Nonlinear vector waves in the atomic chain model

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Happy Birthday to V.E.Z.!

Gorky School on Nonlinear Waves

March 1972

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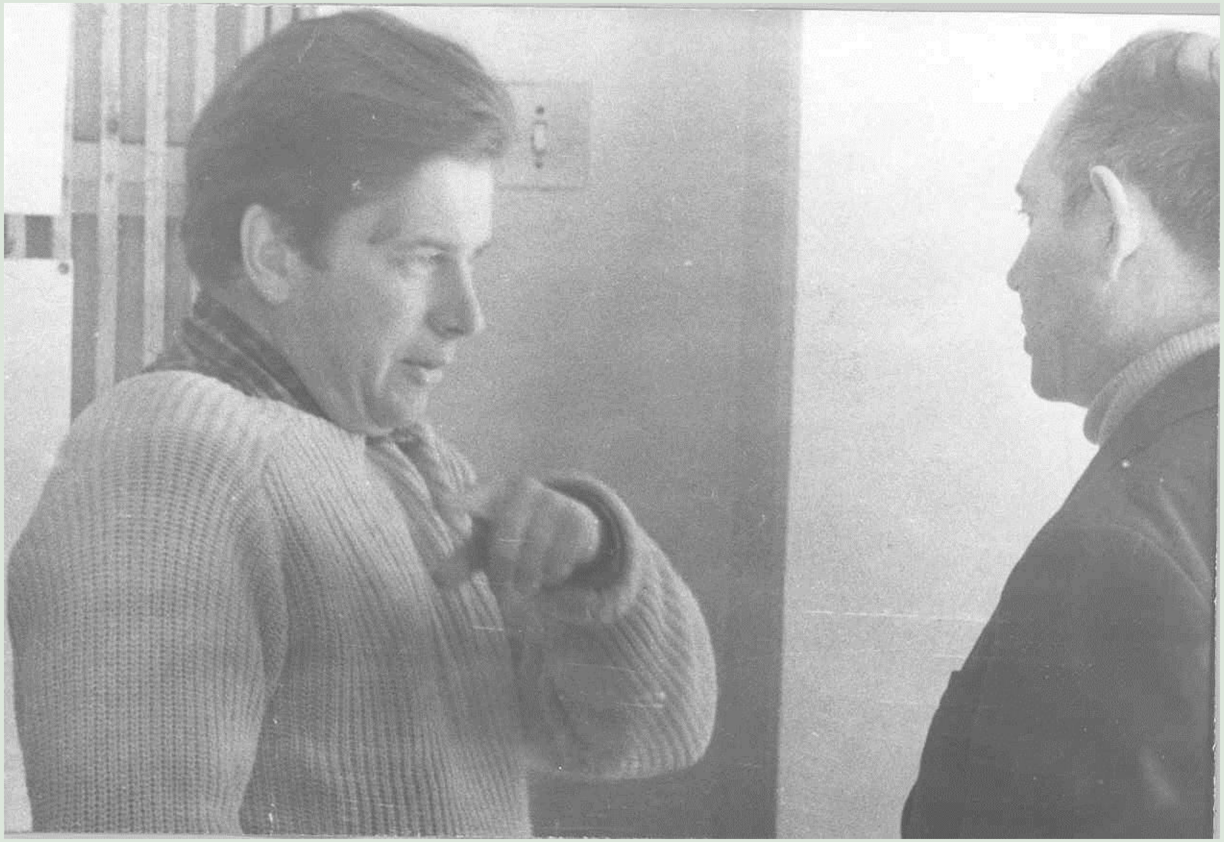


Gorky School on Nonlinear Waves

March 1972 (with Semen Moiseev)

Happy Birthday to V.E.Z.!

Sydney, Australia, ICAM-2003

(with Stuart Anderson and Yury Stepanyants)

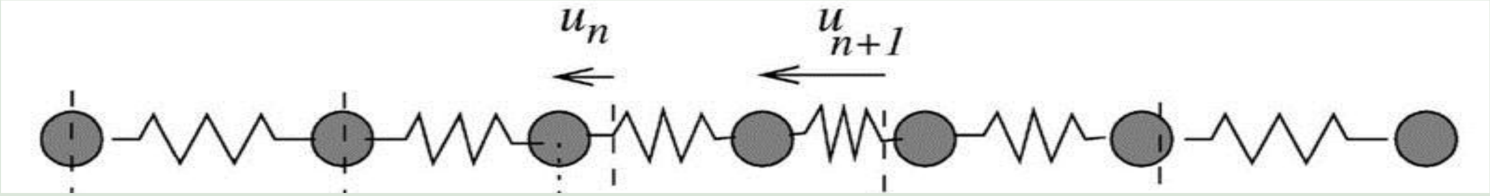
Study of Anharmonic Chains

The theory of such discrete structures remains very topical due to their numerous applications:

- theoretical physics [theory of crystal heat transport]
- molecular physics [transport of excitations in molecules]
- X-ray spectroscopy
- ultrasound diagnostics of solids
- application to electric transmission lines
- dusty plasma, etc.

The FPU Model

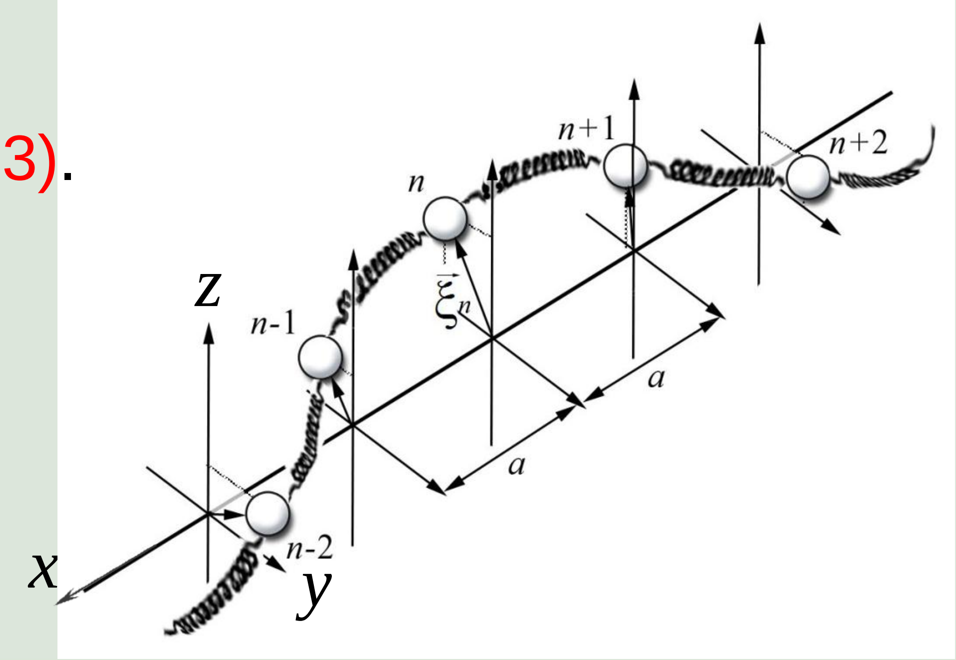
In the one-dimensional case in application to a chain of atoms the equation of motion for longitudinal modes is scalar describing atom vibrations in the direction of wave propagation (*Fermi, Pasta, Ulam, 1955; Toda, 1989*).



Transverse Modes of the Atomic Chain

When the transverse modes are considered the equation of motion becomes vector describing particle displacements in two perpendicular directions transverse to the direction of wave propagation

(*Gorbacheva & Ostrovsky*, 1983).



Transvers Modes on a Particle Chain

Steve Mould: Amazing bead chain experiment in slow motion, YouTube, *http://youtu.be/6ukMId5fIi0*

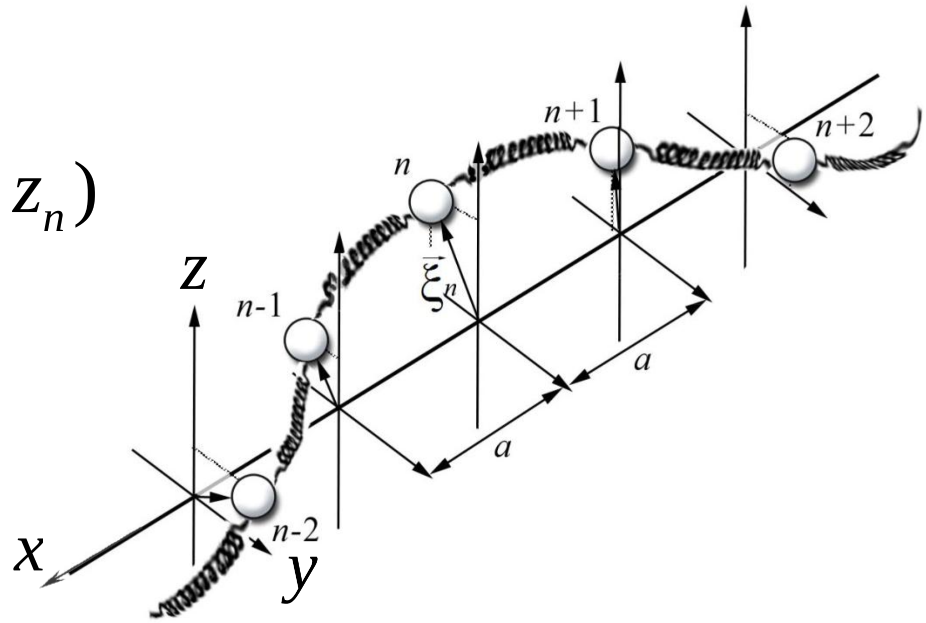
Helical Waves on the Chain of Beads

Vector Equation of Motion

Infinite chain of equal mass atoms:

$$m\frac{d^2\vec{\xi}_n}{dt^2} = \mathbf{F}_{n-2} + \mathbf{F}_{n-1} + \mathbf{F}_{n+1} + \mathbf{F}_{n+2}$$

$$\vec{\xi}_n = (y_n, z_n)$$



β_j – coupling constants,

T – uniform tension of the chain,

K – analogue of Hooke’s constant,

α – local angle between the chain and the x-axis,

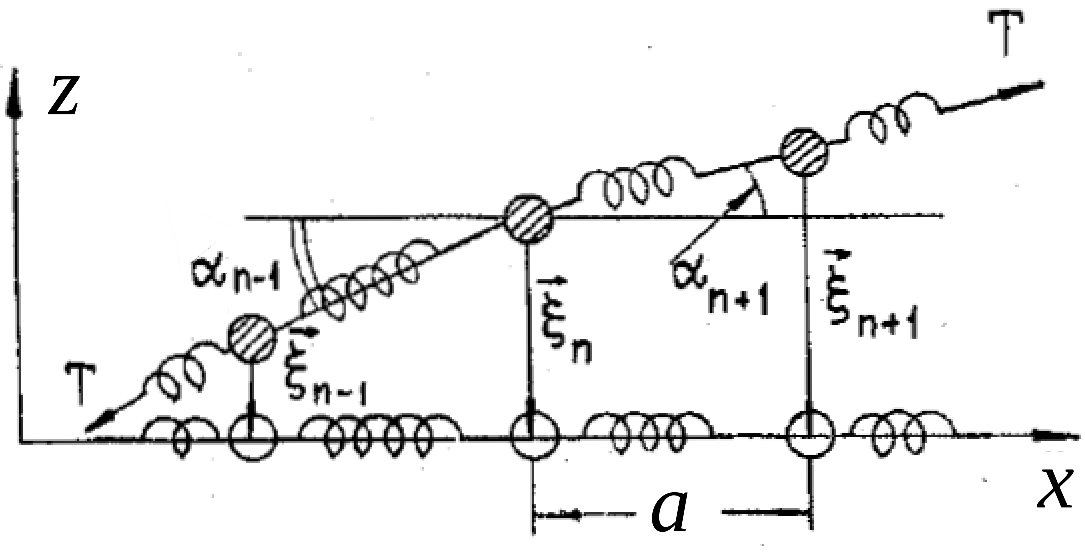
j = 1 – for nearest two neighbor atoms and j = 2 for the next two atoms.

Vector Equation of Motion

The expression for the force:

$$m\frac{d^2\vec{\xi}_n}{dt^2} = \mathbf{F}_{n-2} + \mathbf{F}_{n-1} + \mathbf{F}_{n+1} + \mathbf{F}_{n+2}$$

$$F_{n\pm1} = \pm\beta_1\left[T + aK\left(\frac{1}{\cos\alpha_{n\pm1}} - 1\right)\right]\sin\alpha_{n\pm1}$$



Vector Equation of Motion

$$m\frac{d^2\vec{\xi}_n}{dt^2} = \mathbf{F}_{n-2} + \mathbf{F}_{n-1} + \mathbf{F}_{n+1} + \mathbf{F}_{n+2}$$

$$F_{n\pm 1} = \pm\beta_1\left[T + aK\left(\frac{1}{\cos\alpha_{n\pm 1}} - 1\right)\right]\sin\alpha_{n\pm 1}$$

In the case of small angles α the forces are:

$$\mathbf{F}_{n\pm j} \approx \pm\frac{\vec{\xi}_{n\pm j} - \vec{\xi}_n}{ja}\left[T + \frac{jaK - T}{2(ja)^2}\left|\vec{\xi}_{n\pm j} - \vec{\xi}_n\right|^2\right]$$

Vector Equation of Motion

Finally the equation of motion in the dimensionless variables

reads:

$$m\frac{d^2\vec{\xi}_n}{dt^2} = \mathbf{F}_{n-2} + \mathbf{F}_{n-1} + \mathbf{F}_{n+1} + \mathbf{F}_{n+2}$$

$$\frac{d^2\bar{\xi}_n}{d\tau^2} = \bar{\xi}_{n+1} - 2\bar{\xi}_n + \bar{\xi}_{n-1} + \frac{\mu-1}{2}\left[\left|\bar{\xi}_{n+1} - \bar{\xi}_n\right|^2\left(\bar{\xi}_{n+1} - \bar{\xi}_n\right) - \left|\bar{\xi}_n - \bar{\xi}_{n-1}\right|^2\left(\bar{\xi}_n - \bar{\xi}_{n-1}\right)\right]$$

$$+$$

$$\frac{\beta_2}{2}\left\{\bar{\xi}_{n+2} - 2\bar{\xi}_n + \bar{\xi}_{n-2} + \frac{2\mu-1}{8}\left[\left|\bar{\xi}_{n+2} - \bar{\xi}_n\right|^2\left(\bar{\xi}_{n+2} - \bar{\xi}_n\right) - \left|\bar{\xi}_n - \bar{\xi}_{n-2}\right|^2\left(\bar{\xi}_n - \bar{\xi}_{n-2}\right)\right]\right\}$$

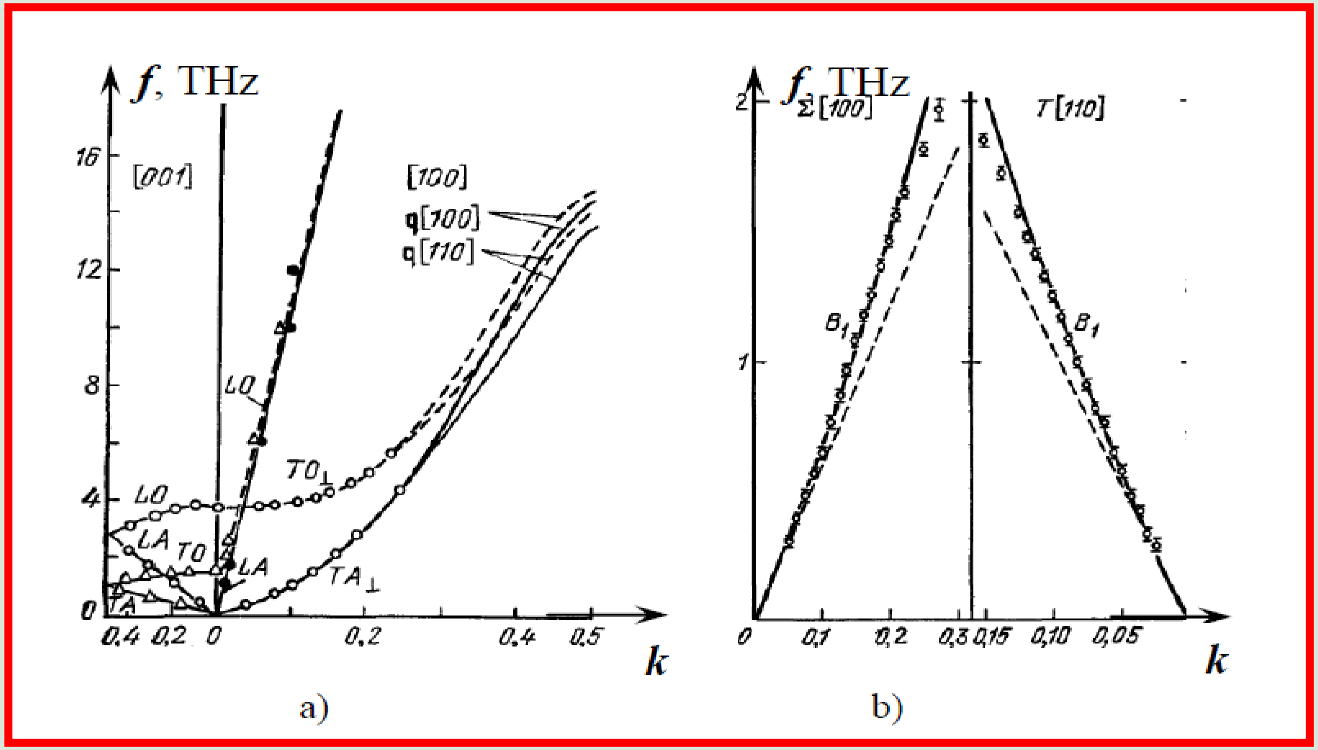
$$\tau = t\sqrt{T/am}, \qquad \bar{\xi}_n = \vec{\xi}_n/a, \qquad \mu = aK/T$$

Dispersion Law for Flexural Modes

- It is a matter of experimental fact that in many cases the transverse flexural modes in crystals demonstrate the quadratic dispersion law in $\omega \sim k^2$ in the long-wave approximation, whereas typically the dispersion low in the long wave approximation is $\omega \sim k$.
- The quadratic dispersion law occurs in anisotropic crystals with strong difference between the inlayer and interlayer forces; e.g., in the graphite (*Nicklow et al*., 1972).

Experimental Observation

Nicklow, Wakabayashi, Smith.
Phys. Rev. B, 1972, v. 5, 4951–4962.



Quadratic phonon dispersion in graphite C (a) and linear phonon dispersion in GaS (b). The wavenumber is given in relative units.

Dispersion Relation

For small perturbations of infinitesimal amplitude the dispersion relation reads:

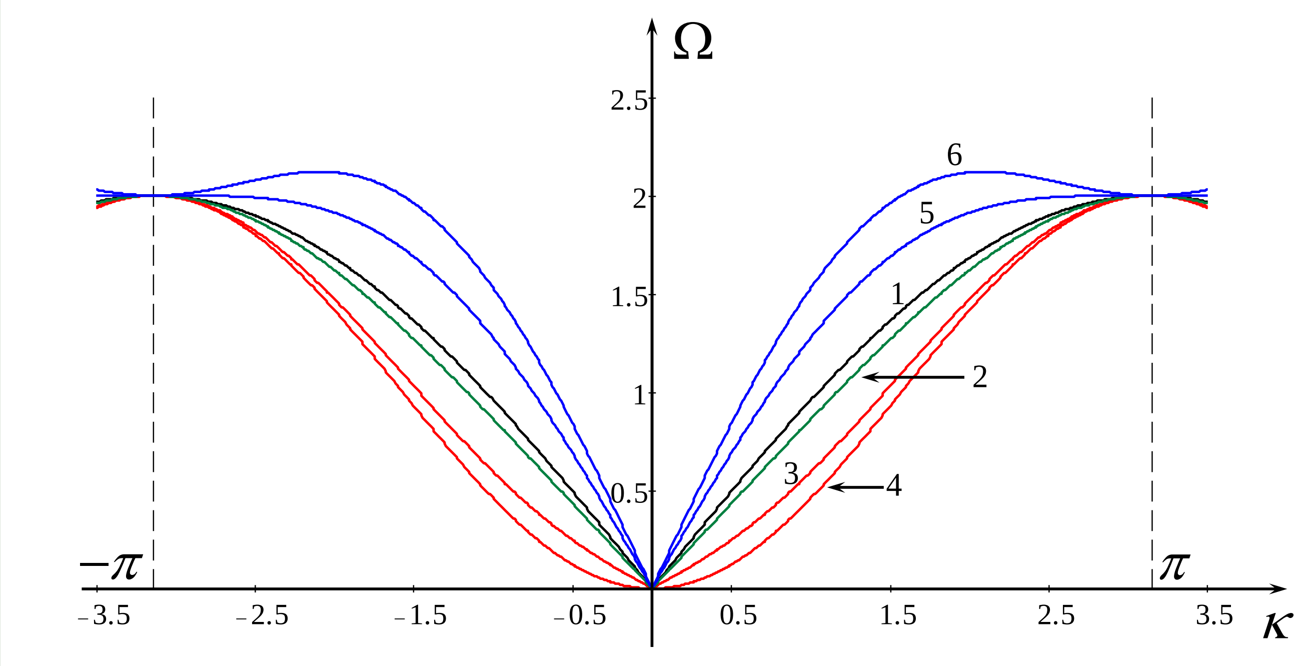
$$\omega^2 = 4\sin^2\frac{\kappa}{2}\left(1+2\beta_2\cos^2\frac{\kappa}{2}\right)$$

I.M. Lifshitz (1952) pointed out that the quadratic dispersion law in crystals can be obtained if the influence of next particles are taken into consideration.

$$1)\ \beta_2 = 0, \quad \omega = 2\sin\frac{\kappa}{2}$$

$$2)\ \beta_2 = -\frac{1}{2}, \quad \omega = 2\sin^2\frac{\kappa}{2}$$

Graphic of the Dispersion Relation



Dispersion relation in the first Brillouin zone, $-\pi \leq k \leq \pi$, for different values of the coupling constant β_2: line 1 – $\beta_2 = 0$, line 2 – $\beta_2 = -1/8$, line 3 – $\beta_2 = -0.4$, line 4 – $\beta_2 = -0.5$, line 5 – $\beta_2 = 0.5$, and line 6 – $\beta_2 = 1.0$.

Dispersion Relation in the Long Wave Approximation

In the long-wave approximation, $\kappa << 1$, the dispersion relation reads:

$\beta_2 \neq -½$:

$$\omega \approx \sqrt{1+2\beta_2}\,\kappa - \frac{1+8\beta_2}{24\sqrt{1+2\beta_2}}\kappa^3 + \ldots$$

$\beta_2 = -½$:

$$\omega \approx \frac{\kappa^2}{2} - \frac{\kappa^4}{24} + \ldots$$

$\beta_2 = -⅛$:

$$\omega \approx \frac{\sqrt{3}}{2}\kappa - \frac{\sqrt{3}}{360}\kappa^5 + \ldots$$

Nonlinear PDEs

In the long-wave approximation the governing equation

$$\frac{d^2\overline{\xi}_n}{d\tau^2} = \overline{\xi}_{n+1} - 2\overline{\xi}_n + \overline{\xi}_{n-1} + \frac{\mu-1}{2}\left[\left|\overline{\xi}_{n+1} - \overline{\xi}_n\right|^2\left(\overline{\xi}_{n+1} - \overline{\xi}_n\right) - \left|\overline{\xi}_n - \overline{\xi}_{n-1}\right|^2\left(\overline{\xi}_n - \overline{\xi}_{n-1}\right)\right]$$

$$+$$

$$\frac{\beta_2}{2}\left\{\overline{\xi}_{n+2} - 2\overline{\xi}_n + \overline{\xi}_{n-2} + \frac{2\mu-1}{8}\left[\left|\overline{\xi}_{n+2} - \overline{\xi}_n\right|^2\left(\overline{\xi}_{n+2} - \overline{\xi}_n\right) - \left|\overline{\xi}_n - \overline{\xi}_{n-2}\right|^2\left(\overline{\xi}_n - \overline{\xi}_{n-2}\right)\right]\right\}$$

reduces to the PDE:

$$\frac{\partial^2\overline{\xi}}{\partial\tau^2} - (1+2\beta_2)\frac{\partial^2\overline{\xi}}{\partial x^2} = \frac{1+8\beta_2}{12}\frac{\partial^4\overline{\xi}}{\partial x^4} + \frac{1+32\beta_2}{360}\frac{\partial^6\overline{\xi}}{\partial x^6} + \frac{\mu(1+4\beta_2)-(1+2\beta_2)}{2}\frac{\partial}{\partial x}\left(\left|\frac{\partial\overline{\xi}}{\partial x}\right|^2\frac{\partial\overline{\xi}}{\partial x}\right)$$

Varios Model Vector Equations

The basic equation can be presented in terms of $\mathbf{u} = \partial\overline{\boldsymbol{\xi}}/\partial x$:

$$\frac{\partial^2\mathbf{u}}{\partial\tau^2} - (1+2\beta_2)\frac{\partial^2\mathbf{u}}{\partial x^2} - \frac{1+8\beta_2}{12}\frac{\partial^4\mathbf{u}}{\partial x^4} - \frac{1+32\beta_2}{360}\frac{\partial^6\mathbf{u}}{\partial x^6} - \frac{\mu(1+4\beta_2)-(1+2\beta_2)}{2}\frac{\partial^2}{\partial x^2}\left(|\mathbf{u}|^2\mathbf{u}\right) = 0$$

If $\beta_2 \neq -1/2$ and $\beta_2 \neq -1/8$, then for the unidirectional wave propagation the equation can be further reduced to the vector mKdV equation (*Karney, Sen & Chu*, 1979; *Gorbacheva & Ostrovsky*, 1983; *Destrade & Saccomandi*, 2008):

$$\frac{\partial\mathbf{u}}{\partial\tau} + c_0\frac{\partial\mathbf{u}}{\partial x} + \frac{1+8\beta_2}{24c_0}\frac{\partial^3\mathbf{u}}{\partial x^3} + \frac{\mu(1+4\beta_2)-c_0^2}{4c_0}\frac{\partial}{\partial x}\left(|\mathbf{u}|^2\mathbf{u}\right) = 0, \quad c_0 = \sqrt{1+2\beta_2}$$

Vector mKdV Equations

The derived vector mKdV equation in non-integrable, but is very close to the completely integrable equation:

$$\frac{\partial \mathbf{u}}{\partial \tau} + \alpha \frac{\partial}{\partial x}\left(|\mathbf{u}|^2 \mathbf{u} \right) + \beta \frac{\partial^3 \mathbf{u}}{\partial x^3} = 0;$$

$$\frac{\partial \mathbf{u}}{\partial \tau} + \alpha |\mathbf{u}|^2 \frac{\partial \mathbf{u}}{\partial x} + \beta \frac{\partial^3 \mathbf{u}}{\partial x^3} = -\alpha \mathbf{u} \frac{\partial |\mathbf{u}|^2}{\partial x}$$

$$\alpha = \frac{\mu\left(1+4\beta_2\right) - c_0^2}{4c_0}, \quad \beta = \frac{1+8\beta_2}{24c_0}, \quad c_0 = \sqrt{1+2\beta_2}$$

Other Model Equations

If $\beta_2 \neq -1/2$, but close to $\beta_2 = -1/8$, then we have:

$$\frac{\partial^2 \mathbf{u}}{\partial \tau^2} - c_0^2 \frac{\partial^2 \mathbf{u}}{\partial x^2} - \frac{1+8\beta_2}{12}\frac{\partial^4 \mathbf{u}}{\partial x^4} - \frac{1+32\beta_2}{360}\frac{\partial^6 \mathbf{u}}{\partial x^6} - \frac{\mu\left(1+4\beta_2\right) - c_0^2}{2}\frac{\partial^2}{\partial x^2}\left(\left|\mathbf{u}\right|^2 \mathbf{u}\right) = 0$$

Or for unidirectional wave propagation:

$$\frac{\partial \mathbf{u}}{\partial \tau} + c_0 \frac{\partial \mathbf{u}}{\partial x} + \frac{1+8\beta_2}{24 c_0}\frac{\partial^3 \mathbf{u}}{\partial x^3} + \frac{1+32\beta_2}{720 c_0}\frac{\partial^5 \mathbf{u}}{\partial x^5} + \frac{\mu\left(1+4\beta_2\right) - c_0^2}{4 c_0}\frac{\partial}{\partial x}\left(\left|\mathbf{u}\right|^2 \mathbf{u}\right) = 0$$

The Critical Case

In the critical case when $\beta_2 = -1/2$, and $\omega \sim k^2$,

the basic vector equation reduces to:

$$\frac{\partial^2 \mathbf{u}}{\partial \tau^2} + \frac{1}{4}\frac{\partial^4 \mathbf{u}}{\partial x^4} + \frac{\mu}{2}\frac{\partial^2}{\partial x^2}\left(\left|\mathbf{u}\right|^2 \mathbf{u}\right) = 0$$

This equation can be treated as the vector version of the '*second order cubic Benjamin–Ono (socBO) equation*'.

The similar (but scalar) equation with the quadratic nonlinearity has been studied in (*Hereman et al.*, 1986; *Taghizadeh et al.*, 2011; *Najafi*, 2012).

The Nonlinear Pseudo-Diffusion Vector Equation

For waves propagating in one direction only, the socBO equation can be further simplified to the nonlinear 'pseudo-diffusion' vector equation:

$$\frac{\partial\left(\hat{\mathrm{H}}\mathbf{u}\right)}{\partial\tau} - \frac{1}{2}\frac{\partial^2\mathbf{u}}{\partial x^2} - \frac{\mu}{2}\left|\mathbf{u}\right|^2\mathbf{u} = 0$$

where $\hat{\mathrm{H}}$ – is the Hilbert transform operator:

$$\hat{\mathrm{H}}\{f\} = \frac{1}{\pi}\,⨍_{-\infty}^{+\infty}\frac{f(x')}{x'-x}\,dx'; \quad \hat{\mathrm{H}}^{-1} = -\hat{\mathrm{H}}.$$

Stationary Waves

Consider stationary solutions to the main equation of

nonlinear vector string, $\mathbf{u} = \mathbf{u}(s = x - Vt)$:

$$\frac{\partial^2 \mathbf{u}}{\partial \tau^2} - c_0^2 \frac{\partial^2 \mathbf{u}}{\partial x^2} - \alpha \frac{\partial^2}{\partial x^2}\left(|\mathbf{u}|^2 \mathbf{u}\right) - \beta \frac{\partial^4 \mathbf{u}}{\partial x^4} = 0$$

$$\frac{d^2 \mathbf{u}}{dx^2} + \frac{c_0^2 - V^2}{\beta} \mathbf{u} + \frac{\alpha}{\beta} |\mathbf{u}|^2 \mathbf{u} = 0$$

Energy integral:

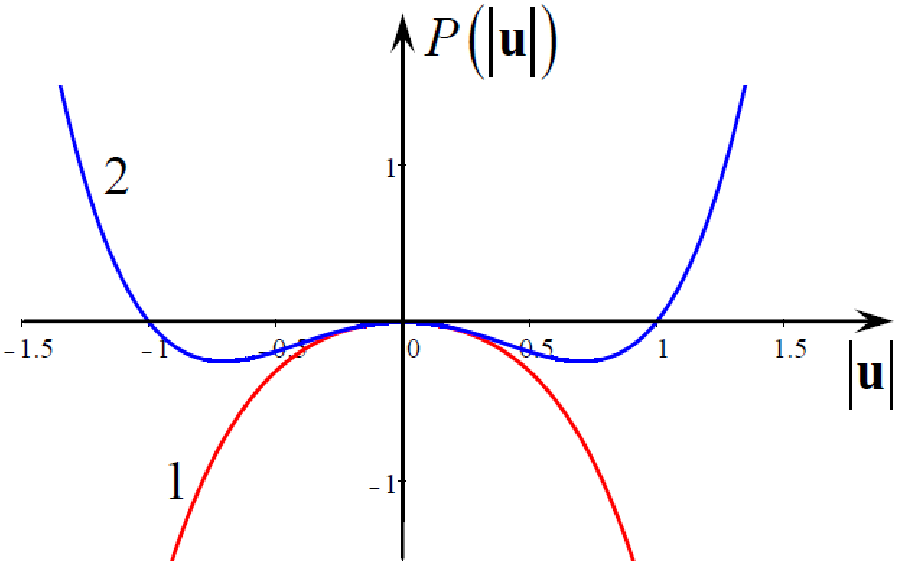
$$\frac{1}{2}\left|\frac{d\mathbf{u}}{ds}\right|^2 + \frac{c_0^2 - V^2}{\beta} |\mathbf{u}|^2 + \frac{\alpha}{\beta} |\mathbf{u}|^4 = E$$

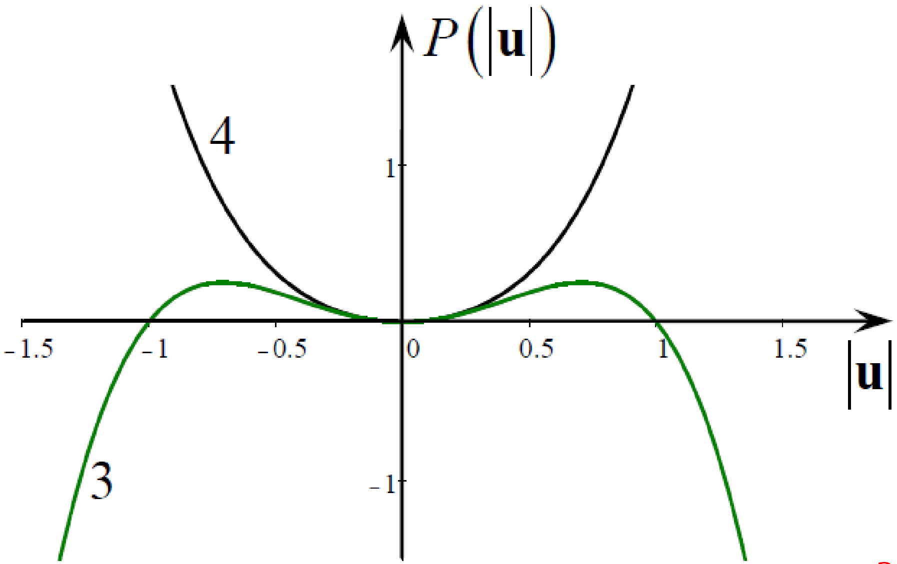
Analysis of the Energy Integral

Mechanical interpretation of the energy integral:

$$\frac{1}{2}\left|\frac{d\mathbf{u}}{ds}\right|^2 + \frac{c_0^2 - V^2}{\beta}\left|\mathbf{u}\right|^2 + \frac{\alpha}{\beta}\left|\mathbf{u}\right|^4 = E$$

The potential function: $P\left(\left|\mathbf{u}\right|\right) = \frac{c_0^2 - V^2}{\beta}\left|\mathbf{u}\right|^2 + \frac{\alpha}{\beta}\left|\mathbf{u}\right|^4$





Solitary Waves

Let us look for a solution to the equation

$$\frac{d^2\mathbf{u}}{dx^2}+\frac{c_0^2-V^2}{\beta}\mathbf{u}+\frac{\alpha}{\beta}|\mathbf{u}|^2\mathbf{u}=0$$

in the form $\mathbf{u} = (R\cos\varphi, R\sin\varphi)$;

then denoting $X = \varphi'$ we obtain:

$$\beta\left[R''-RX^2\right]+\alpha R^3+\left(c_0^2-V^2\right)R=0; \qquad R^2X=I=const$$

$$R''+\frac{\alpha}{\beta}R^3+\frac{c_0^2-V^2}{\beta}R-\frac{I^2}{R^3}=0$$

Stationary Solitary Waves

The analysis of the derived equation

$$R'' + \frac{\alpha}{\beta} R^3 + \frac{c_0^2 - V^2}{\beta} R - \frac{I^2}{R^3} = 0$$

shows that stationary solitary waves are possible

only in the form of plane solitons when $I = 0$.

$$\frac{1}{2}\left(R'\right)^2 + \frac{\alpha}{4\beta} R^4 + \frac{c_0^2 - V^2}{2\beta} R^2 + \frac{I^2}{2R^2} = E$$

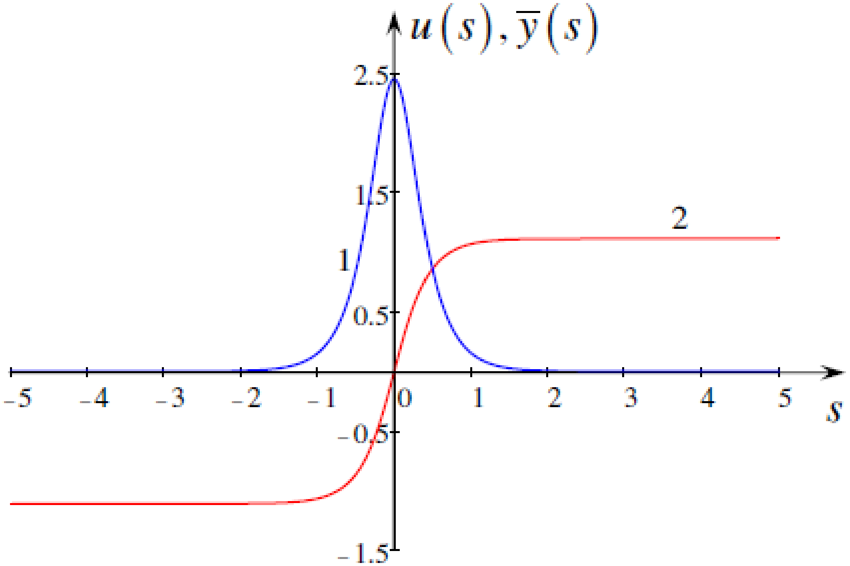
Stationary Solitary Waves

Plane soliton solution:

$$u(s) = \frac{A_s}{\cosh(s/\Delta_s)}, \quad \bar{y}(s) = 2A_s\Delta_s\left[\tan^{-1}\left(e^{-s/\Delta_s}\right) - C\right]$$

$$\Delta_s = \frac{1}{|A_s|}\sqrt{\frac{1+8\beta_2}{3\left[\mu(1+4\beta_2) - c_0^2\right]}}$$

$$V^2 = c_0^2 + \frac{A_s^2}{4}\left[\mu(1+4\beta_2) - c_0^2\right]$$



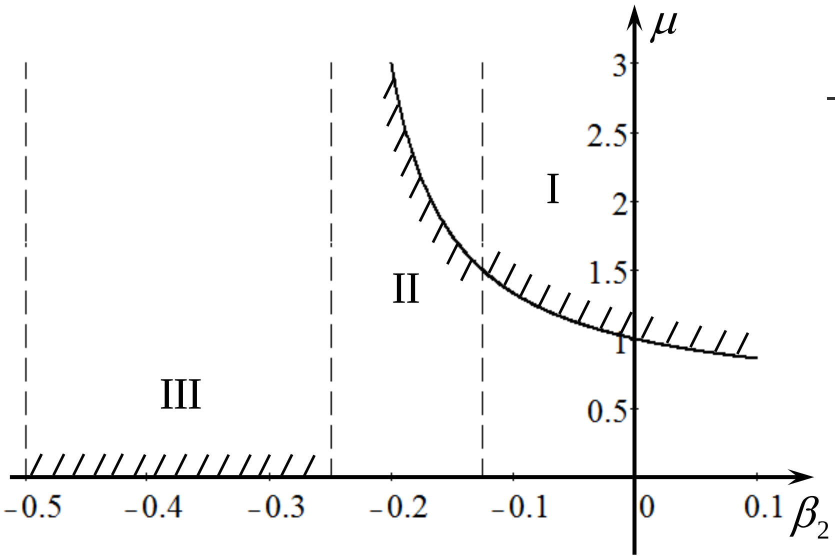
Stationary Solitary Waves

Existence of plane solitons:

1) Fast solitons, $|V| > c_0$; $\beta_2 > -1/8, \quad \mu > \dfrac{1+2\beta_2}{1+4\beta_2}$

2) Slow solitons, $|V| < c_0$; $-1/4 < \beta_2 < -1/8, \quad \mu < \dfrac{1+2\beta_2}{1+4\beta_2}$

$-1/2 < \beta_2 < -1/4, \quad \mu > 0$



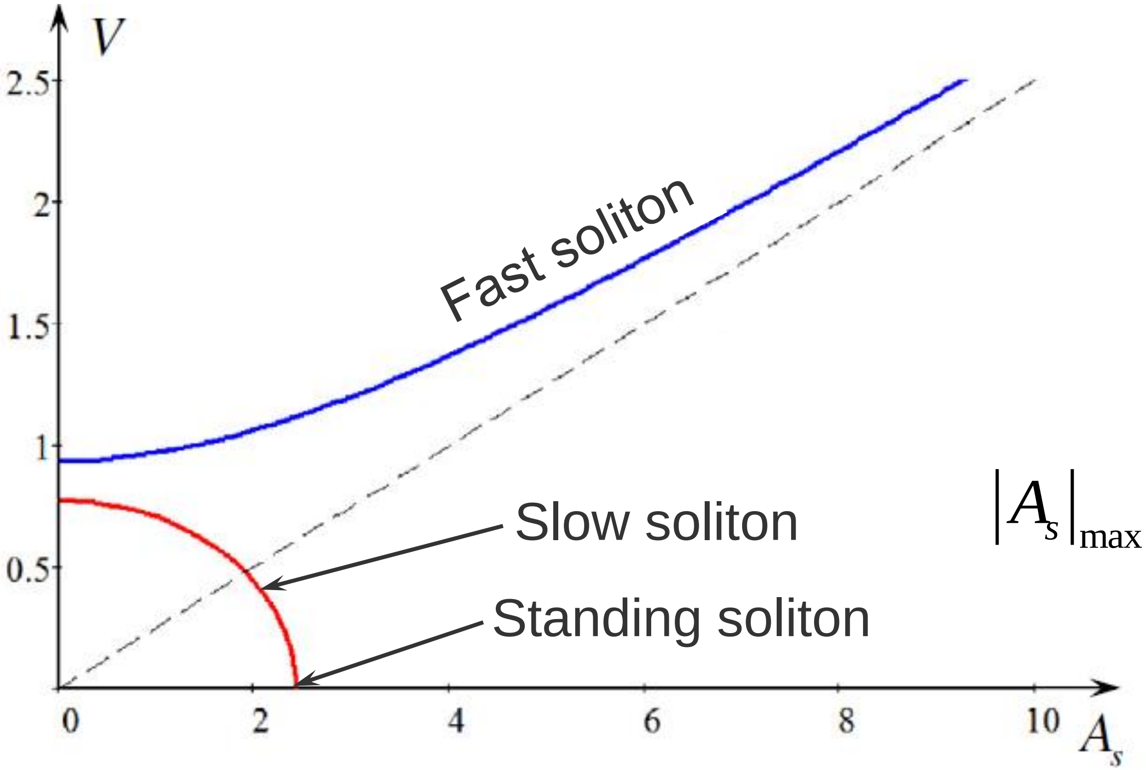
Fast solitons exist in the domain I

Slow solitons exist in the domains II and III

Stationary Solitary Waves

Dependence of soliton speed on amplitude:

$$V^2 = c_0^2 + \frac{A_s^2}{4}\left[\mu\left(1+4\beta_2\right) - c_0^2\right]$$



$$\left|A_s\right|_{\max} = \frac{2c_0}{\sqrt{c_0^2 - \mu\left(1+4\beta_2\right)}}$$

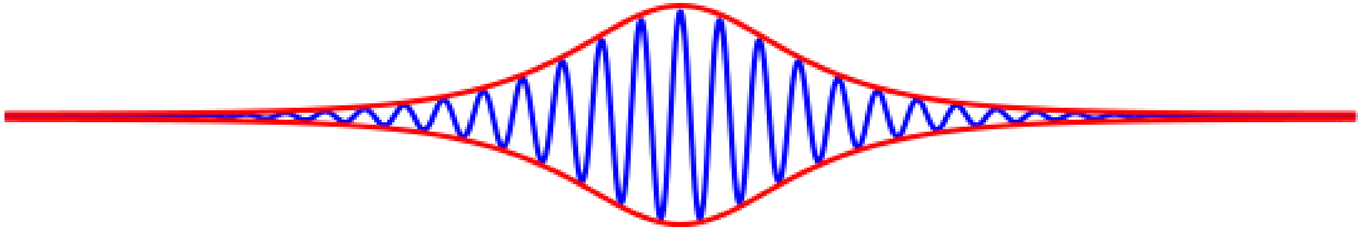
Non-Stationary Solitary Waves

I. Plane breathers in the mKdV equation

$$u(x,\tau) = -4q\sqrt{\frac{1+8\beta_2}{\mu(1+4\beta_2)-c_0^2}}\,\mathrm{sech}\Psi\,\frac{\cos\Phi-(q/p)\sin\Phi\tanh\Psi}{1+(q/p)^2\sin^2\Phi\,\mathrm{sech}^2\Psi},$$

$$\Phi = 2px + \frac{\delta}{24c_0}(1+8\beta_2)\tau + \varphi_0, \quad \Psi = 2qx + \frac{\gamma}{24c_0}(1+8\beta_2)\tau + \psi_0,$$

$$\delta = 8p\left(p^2-3q^2\right), \quad \gamma = 8q\left(3p^2-q^2\right).$$



Non-Stationary Solitary Waves

II. Helical solitons – clockwise rotating soliton

$$\mathbf{u} = Re^{i\psi}\mathbf{e} + Re^{-i\psi}\mathbf{e}^{*}$$

$$\mathbf{e} = (0, 1/2, i/2), \quad \mathbf{e}^{*} = (0, 1/2, -i/2).$$

$$R(s) = \frac{A_h}{\cosh(s/\Delta_h)}, \qquad \psi(s,\tau) = \frac{C(\tau)}{A_h^2}\sqrt{\frac{1+8\beta_2}{3\left[\mu(1+4\beta_2)-c_0^2\right]}}\sinh(s/\Delta_h)$$

$$\Delta_h = \frac{1}{|A_h|}\sqrt{\frac{1+8\beta_2}{3\left[\mu(1+4\beta_2)-c_0^2\right]}}$$

$$V_h = \frac{\mu(1+4\beta_2)-c_0^2}{8c_0}A_h^2$$

Interactions of Solitary Waves

The numerical modelling of wave dynamics was undertaken by direct simulation of the differential-difference set of vector equations on the basis of the fourth order Runge–Kutta method.

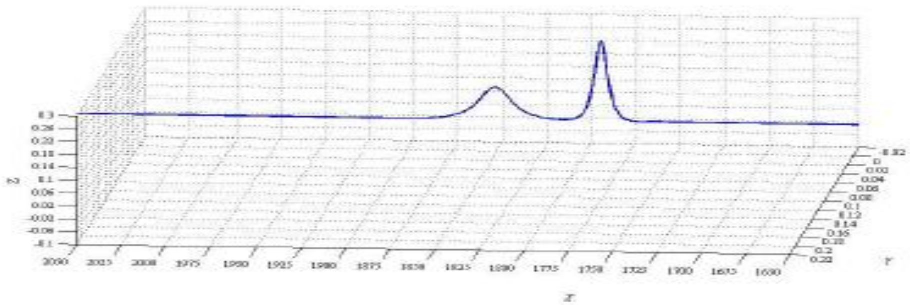
$$\frac{d^2\bar{\xi}_n}{d\tau^2} = \bar{\xi}_{n+1} - 2\bar{\xi}_n + \bar{\xi}_{n-1} + \frac{\mu-1}{2}\left[\left|\bar{\xi}_{n+1}-\bar{\xi}_n\right|^2\left(\bar{\xi}_{n+1}-\bar{\xi}_n\right) - \left|\bar{\xi}_n-\bar{\xi}_{n-1}\right|^2\left(\bar{\xi}_n-\bar{\xi}_{n-1}\right)\right]$$

$$+$$

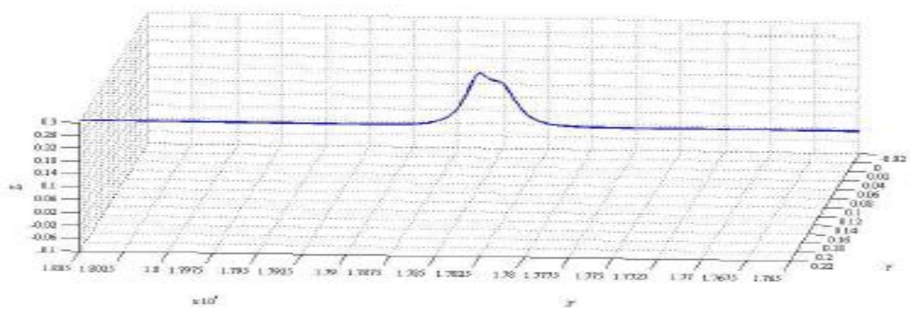
$$\frac{\beta_2}{2}\left\{\bar{\xi}_{n+2} - 2\bar{\xi}_n + \bar{\xi}_{n-2} + \frac{2\mu-1}{8}\left[\left|\bar{\xi}_{n+2}-\bar{\xi}_n\right|^2\left(\bar{\xi}_{n+2}-\bar{\xi}_n\right) - \left|\bar{\xi}_n-\bar{\xi}_{n-2}\right|^2\left(\bar{\xi}_n-\bar{\xi}_{n-2}\right)\right]\right\}$$

Interaction of Plane Solitary Waves

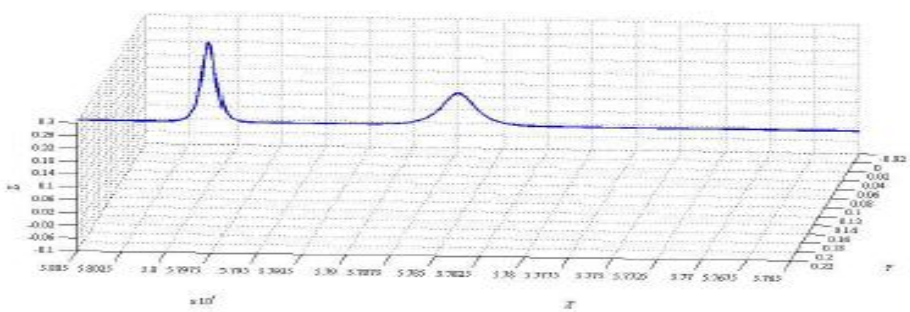
Elastic interactions between solitons propagating in the same plane



a)

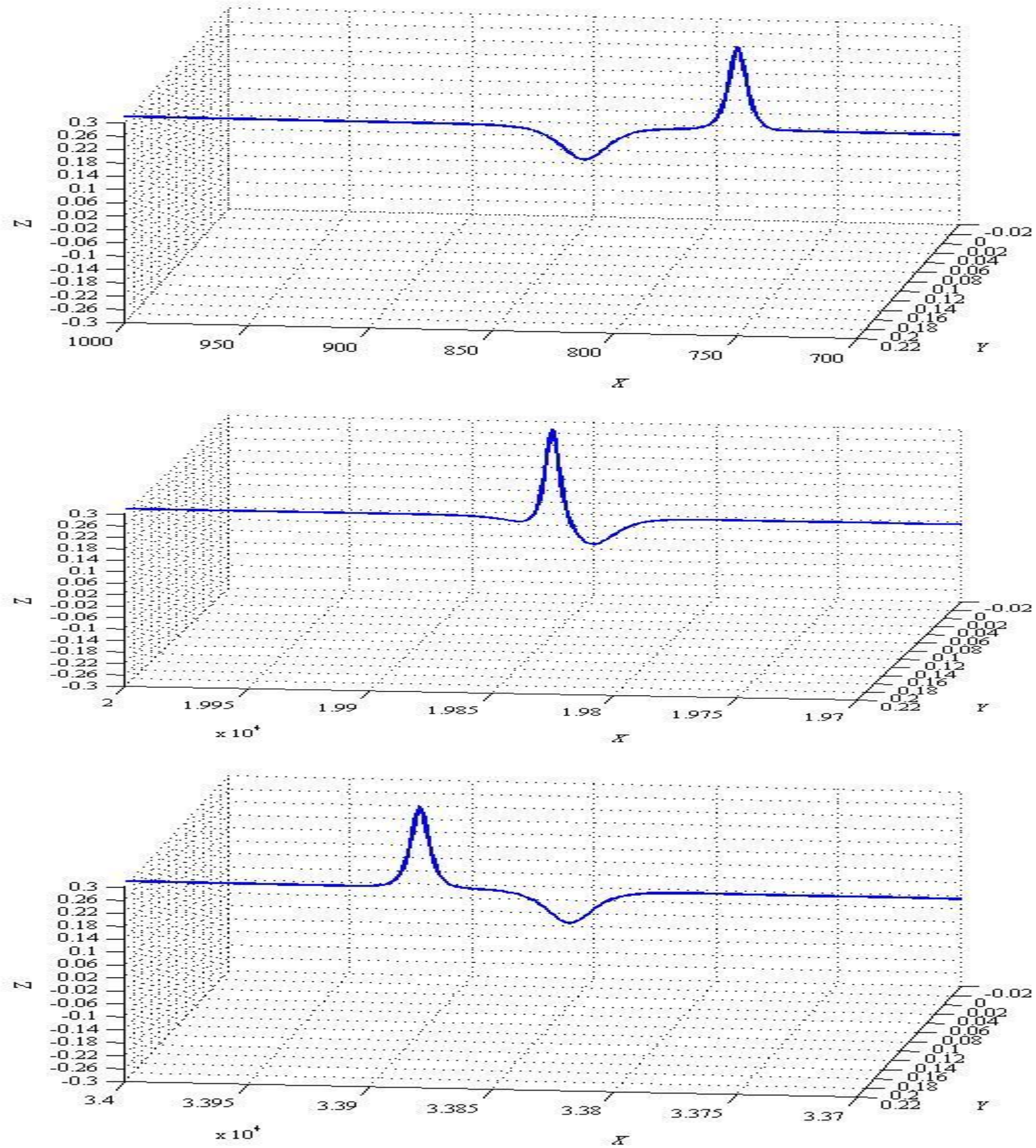


b)



c)

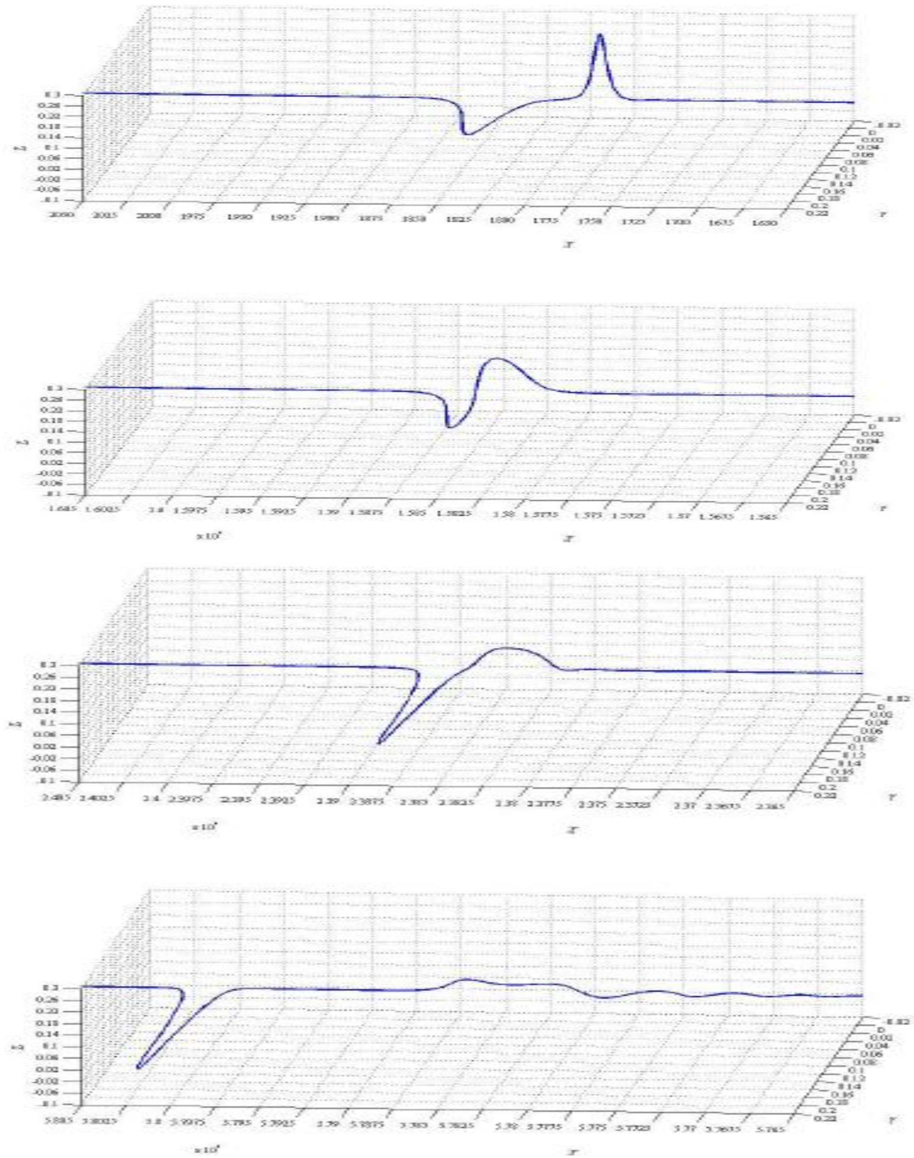
Interaction of Plane Solitary Waves



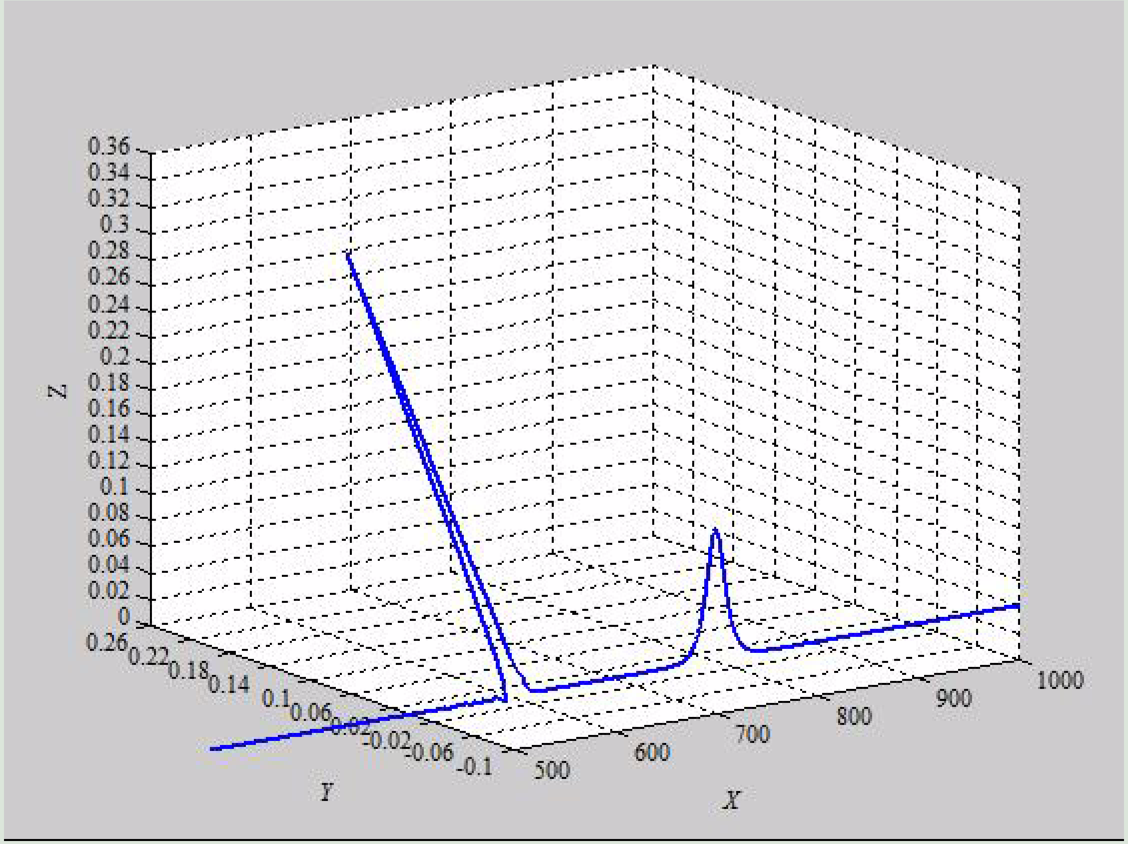
Interaction of Plane Solitary Waves

Inelastic interactions between solitons propagating in different planes

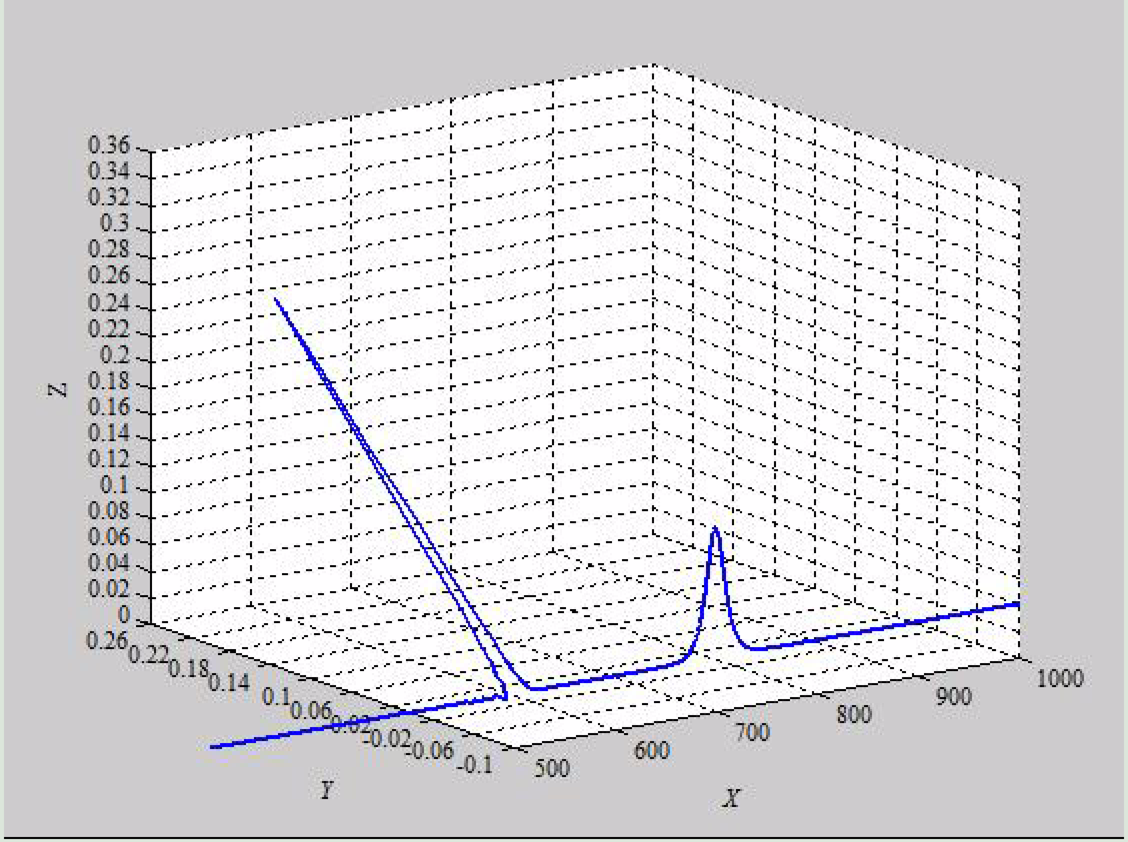
- The larger-amplitude soliton overtaking the smaller one transfers its energy to the smaller soliton and then decays.
- In the meantime, the smaller-amplitude soliton acquiring energy from the bigger one becomes taller and moves ahead.



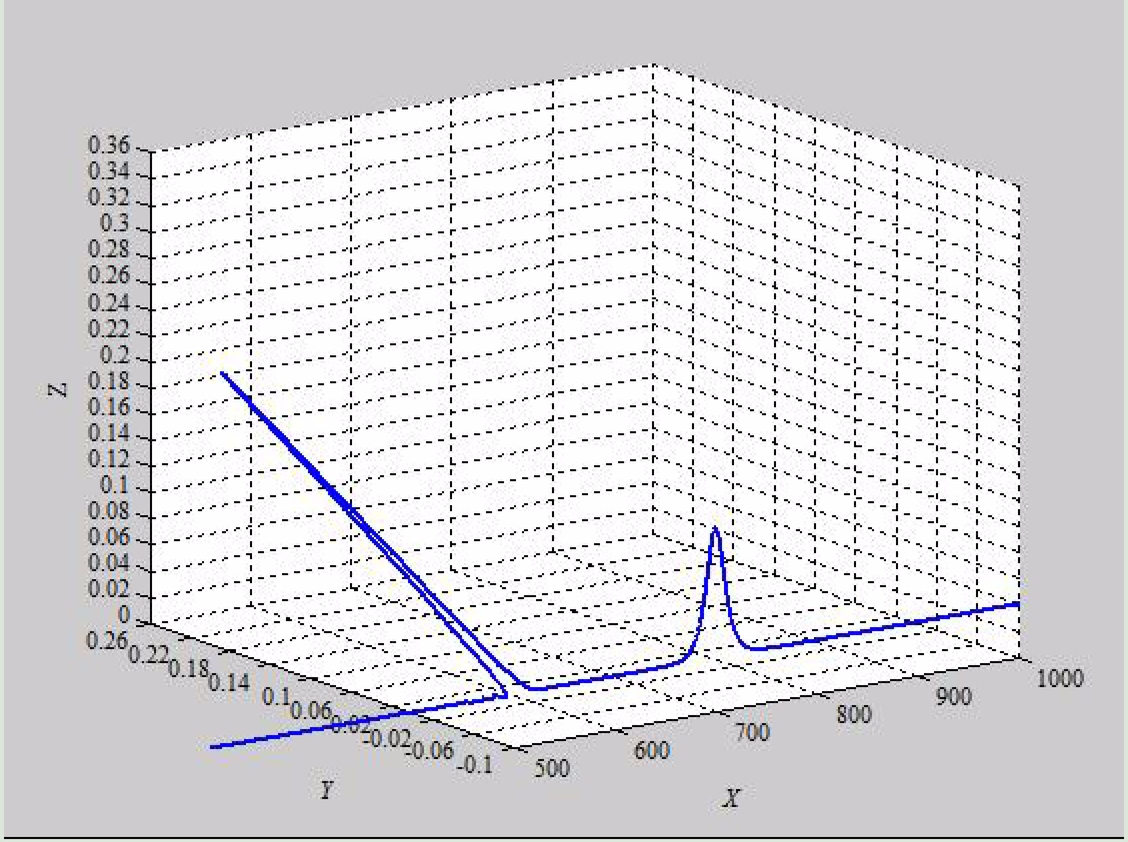
Inelastic Soliton Interaction at 30˚



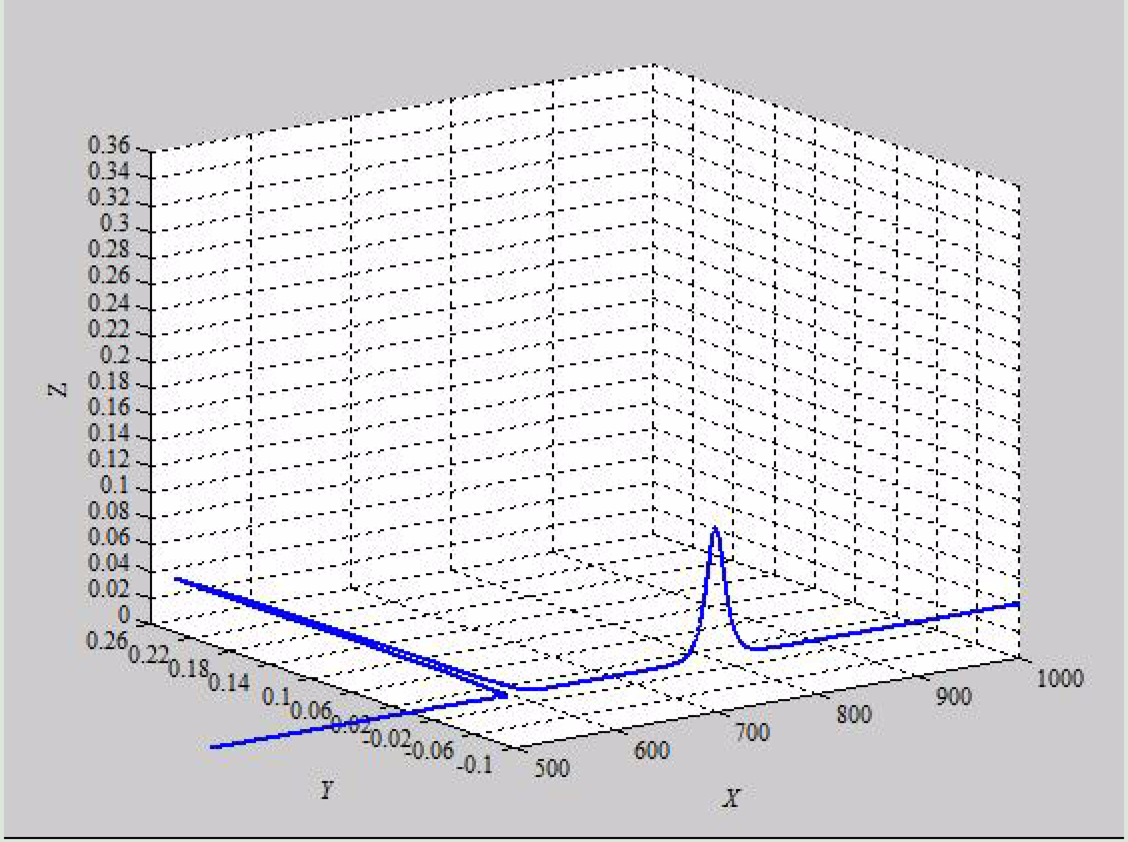
Inelastic Soliton Interaction at 45˚



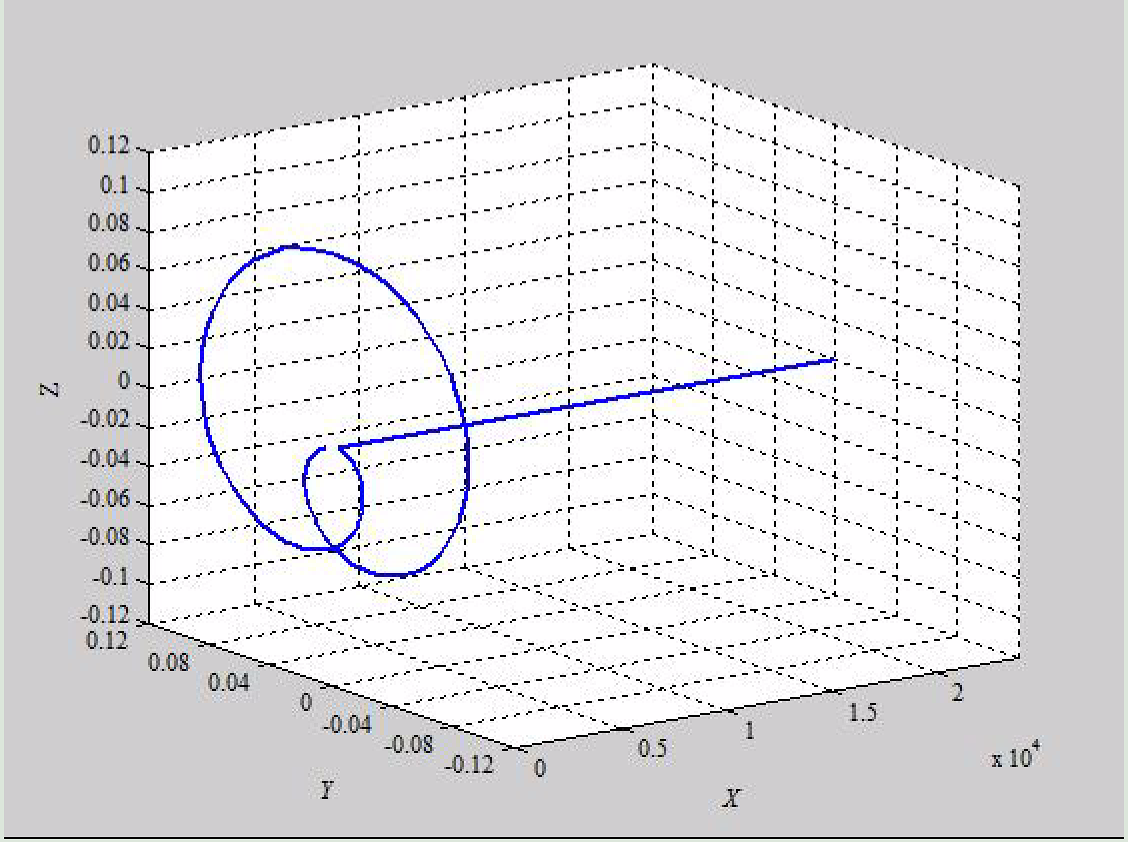
Inelastic Soliton Interaction at 60°



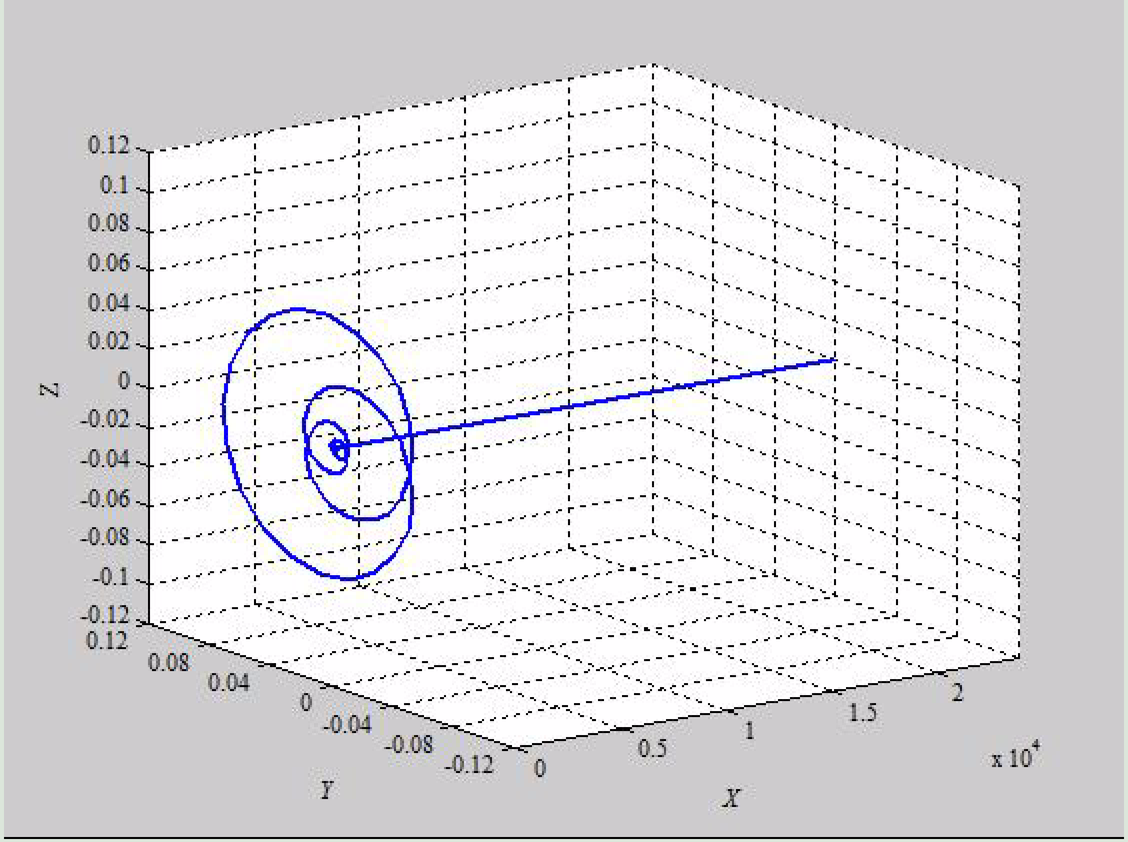
Inelastic Soliton Interaction at 90˚



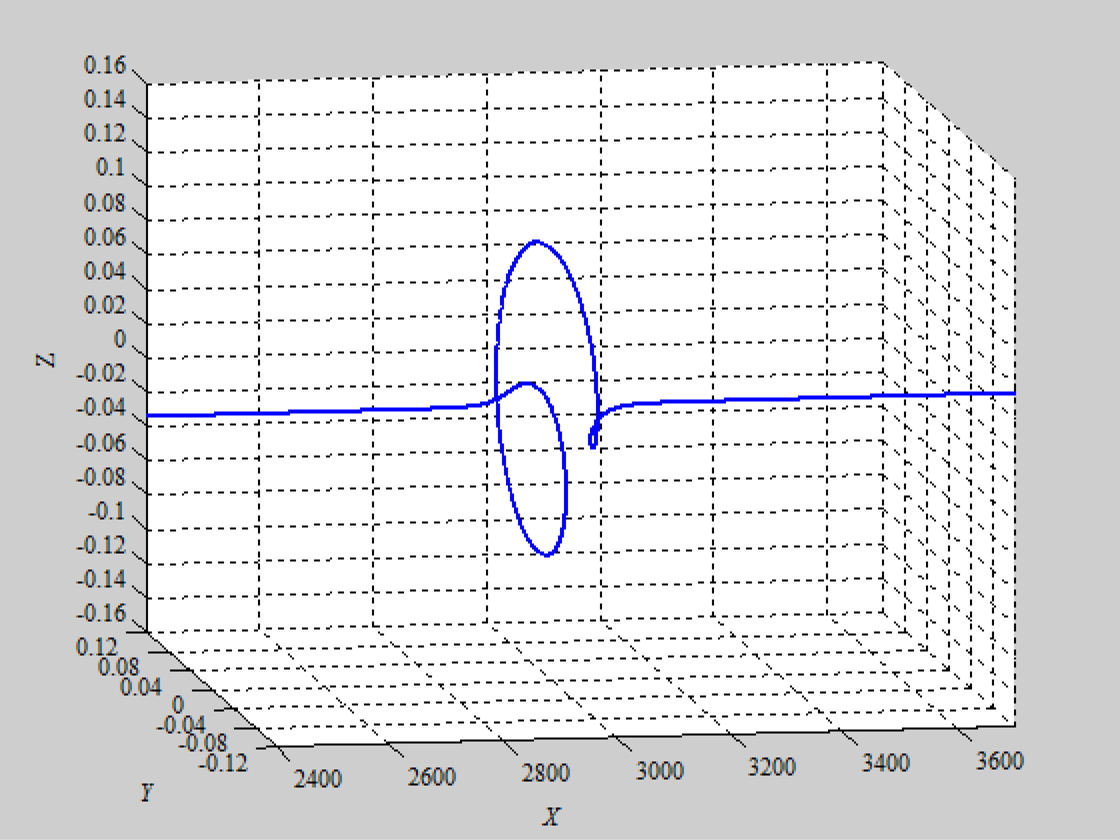
Helical Soliton



Non-Stationary Dynamics



Breakdown of a Helical Perturbation



Conclusion

- It has been shown that flexural transverse waves in an anharmonic chain of atoms can be described by general vector differential-difference equation which can be reduced to the "string equation" in the long-wave approximation.
- The basic differential-difference equation takes into account the interaction of each atom with two nearest neighbours from both sides.
- The dispersion relation in the long-wave approximation may be both linear and quadratic depending on the relationship between the bonds.

Conclusion

- Two solitons of the same or opposite polarities interact elastically similar to the scalar mKdV solitons, but interaction of two solitons lying initially in the nonparallel planes is essentially inelastic.
- Helical soliton solution has been constructed.
- Examples of non-stationary dynamics of helical initial perturbations were obtained.

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