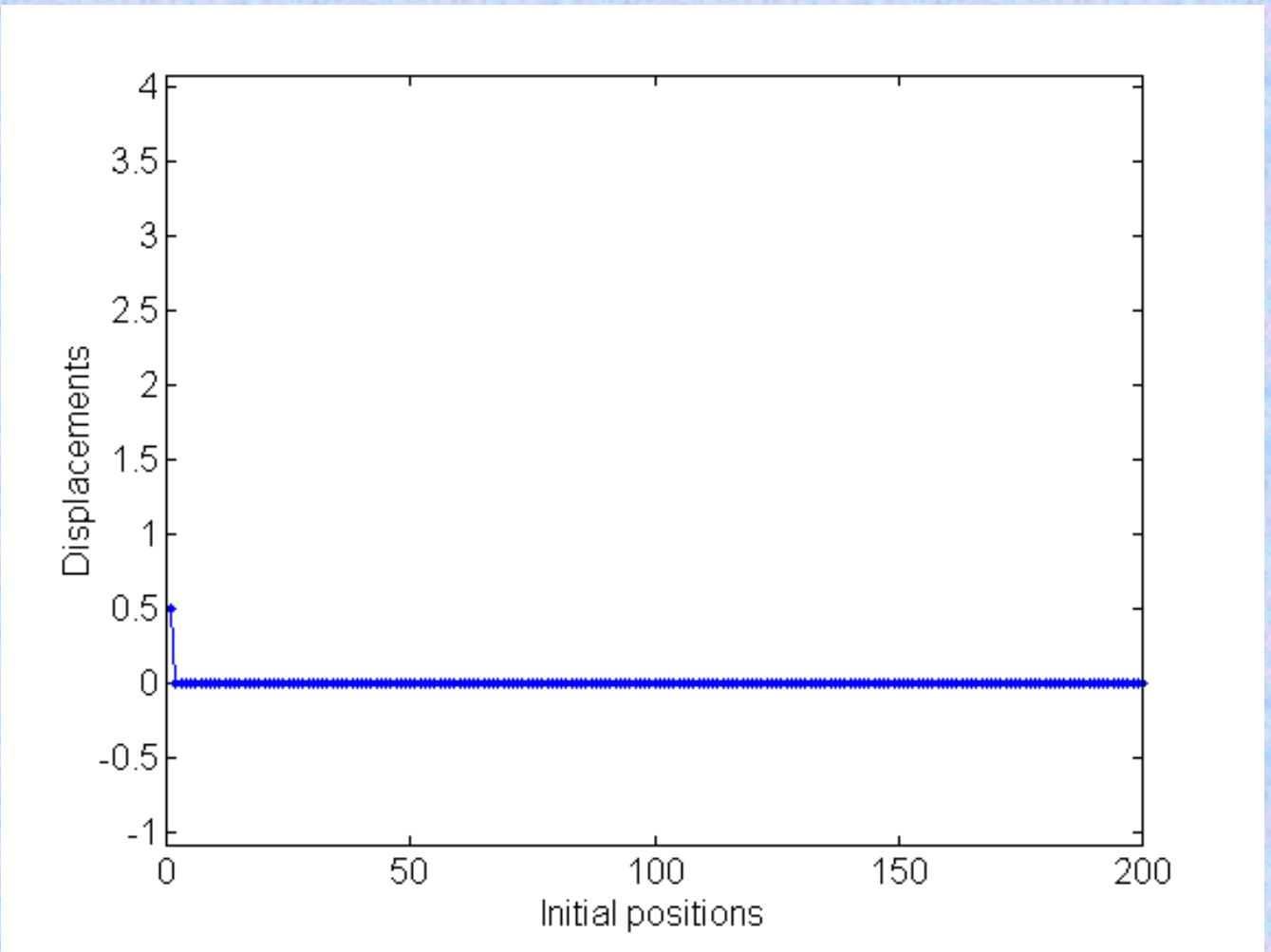
$$V = 4.1c$$



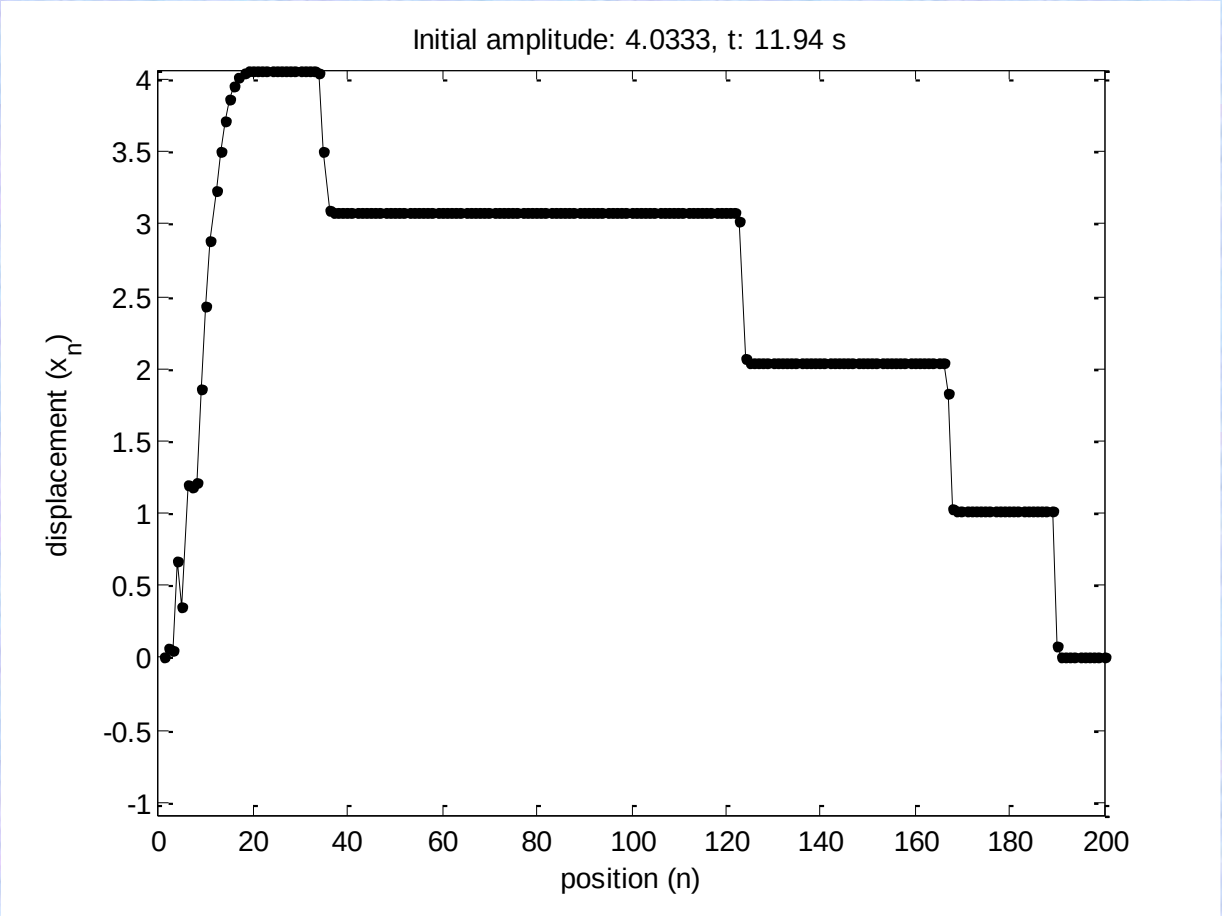
Three kinks. Energy-time



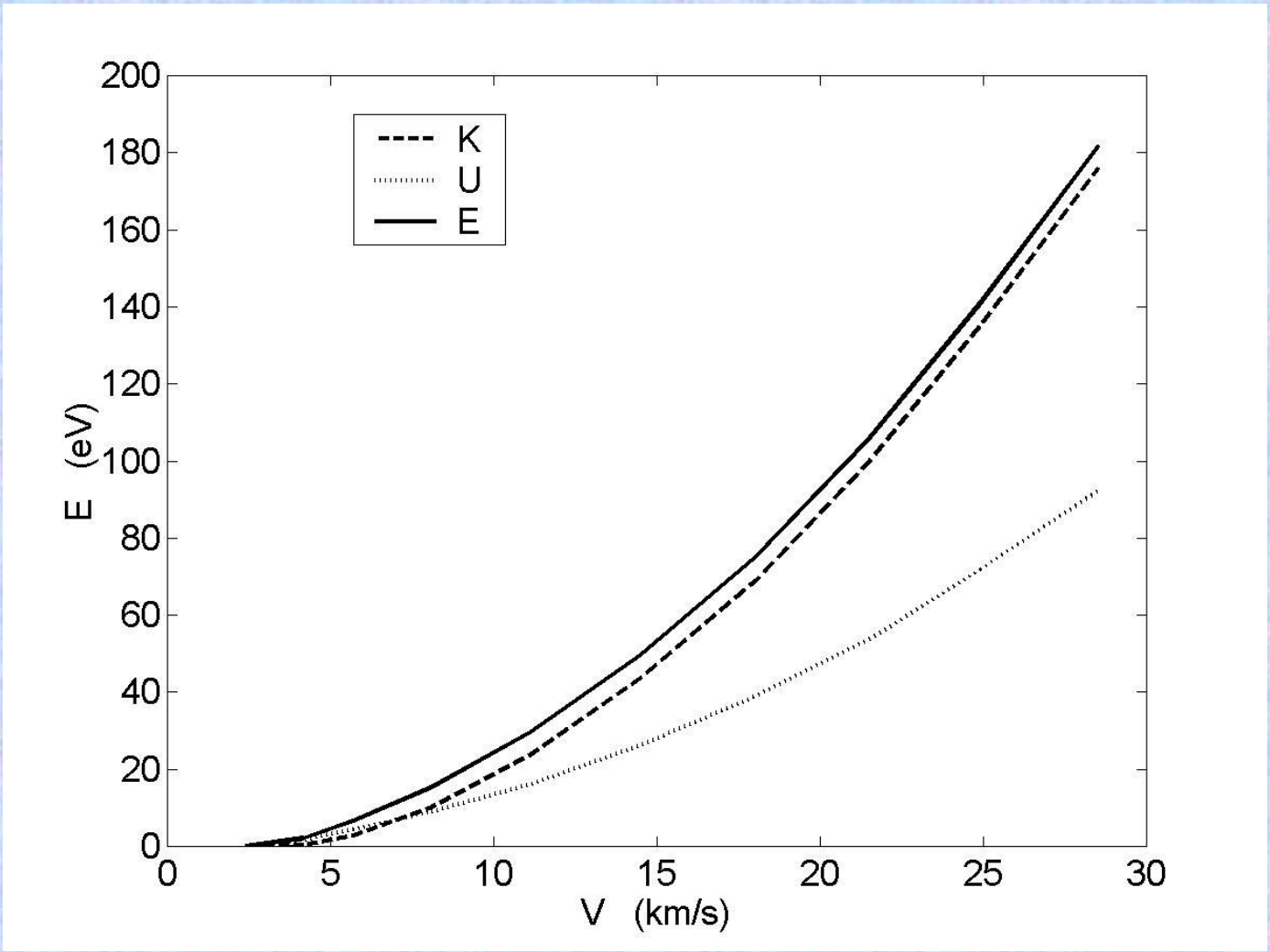
Four kinks. Video



Four kinks. Profile

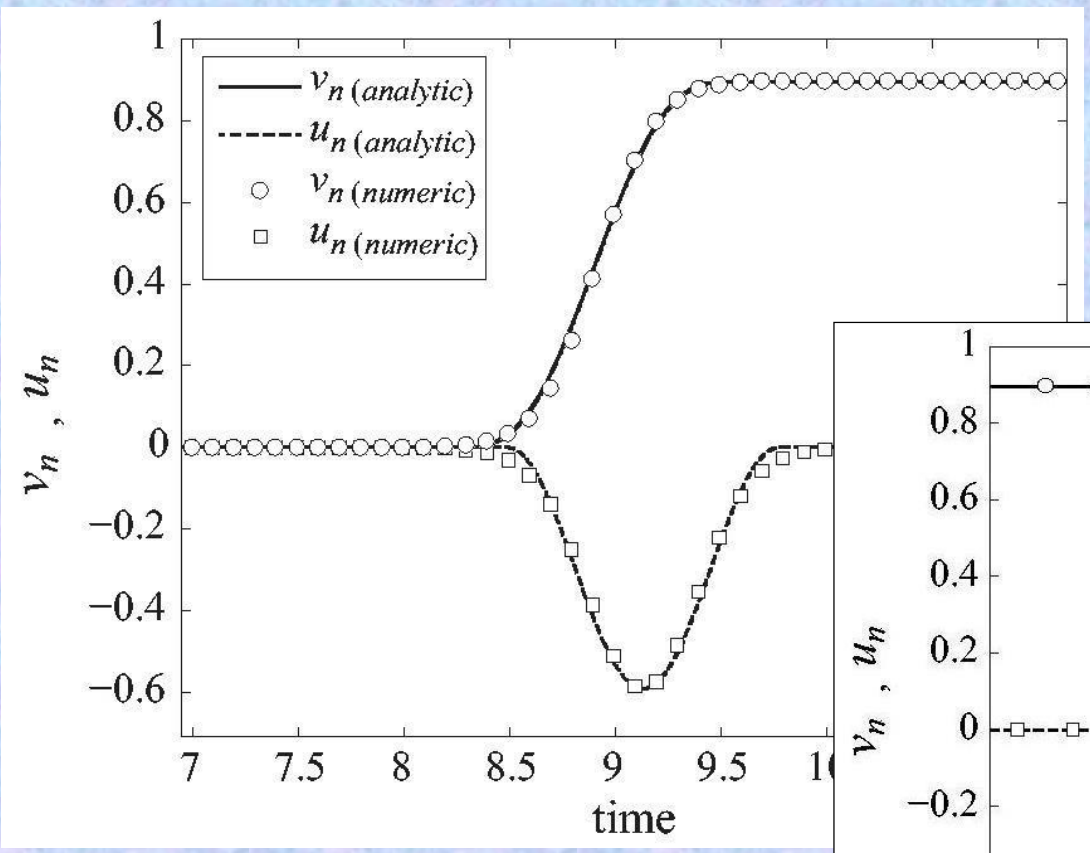


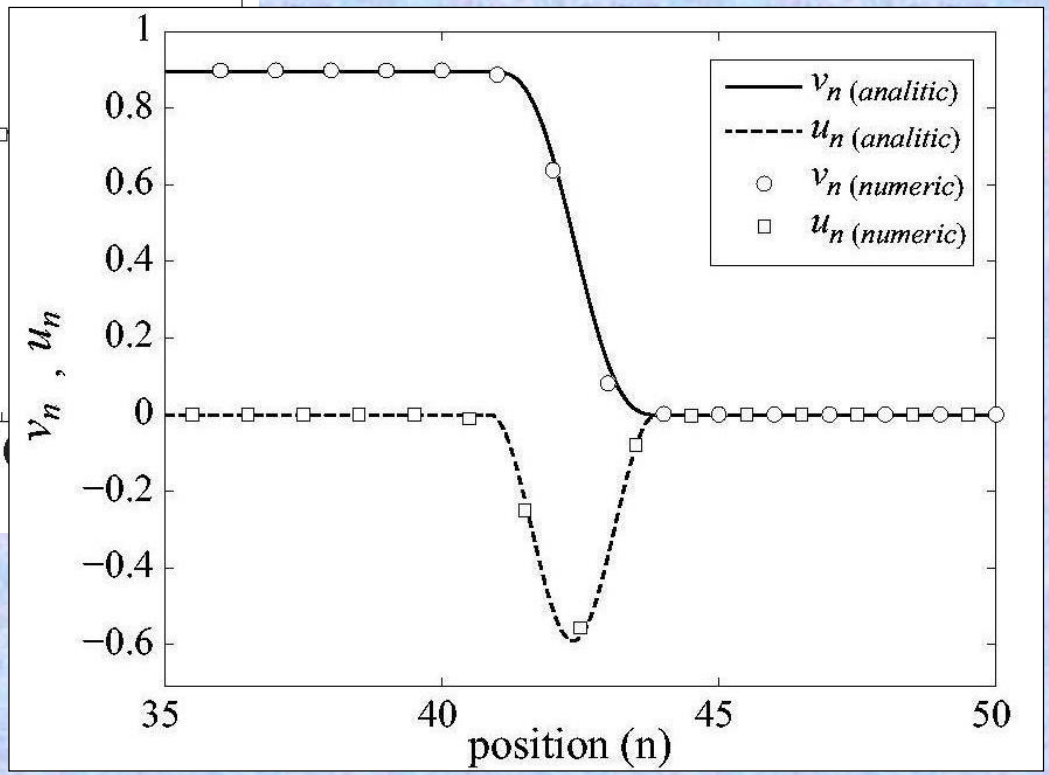
Physical units, energies versus velocity



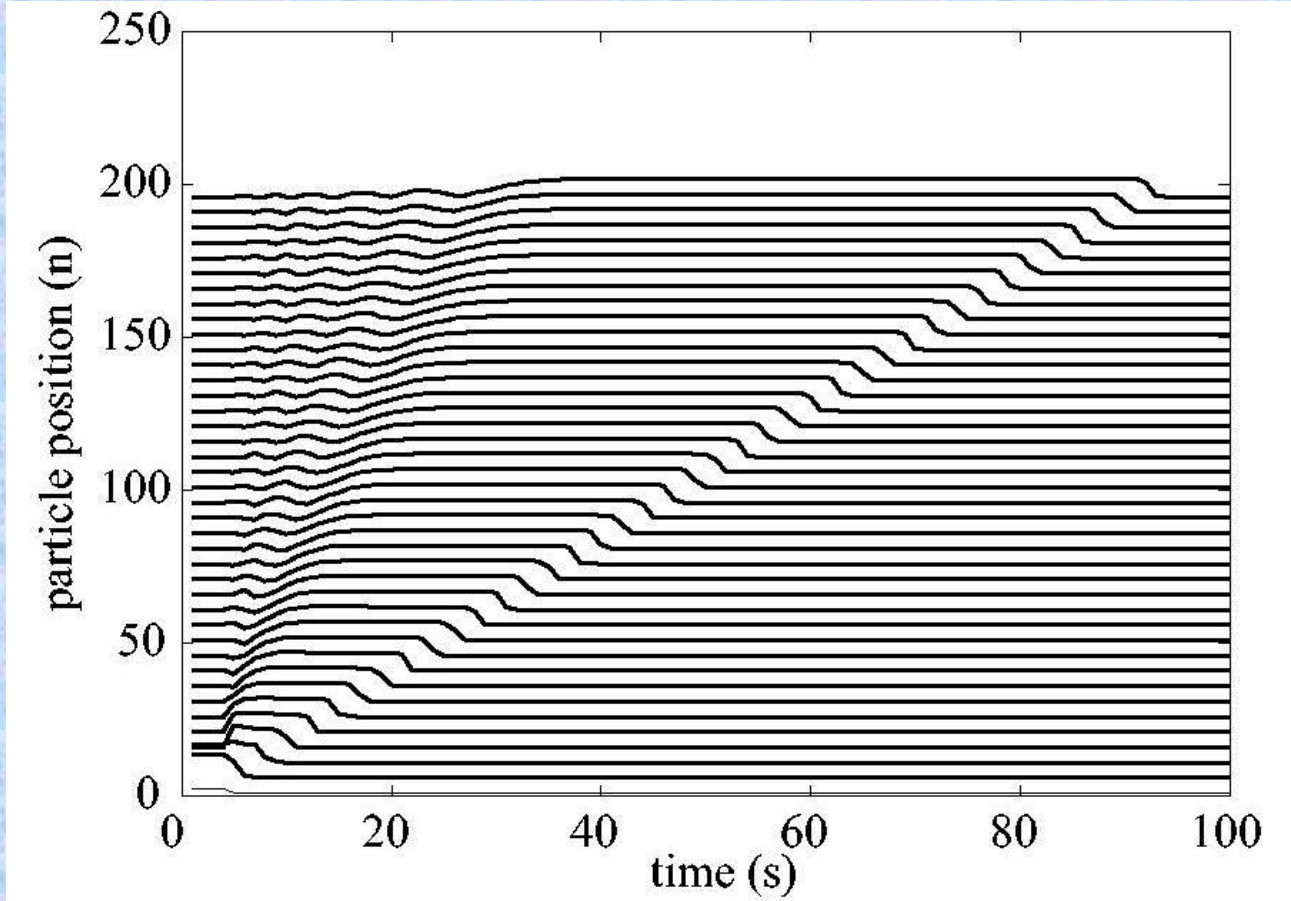
How good is the RWA description?

Very good agreement for intermediate velocities



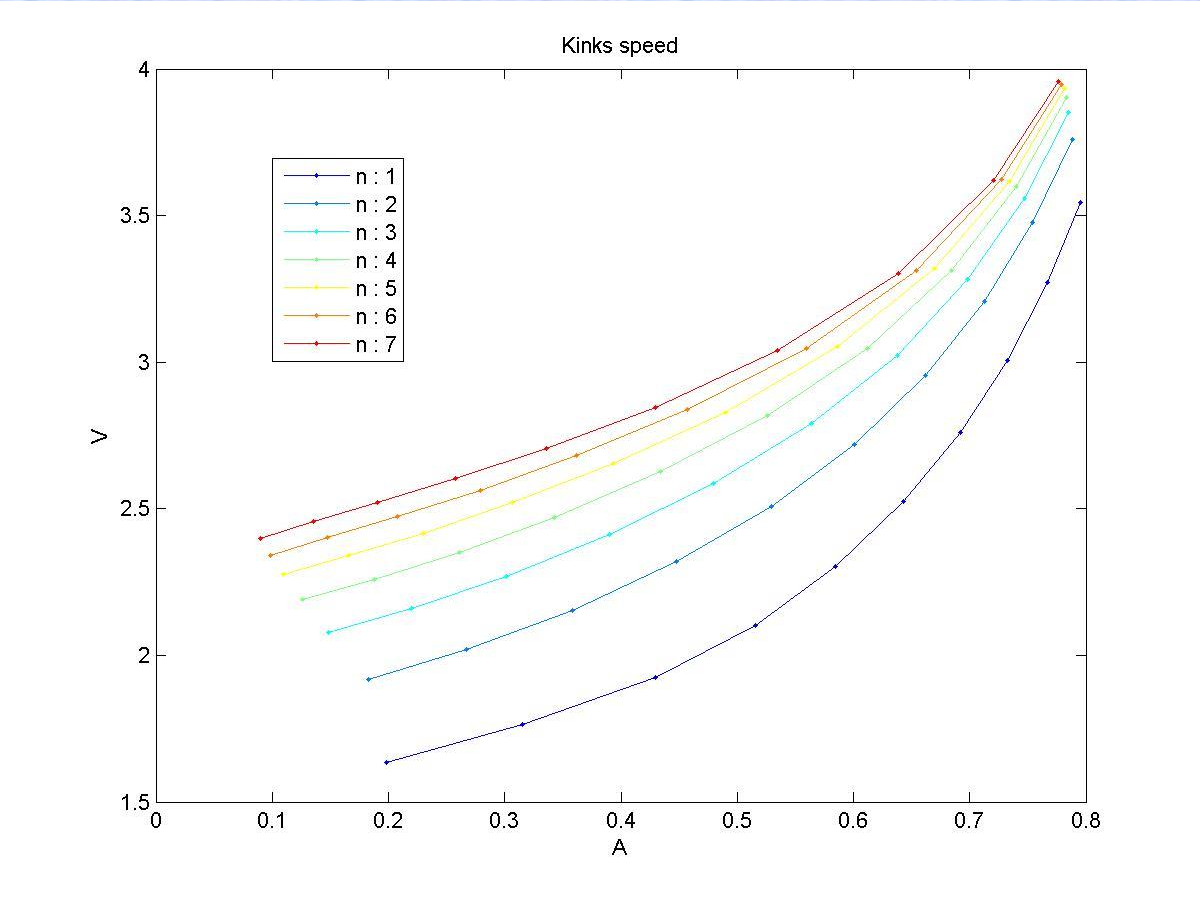


With more neighbours kinks also exist



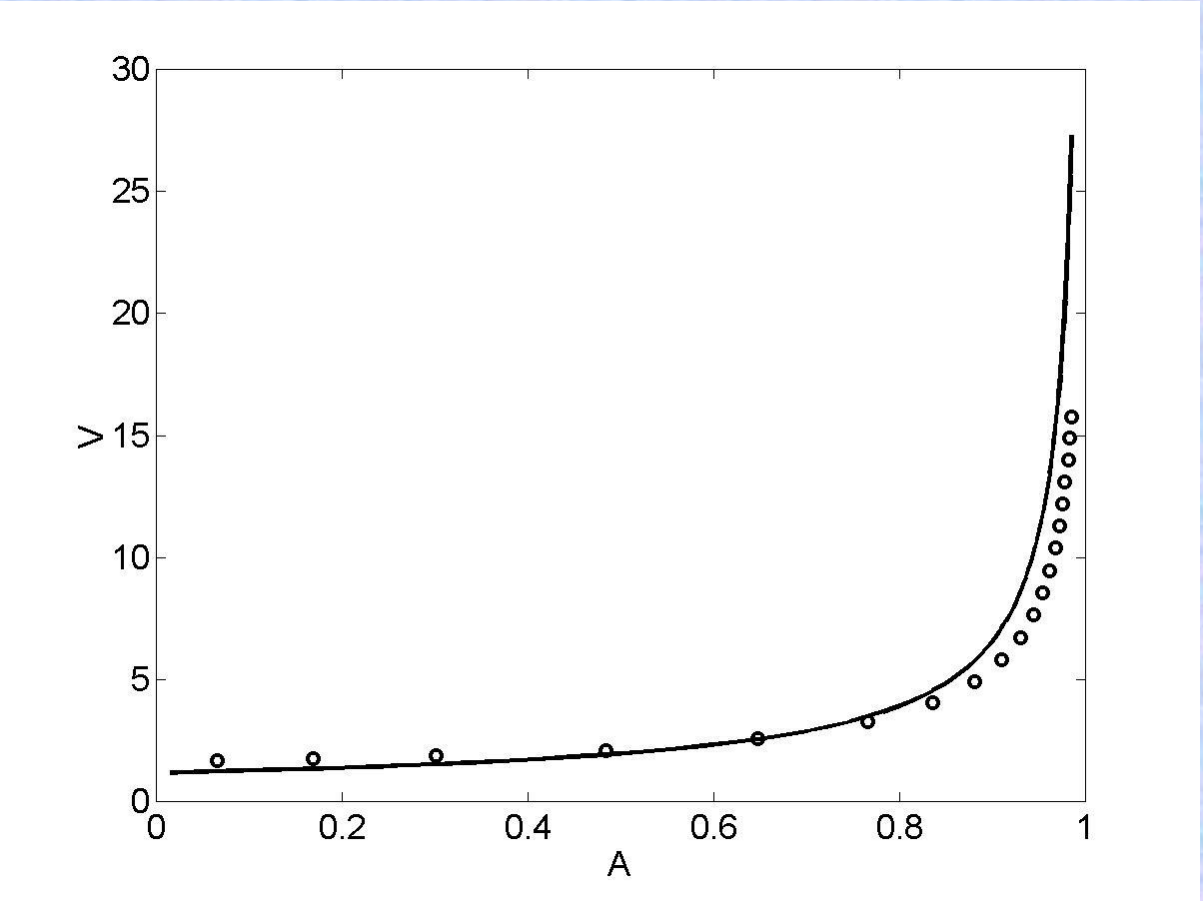
Up to 30 neighbours kinks exist, although more energy is needed

V=V(A) with several neighbours



Up to 30 neighbours, kinks have been obtained

The distances between atoms are not realistic



Need to consider a short range potential

ZBL potential used in particle collisions

Ziegler Biersack Litmark (ZBL) potential for high energy collisions

$$V(r) = \frac{Z_1 Z_2 e^2}{4\pi\varepsilon_0 r} f(\frac{r}{a}) \qquad a = \frac{0.98856\ \mathrm{a_B}}{Z_1^{0.23} + Z_2^{0.23}}$$

$\mathrm{a_B}$ Bohr radius

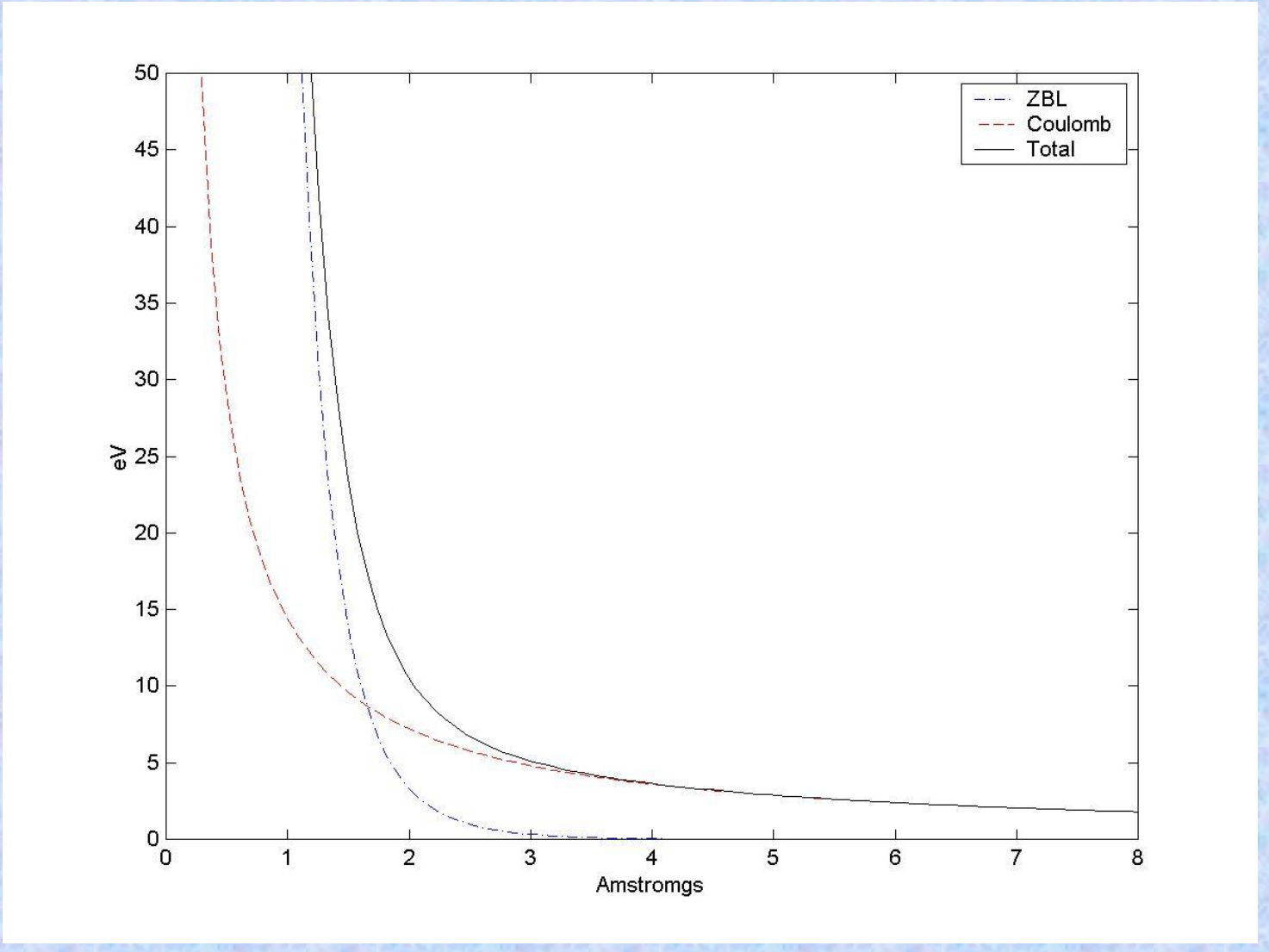
$$f(x) = \sum_{i=1}^{4} a_i \exp(-b_i x)$$

Ziegler JF, Biersack JP, Littmark U, The Stopping and Range of Ions in Matter (Pergamon, New York, 1985)

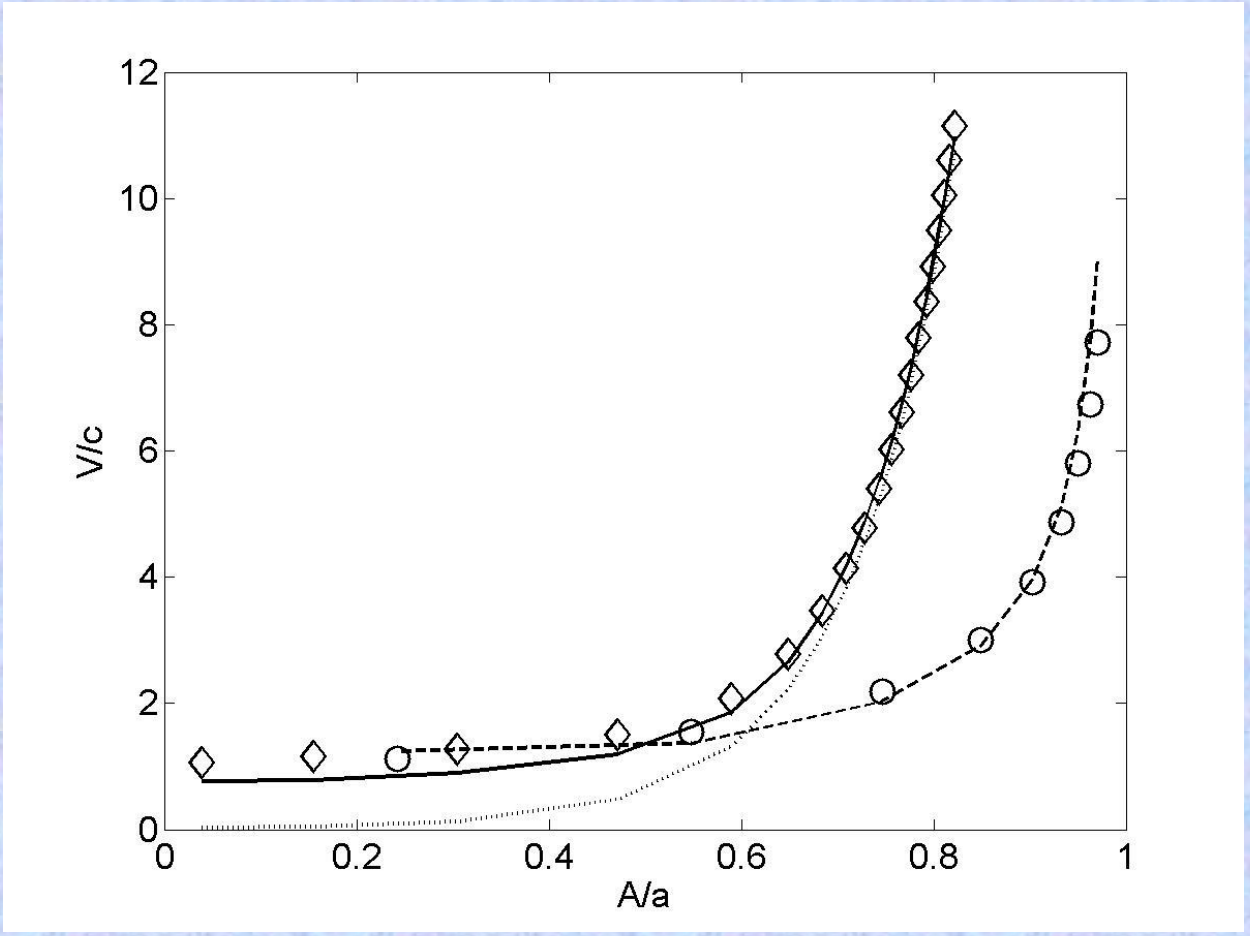
Up to 200 KeV:

$$V(r) = \frac{2650\mathrm{eVA}}{r} \exp(-\frac{\mathrm{r}}{0.3\mathrm{A}}) \qquad V(x) = \frac{184}{x} \exp(-\frac{\mathrm{x}}{0.06})$$

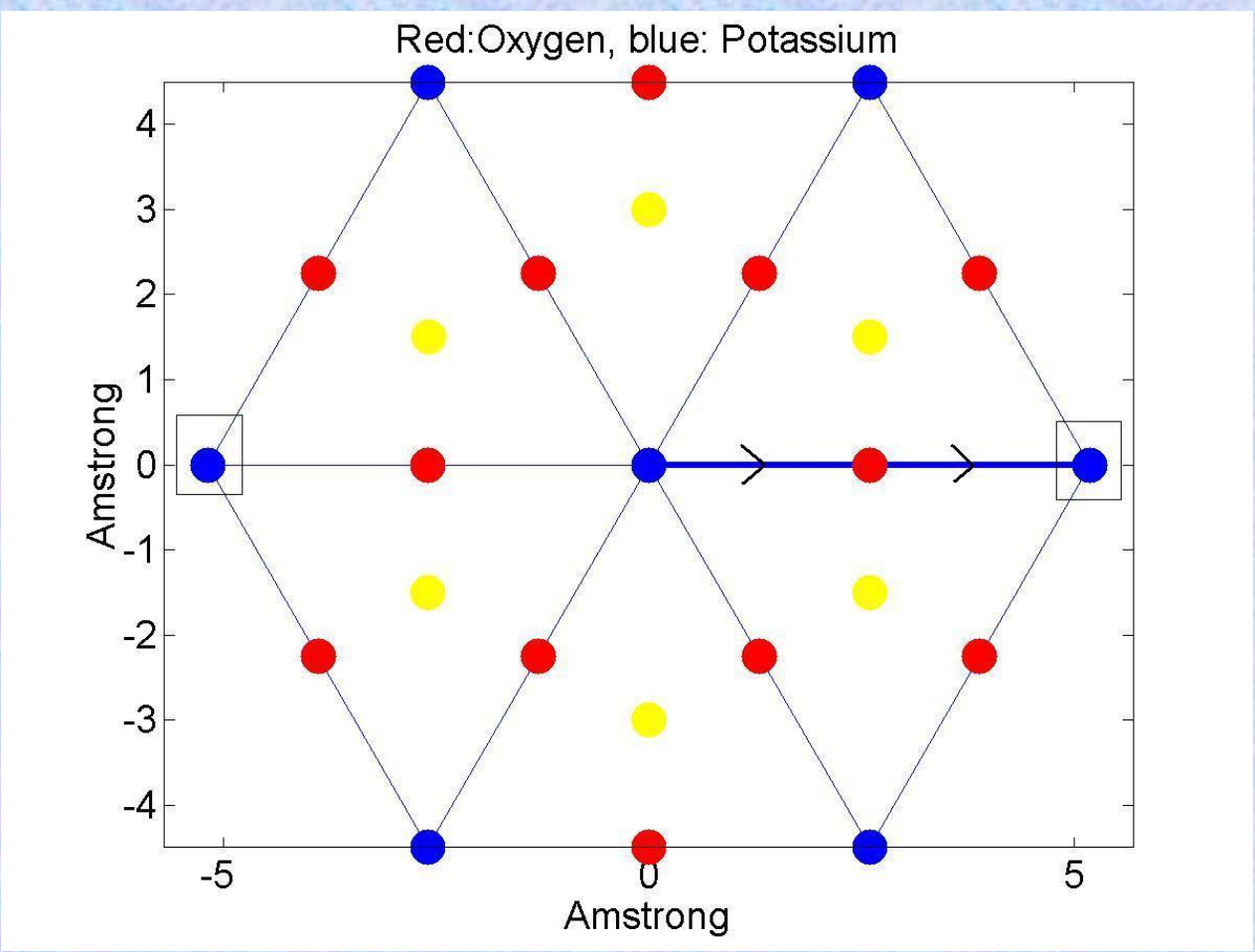
ZBL + Coulomb potential



Kink velocities ZBL + Coulomb potential



Substrate potential (1)



K^{+}

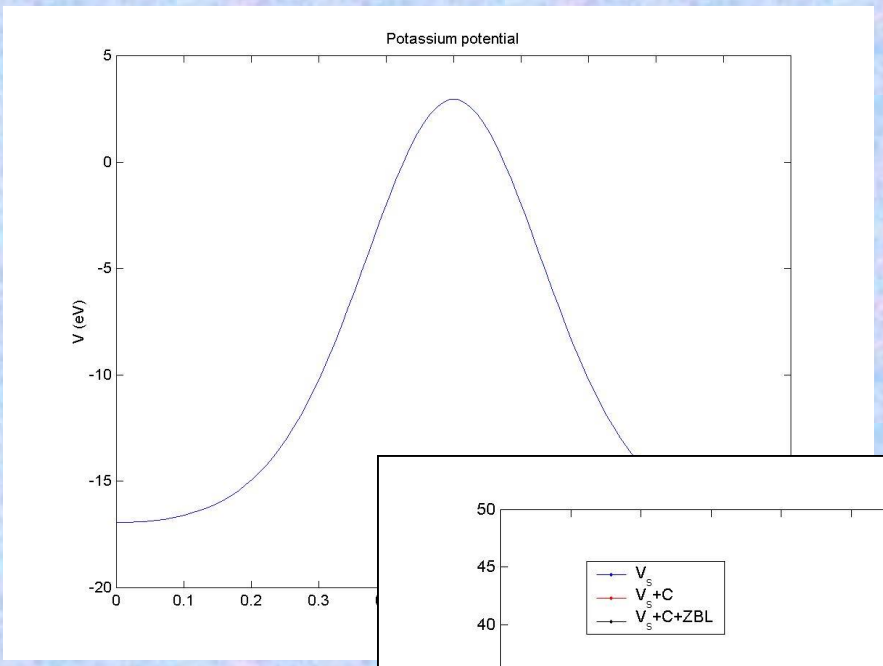
O^{-2}

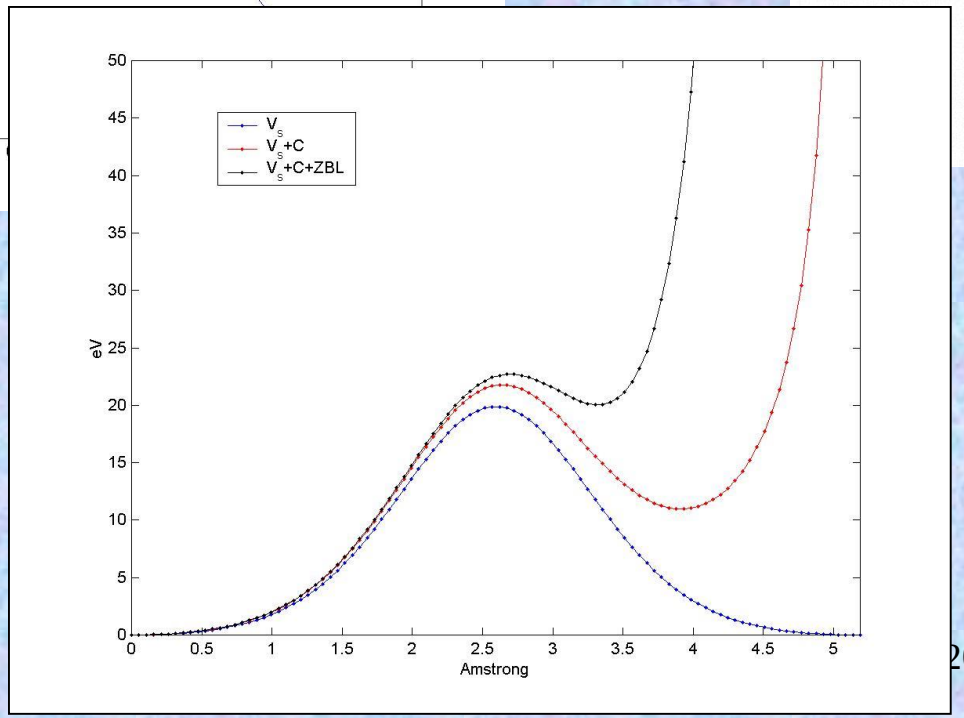
$Si^{+2.75}$

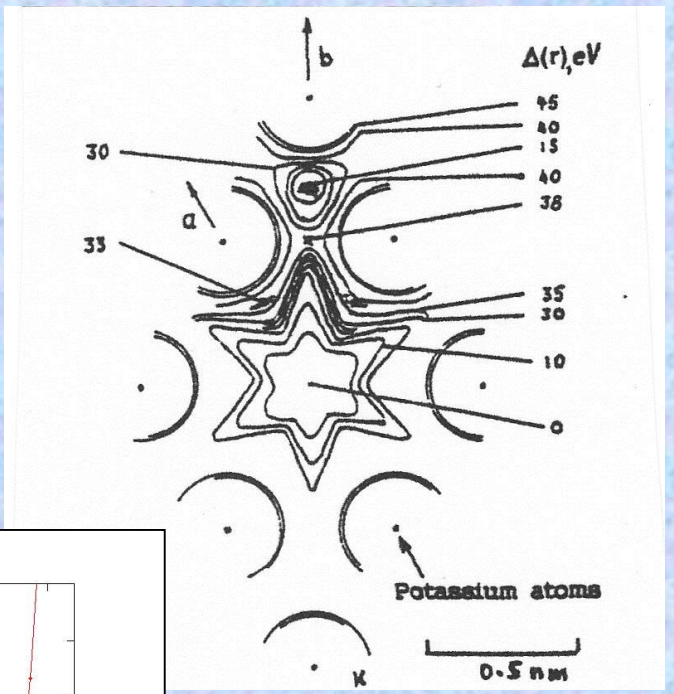
K+ not included

O and Si in planes above and below.
Coulomb and Born Mayer potentials.

Substrate potential +ZBL+ Coulomb





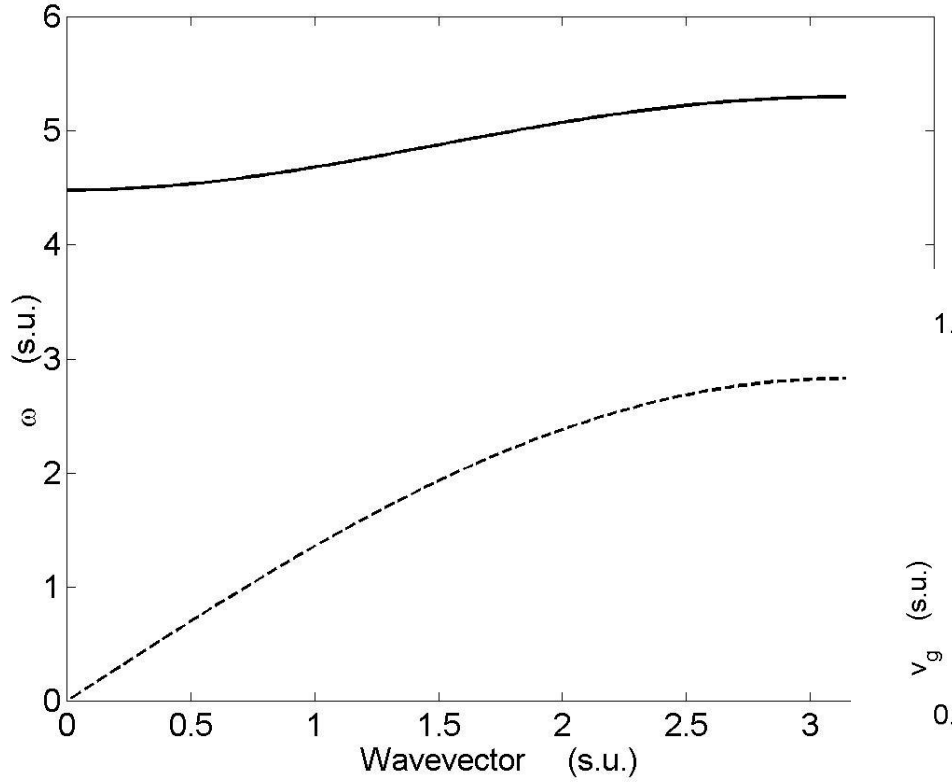


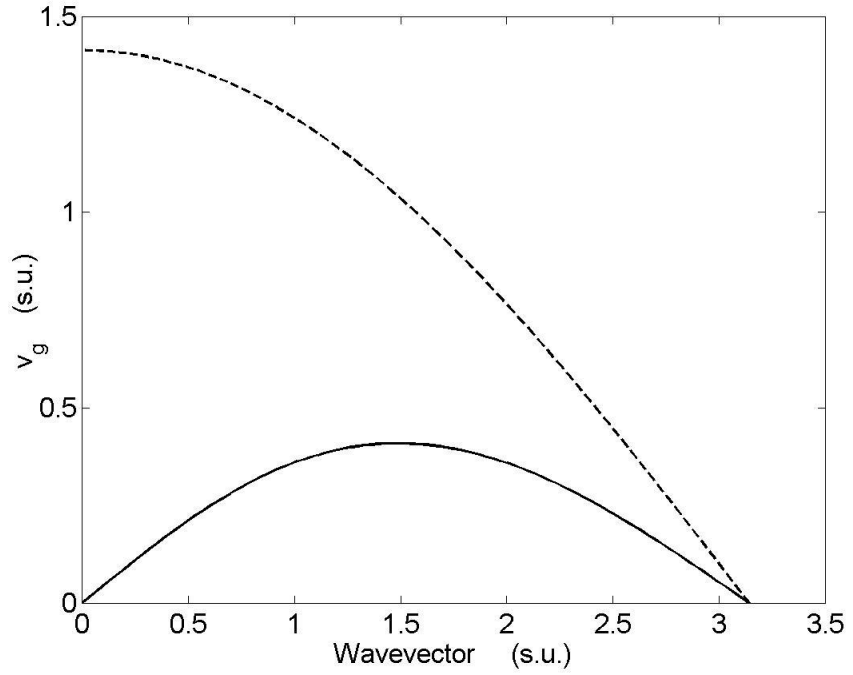
Russell&Collins
Rad. Meas. 25 (1995) 667

Phonon spectrum and group velocity with substrate

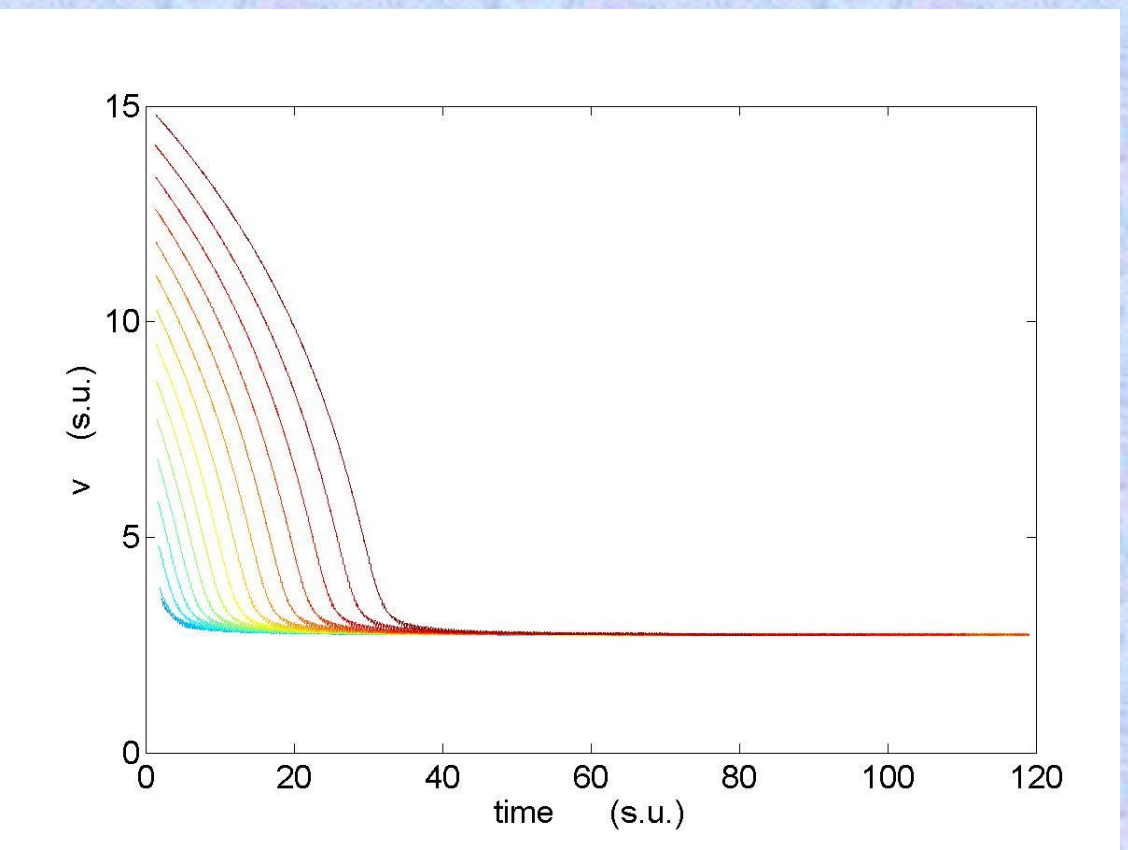
Substrate _____

No substrate -----





Lattice kinks or crowdions with limit velocity



V ~2c =8km/s , E=28 eV

Recoil of K^+ is 40 eV.
Typical ejection energies are between 3-8 eV.

Crowdions in MD for Ni in 2D and 3D:
AM Iskandarov, Comp. Mat. Sci (2009) 429


Μικε Ρυσσελλωιτη της εξπεραμ εντολεθυιπμ εντ


Altea, Alicante, Spain, September 2013



Conference Quodons in Mica 18-21-Sep-2013

Chairman: JFR Archilla/V. Sánchez-Morcillo
Scientific Committee:
Y. Kosevich, V. Dubinko....

Participants:
S. Flach, G. Tsironis,….

Nonlinear localized travelling excitations in crystals
Meeting in honor of Prof. Mike Russell, Altea,Alicante

http://www.quodons.webs.upv.es

Conclusions

• Mica has a recording capability of charged particles and lattice excitations

•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

• The are are very energetic and localized lattice kinks travelling in Coulomb's chains with muscovite parameters, with properties well described by the theory

• Lattice kinks select their own energy and velocity.

•The energy of the lattice kinks is between the surface binding energy and the energy available from K^{40} decay.

• Coulomb's lattice kinks are 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.

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.

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