Інститут теоретичної фізики
ім. М.М.Боголюбова

Bogolyubov Institute for Theoretical Physics, Kiev, Ukraine

SOLITON ASSISTED HYPERCONDUCTIVITY OF LOW-DIMENSIONAL SYSTEMS:
role of electron-phonon coupling and lattice anharmonicity

Larissa Brizhik

brizhik@bitp.kiev.ua

Thanks to

- **The Organizers**
- **The Institute of Mathematics of the University of Sevilla and NoLineal 2016**
- **Co-authors**

A. Chetverikov (Chernyshevsky State University, Saratov, Russia)

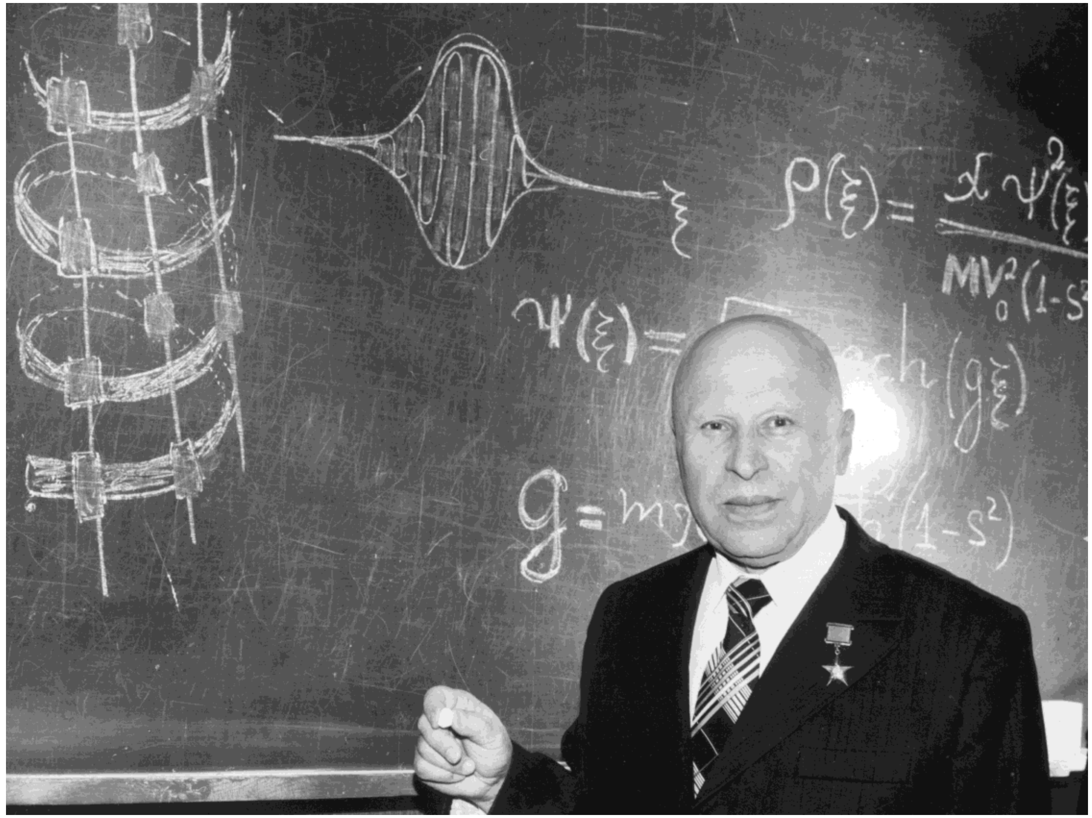
W. Ebeling (Humboldt Universität , Berlin, Germany)

A. Eremko (Bogolyubov Inst. Theoret. Physics, Kyiv, Ukraine)

G. Roepke (Universität Rostock, Rostock, Germany)

M. G. Velarde (Instituto Pluridisciplinar, Universidad Complutense, Madrid, Spain)

- **Mike Russell and Juan Archilla for stimulating discussions**



Alexander Davydov (26.12.1912-19.02.1993)

"*...the nonlinear states are as fundamental, as are quasi-particles in linear theories*"

(Davydov, **Theory of Molecular Solitons**, Dordrecht, Reidel, 1985)

Scope

- Davydov’s soliton and electrosoliton, localized 1D modes, quodons
- Bisoliton
- Bisolectron in a lattice with cubic or quartic anharmonicity
- Account of the Coulomb repulsion
- Supesonic bisolectron
- Conclusions

Low-dimensional systems

There is a large class of **low-dimensional systems**, which demonstrate **nonlinear properties and hyperconductivity**.

Some examples:

macromolecules (proteins and DNA) ;

polydiacetylene (Wilson, J Phys C16, 6739 (1983).; Donovan, Wilson, Phil Mag B 44, 9, 31(1981); J Phys C 18, L-51 (1985); Gogolin, JETP Lett 43, 511 (1986));

conducting polymers and platinum chain compounds (P. Monceau (Ed.), Electronic Properties of Inorganic Quasi-One-Dimensional Compounds, Part II (Reidel, Dordrecht)

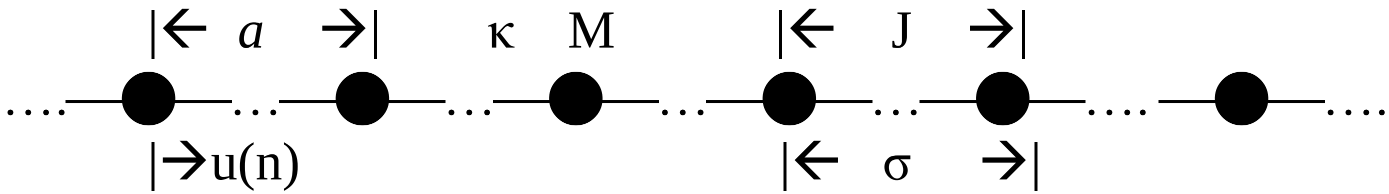
Bechgaard salts, salts of transition metals (PbSe,PbTe,PbS) (Streetman,. Banerjee, Solid State Electronic Devices, Prentice-Hall, N.J.; Zhang et al PRB 80, 024303 (2009); Madelung, Roessler Schultz (Eds.), PdO Crystal Structure, Lattice Parameters, Thermal Expansion. V. 41D, Springer, Berlin, 1998; Androulakis et al PRB 83 195209 (2011));

superconducting cuprates (Falter et al, PRB 64, 054516 (2001); Bohnen et al Europhys Lett 64, 104 (2003); Devereaux et al, PRL 93 117004 (2004); Reznik et al Nature 440, 1170 (2006); Kresin et al Rev Mod Phys 81, 481 (2009); Newns, Tsuei, Nature Physics 3, 184 (2007).

Many of them find numerous applications in **microelectronics and nanotechnologies**, or play important role in **living systems**.

Molecular (Davydov's) solitons

- Role of **electron-lattice coupling**
- Consider an isolated molecular **chain**



- **Nonlinear system**: (electron & lattice deformation) + **interaction**
- **Self-trapping** of electrons (molecular excitation) in the **self-induced** local deformation of the chain (comp. **polaron**)
- System of **nonlinear** coupled equations can be reduced to the **Nonlinear Schrödinger equation**

$$i\hbar \frac{\partial \Psi}{\partial t} + J \frac{\partial^2 \Psi}{\partial \xi^2} + 2Jg|\Psi|^2 \Psi = E\Psi,$$

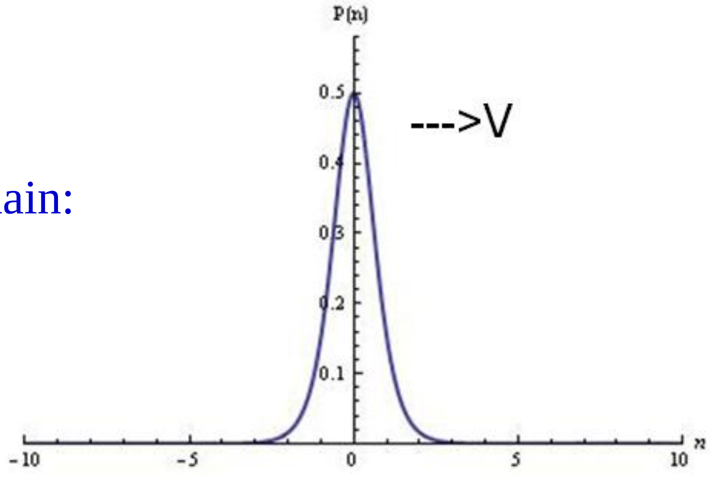
$$g = \frac{\sigma^2}{2J\kappa(1-s^2)}, \qquad s^2 = V^2 / V_{ac}^2$$

- **Soliton** solution:

$$\Psi_s(x,t) = \frac{1}{2}\sqrt{g}\, \frac{\exp\left[i\left(kx - \Phi_s(t)\right)\right]}{\cosh\left[g(x - Vt/a)/2\right]}$$

Soliton profile

Probability of electron localization in a molecular chain:



- **Soliton** – self-trapped localized state of an electron or molecular excitation in a one-dimensional molecular chain. It is a bound state of a quasiparticle and local chain deformation. It is formed in the result of the quasiparticle self-trapping by the local deformation created by the particle itself.

- **Stability**: soliton has **the energy** lower than the energy of a free electron! It propagates (almost) **without energy dissipation** and provides **coherent electron (energy) transport** at $T<T_{cr}$

- Existence of **optimal temperature** T_0 (comp. **hyperconductivity)**

Bisoliton

- **Self-trapping** of **two** extra electrons (holes) with opposite spins in the self-induced local deformation of a chain:

$$H = H_e + H_{ph} + H_{\text{int}} =$$
$$\sum_{k,\sigma} E(k) a^+_{k,\sigma} a_{k,\sigma} + \frac{1}{2}\sum_q [P^+_q P_q + \omega^2(q) Q^+_q Q_q] + \frac{1}{\sqrt{N}} \sum_{k,q,\sigma} \chi(k,q) a^+_{k+q,\sigma} a_{k,\sigma} Q_q$$

- At intermediate value of electron-phonon interaction (**adiabatic approximation**) the vector state is:

$$\left|\Psi(t)\right\rangle = \sum \psi_{n,m}(t) e^{S(t)} B_n^{\,+} B_m^{\,+} \left|0\right\rangle$$

- which leads to **bisoliton** (large polaron) **state**

Bisoliton

The Hamiltonian leads to the system of nonlinear equations which in the **contnuum approximation** can be reduced to **nonlinear** coupled equations can be reduced to the **2-component Nonlinear Schrödinger equation**

$$i\hbar\frac{\partial\Psi_j}{\partial t}+J\frac{\partial^2\Psi_j}{\partial\xi j^2}+2J(g_1|\Psi_1|^2+g_2|\Psi_2|^2)\Psi_j=E_j\Psi_j,$$

Here j=1,2 and

$$g_j=\frac{\chi^2}{2J\kappa(1-s_j^2)},\quad s_j^2=\frac{V_j^2}{V_{ac}^2}.$$

*LB, A.S. Davydov, J. LTP, 1984, **10,** 748; J. LTP, 1987, **13,** 1222; Phys. Stat. Sol. (b), 1987, **143**, 689.*

*LB, J. LTP, 1986, **12**, 437-438*

Bisoliton

2-component NLS has two types of solutions:

- **Two** almost independent **isolated solitons** in two separate potential wells:

$$\Psi_j(x,t) = \Psi_s(x + l_j, t), \quad l_1 >> l_2.$$

- **Bisoliton solution** (both electrons (holes) in the common well). The lowest energy state is at V_1=V_2, hence, g_1=g_2. Then

$$i\hbar \frac{\partial \Psi_j}{\partial t} + J \frac{\partial^2 \Psi_j}{\partial \xi_j^2} + 2Jg\left(\left|\Psi_1\right|^2 + \left|\Psi_2\right|^2\right)\Psi_j = E_{bs}\Psi_j.$$

It's solution:

$$\Psi_{bs}(x,t) = \sqrt{\frac{g}{2}} \frac{\exp\left[i\left(kx - \Phi_{bs}(t)\right)\right]}{\cosh\left[g(x - Vt/a)\right]}.$$

Bisoliton vs soliton parameters

- Width:

$$l_s = \pi / g, \qquad l_{bs} = \pi / 2g = l_s / 2.$$

- Mass :

$$m_s = m_e + \delta m = m_e \left(1 + \frac{M\chi^4}{6\hbar^2\kappa^3} \right), \qquad m_{bs} = 2m_s + \Delta m$$

- Energy:

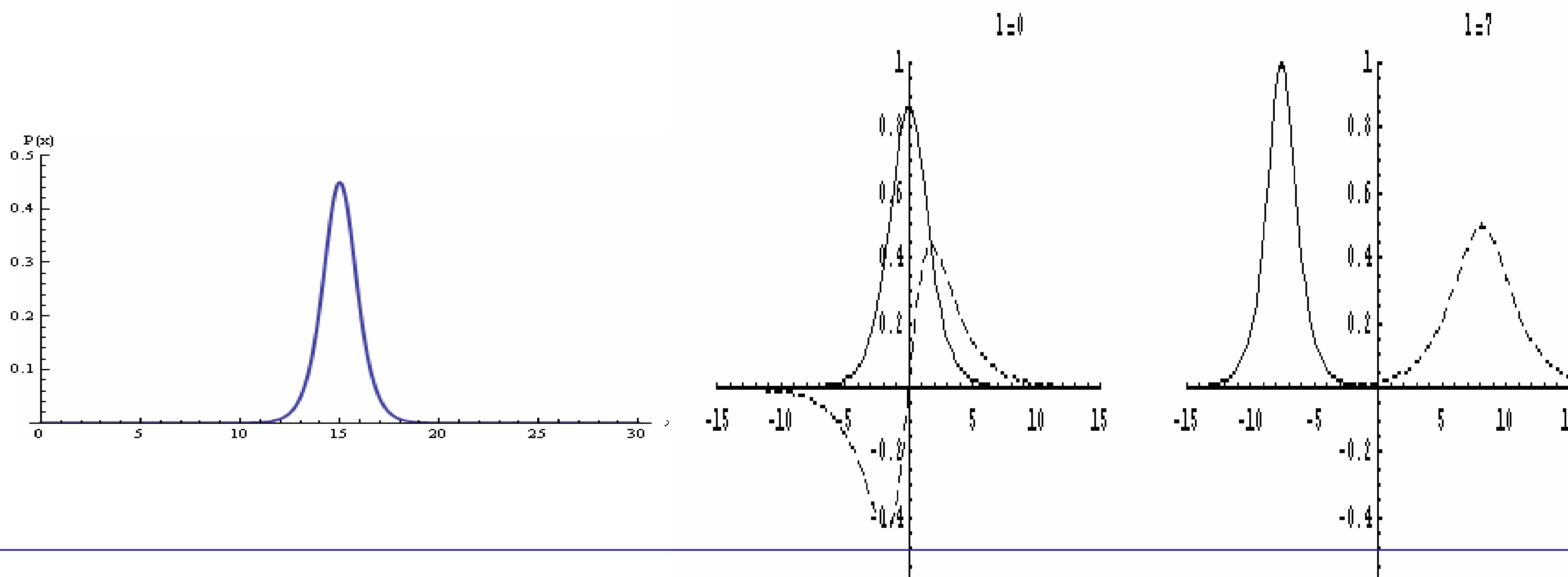
$$E_s(0) = -\frac{1}{12} J g_0^{\ 2}, \qquad E_{bs}(0) = -\frac{2}{3} J g_0^{\ 2} = 8E_s(0),$$

- Binding energy:

$$E_{bind}(V) = 2E_s(V) - E_{bs}(V) = \frac{J g_0^{\ 2}(1-5s^2)}{2(1-s^2)^3} = F(V).$$

Bisoliton wave functions

- **Triplet state:** The Pauli principle does not allow electrons to occupy the same level in a potential well, and, as a result, the two separated potential wells are formed in a chain, with one energy level in each. **(***LB, A.Eremko, PSS (b)* ***182*** *(1994) 89)* . This solution describes also the **1st excited singlet bisoliton state**

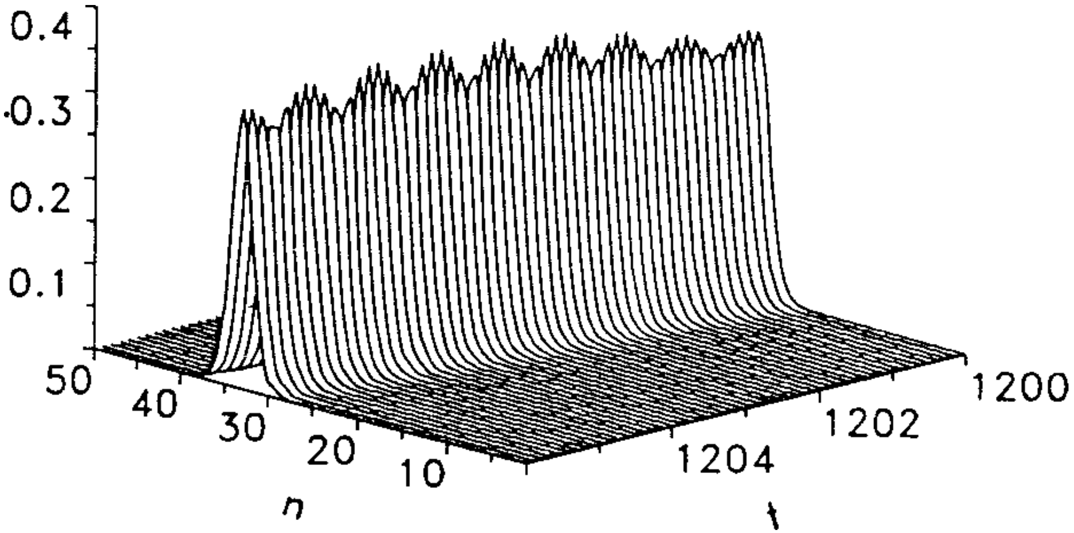


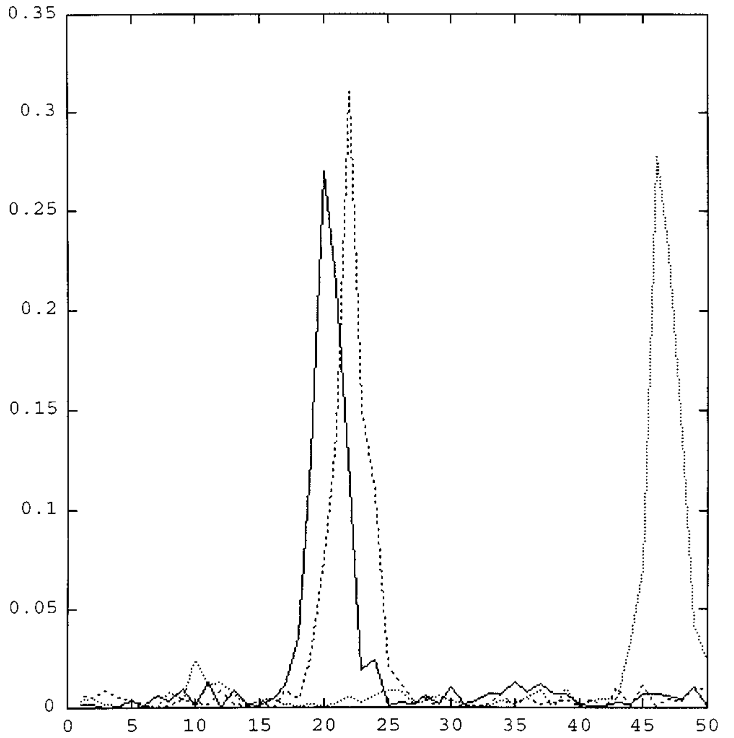
(a) (b) (c)

Charge density distributions in a soliton (a) *singlet bisoliton* (b), *bound triplet states* (c)

Localized modes

- With account of lattice dicretness solitons are **breathers** (comp. **quodons**)





Amplitude of the soliton envelope as a function of the lattice site n *for different times in different time-scales. Right:* t=60 - *solid line*, 80 – *dashed line, and* 100 - *dotted line.*

- **Bisoliton** width depends on its velocity: $l_{bs}(V) = l_{bs}(0)/(1 - V^2/V_{ac}^2)$

Hence, **shrinking** at *V* -> *Vac*.

•**Bisoliton** is stable at $V^2 < V_{ac}^2/5$

Role of lattice anharmonicity:

- In this model a lattice was treated in the **harmonic approximation**
- Role of **anharmonicity** *(A.Davydov, A.Zolotaryuk; A.Zolotaryuk, A.Savin; Y.Gaididei, S.Mingaleev;…)* **->** change of soliton properties, supersonic **solitons**
- Solitons do exist in **anharmonic lattices -** FPU, Toda, …
- **Bisoliton (bisolectron)** in **anharmonic** lattice:

Cubic anharmonicity: *Velarde, Brizhik, Chetverikov, Cruzeiro, Ebeling, Roepke, IJQC 2012,* ***110****, 551-565;*

Quartic anharmonicityy: *Velarde, Brizhik, Chetverikov, Cruzeiro, Ebeling, Roepke, IJQC, 2012,* ***112****,* 2591-2598

Hamiltonian of the system

Consider a 1D chain with 2 extra electrons (j=1,2) . Total Hamiltonian:

$$H = H_{el} + H_{lat} + H_{\text{int}}$$

$$H_{el} = \sum_{j=1,2} \frac{1}{a} \int_{-\infty}^{\infty} \Psi_j^* \left[\mathrm{E}_0 - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} \right] \Psi_j dz \qquad H_{lat} = \frac{1}{a} \int_{-\infty}^{\infty} \left[\frac{M}{2} \left(\frac{\partial \beta}{\partial t} \right)^2 + U(\rho) \right] dz$$

$$H_{\text{int}} = -\chi \sum_{j=1,2} \int_{-\infty}^{\infty} \rho(z,t) \left| \Psi_j(z,.t) \right|^2 dz$$

$\rho(z,t) = -a \partial \beta / \partial z$ - deformation of the chain.

General case of the potential:

$$\frac{\partial U}{\partial \rho}(\rho = 0) = 0 \qquad \frac{\partial^2 U}{\partial \rho^2}(\rho) > 0 \qquad \frac{\partial^2 U}{\partial \rho^2}(\rho = 0) = 1$$

Normalization condition

$$\frac{1}{a} \int_{-\infty}^{\infty} \left| \Psi_j(z,t) \right|^2 dz = 1$$

System of nonlinear equations

- In the continuum approximation we get the system of equations.:

$$i\hbar \frac{\partial \Psi_j}{\partial t} + \frac{\hbar^2}{2m} \frac{\partial^2 \Psi_j}{\partial z^2} + \chi a \rho(z,t) \Psi_j = 0,$$

$$\frac{\partial^2 \beta}{\partial t^2} - V_{ac}^2 \frac{\partial^2 U}{\partial \rho^2} \frac{\partial^2 \beta}{\partial z^2} = \frac{\chi a}{M} \frac{\partial}{\partial z} \left(|\Psi_1|^2 + |\Psi_2|^2 \right),$$

- Translational symmetry --> $\xi=(z-z_0-Vt)/a$

$$\Psi_j(z,t) = \Phi_j(\xi) \exp\left\{ \frac{i}{\hbar} \left[mVz - E_j t - \frac{1}{2} mV^2 t \right] + i\varphi_j(t) \right\}$$

- Introduce dimensionless parameters:

$$\lambda_j = -\frac{E_j}{J}, \qquad \sigma = \frac{\chi a}{J}, \qquad D = \frac{\chi a}{M V_{ac}^2}$$

System of nonlinear equations

- We obtain the **system of equations**

$$\frac{d^2\Phi_j}{d\xi^2} + \sigma\rho(\xi)\Phi_j(\xi) = \lambda_j\Phi_j(\xi),$$

$$\frac{dF(\rho)}{d\rho} = D\left(\Phi_1^2(\xi) + \Phi_2^2(\xi)\right),$$

where F is the ***effective*** lattice potential $F(\rho) = U(\rho) - \frac{1}{2}s^2\rho^2$

From the first equation we get:

$$\left(\frac{d\Phi_j}{d\xi}\right)^2 = \lambda_j\Phi_j^{\,2}(\xi) - \sigma Q_j(\xi)$$

where

$$Q_j(\xi) = \int_{-\infty}^{\xi} \rho(x)\, d\Phi_j^2(x)$$

Lattice deformation

- This gives:

$$\frac{d\rho}{d\xi} = \pm 2 \frac{dF/d\rho}{d^2F/d\rho^2}\sqrt{\lambda - \sigma G(\rho)}$$

Hence,

$$\xi(\rho) = \pm \frac{1}{2\sqrt{\sigma}} \int_{\rho(\xi)}^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho} \frac{1}{\sqrt{G(\rho_0) - G(\rho)}} d\rho$$

Here

$$G(\rho) = \rho - \frac{F(\rho)}{dF/d\rho} \qquad \lambda = \sigma G(\rho_0)$$

- From the normalization condition we have:

$$\int_{-\infty}^{\infty} \Phi^2(\xi) d\xi = \frac{1}{D} \int_0^{\rho_0} \frac{dF}{d\rho} \left| d\xi(\rho) \right| = 1$$

Hence,

$$\int_0^{\rho_0} \frac{d^2F/d\rho^2}{\sqrt{G(\rho_0) - G(\rho)}} d\rho = 2D\sqrt{\sigma} \qquad \Phi_0 = \sqrt{\frac{1}{2D}\left(\frac{dF}{d\rho}\right)\Bigg|_{\rho=\rho_0}}$$

Energy and momentum

- From the Hamiltonian we calculate **the energy**

$$E_{tot}^{(bs)}(V) = mV^2 + E^{(bs)}(V) + W(V)$$

$$E^{(bs)}(V) = -2\lambda J = -2DG(\rho_0)MV_{ac}^2$$

$$W(V) = 2MV_{ac}^2 \int_{-\infty}^{0} \left(F(\rho) + s^2\rho^2\right) d\xi = \frac{MV_{ac}^2}{\sqrt{\sigma}} \int_0^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho} \frac{F(\rho) + s^2\rho^2}{\sqrt{G(\rho_0) - G(\rho)}} d\rho$$

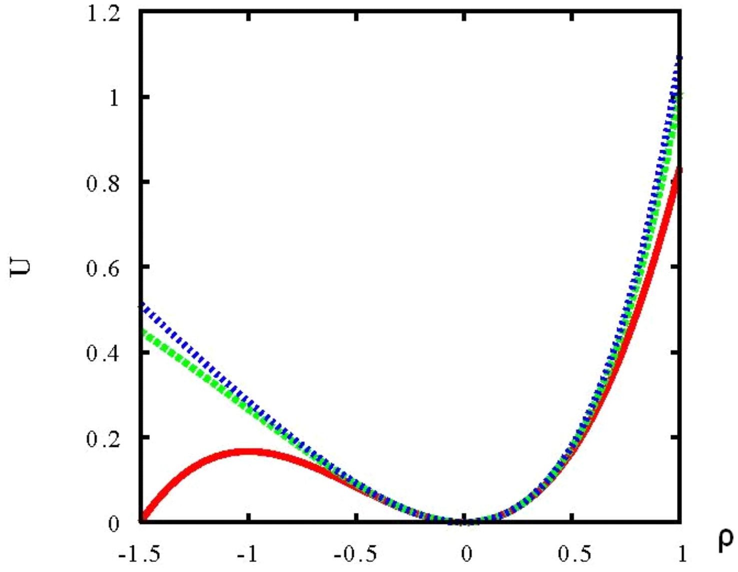
and **momentum** of the system

$$P(V) = \left(2m + M\int_{-\infty}^{\infty} \rho^2 d\xi\right) V = \left(2m + \frac{M}{\sqrt{\sigma}} \int_0^{\rho_0} \frac{d^2F/d\rho^2}{dF/d\rho} \frac{\rho^2}{\sqrt{G(\rho_0) - G(\rho)}} d\rho\right) V$$

Cubic anharmonic potential

- Consider cubic anharmonic potential

$$U(\rho) = \frac{1}{2}\rho^2 + \frac{\alpha}{3}\rho^3$$



Lattice potentials, U, given by Morse (green line), Toda (blue line) and cubic (red line) potentials with suitably rescaled parameters fixing approximately equal their first three derivatives around a common minimum placed at zero in the abscissa which accounts for dimensionless lattice inter-particle equilibrium distance, r.

- The effective potential: $F(\rho) = \frac{1}{2}\alpha\rho^2\left(\frac{2}{3}\rho + \delta_c\right)$ $\delta_c = \frac{1-s^2}{\alpha}$

Quartic anharmonic potential

- Consider lattice with **quartic anharmonic potential**

$$U(\rho) = \frac{1}{2}\rho^2 + \frac{\beta}{4}\rho^4$$

- The effective potential:

$$F(\rho) = \frac{1}{4}\beta\rho^2\left(\rho^2 + 2\delta_q\right) \qquad \delta_q = \frac{1-s^2}{\beta}$$

From the system of equations we get

$$\left(\frac{d\Phi(\xi)}{d\xi}\right)^2 = \frac{1}{2D}\frac{dF}{d\rho}(\lambda - \sigma G)$$

Here

$$G(\rho) = \rho - \frac{F(\rho)}{dF/d\rho} = \frac{\rho}{4}\frac{3\rho^2 + 2\delta}{\rho^2 + \delta}$$

Quartic anharmonic potential

We obtain the equation

$$\frac{d\rho}{d\xi} = \pm 2\sqrt{\sigma}\,\frac{dF/d\rho}{d^2F/d\rho^2}\sqrt{G(\rho_0) - G(\rho)}$$

Integrating it, we get

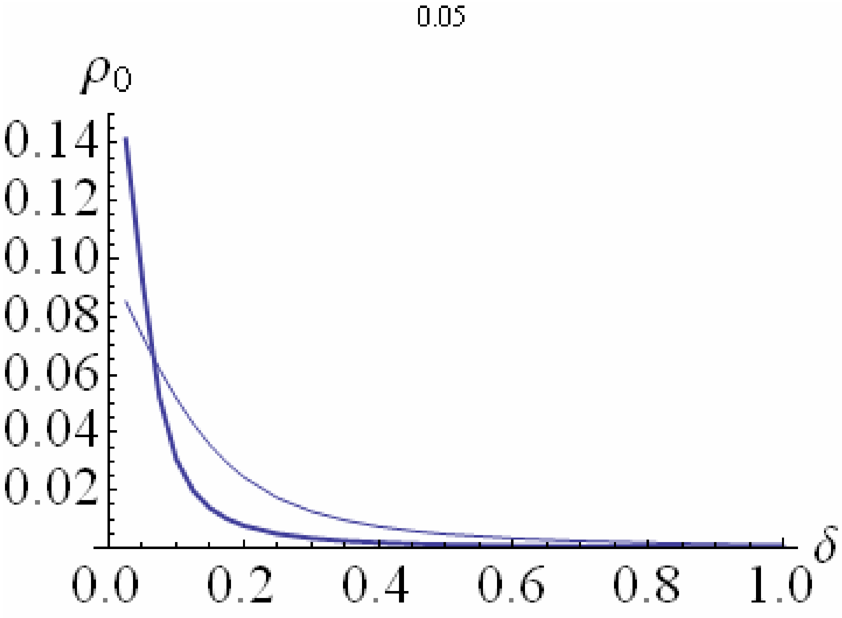
$$\rho(\xi) = \rho_0 Sech^2(\kappa\xi)$$

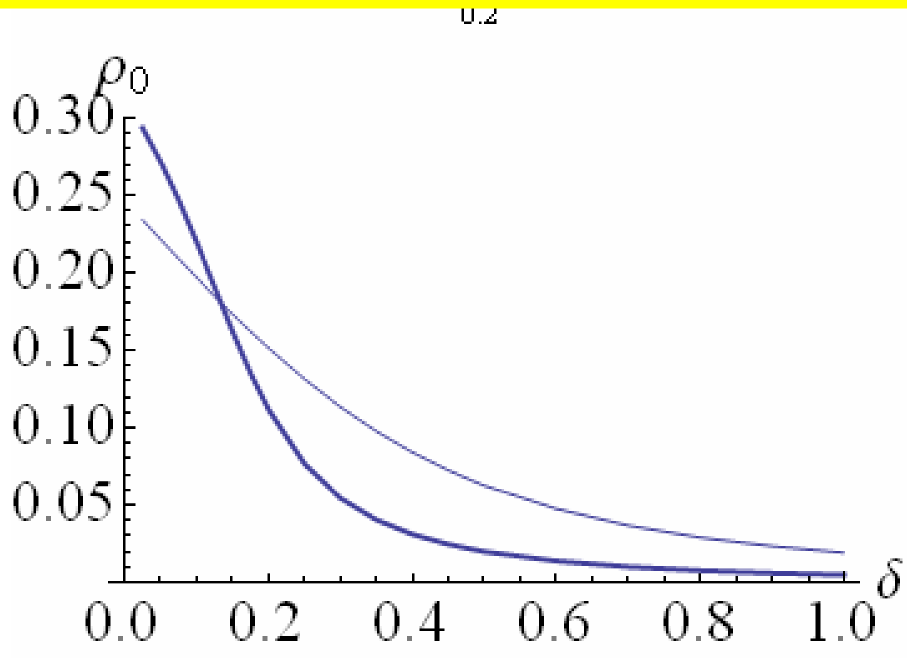
Here ρ_0 is **the maximum value of the deformation**.

The inverse width of the lattice deformation localization is:

$$\kappa = \sqrt{\frac{\sigma\rho_0}{2}}$$

Lattice deformation





Maximum value of the lattice deformation ρ_0*, as a function of the dynamically modulated inverse anharmonic stiffness coefficient* δ *, in lattices with quartic (thick line) and cubic (thin line) anharmonicity for two values of electron-lattice coupling constant. Left figure: G=0.025, right figure: G=*0.1

Here *G* is the dimensionless electron-lattice coupling constant:

$$G^2 = \frac{D^2\sigma}{\alpha^2} \qquad\qquad G^2 = \frac{D^2\sigma}{\beta^2}$$

Cubic anharmonic potential

Bisoliton wave function:

$$\Phi(\xi) = \sqrt{\frac{\rho_0}{2D}} Sech(\kappa\xi)\sqrt{1+s^2+\alpha\rho_0 Sech^2(\kappa\xi)}$$

Bisoliton energy:

$$E^{(bs)}(V) = -DMV_{ac}^2\rho_0 \frac{\frac{4}{3}\rho_0+\delta}{\rho_0+\delta}$$

Energy of the deformation:

$$W(V) \approx \frac{MV_{ac}^2}{3\sqrt{\sigma}}\rho_0^{3/2}\left(\tfrac{8}{15}\alpha\rho_0+1+s^2\right)$$

Cubic anharmonic potential

- Total momentum:

$$P(V) \approx \left(2m + \frac{2M\rho_0^{3/2}}{3\sqrt{\sigma}} \right) \cdot V$$

- **Binding energy** of the bisoliton **is positive**:

$$2E^{(s)}(V) - E^{bs}(V) = \chi a \rho_0^{(s)} \frac{\frac{4}{3}\rho_0^{(s)} + \delta}{\rho_0^{(s)} + \delta} > 0$$

- Bisoliton effective mass

$$\Delta M = M_{eff}^{(bs)} - 2M_{eff}^{(s)} \approx \frac{2M}{3\sqrt{\sigma}} 2.8 {\rho_0^{(s)}}^{3/2}$$

Quartic anharmonic potential

Bisolectron **wave function** and **energy:**

$$\Phi(\xi) = \sqrt{\frac{\rho_0}{2D}} Sech(\kappa\xi)\sqrt{1 - s^2 + \beta\rho_0{}^2 Sech^4(\kappa\xi)}$$

$$E_{tot}^{(bs)}(V) = mV^2 + E^{(bs)}(V) + W(V)$$

$$E^{(bs)}(V) = -\frac{1}{2} DMV_{ac}^2 \rho_0 \frac{3\rho_0{}^3 + 2\delta}{\rho_0{}^2 + \delta}$$

$$W(V) \approx 8 \frac{MV_{ac}^2}{\sqrt{2\sigma}} \rho_0{}^{3/2} \left[\frac{1}{3}\left(s^2 + \frac{1}{2}\delta\beta \right) + \frac{2}{35}\beta\rho_0{}^2 \right]$$

Account of the Coulomb repulsion

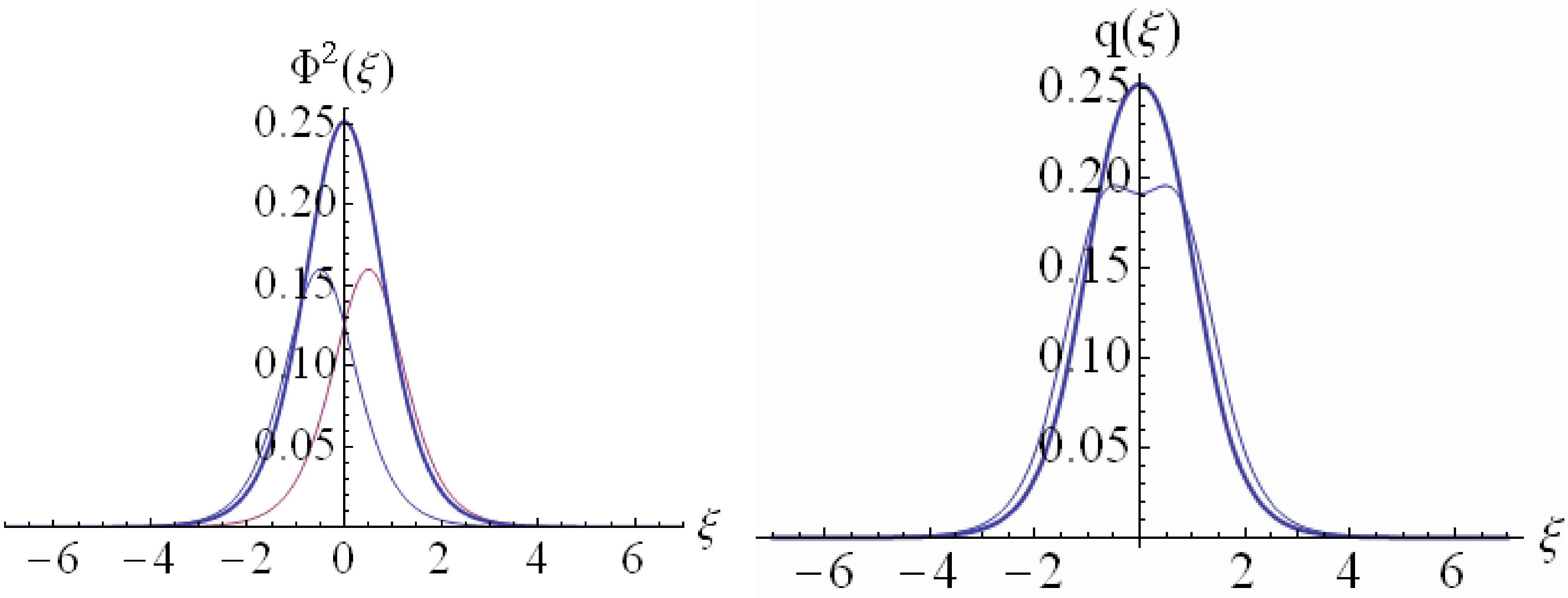
One-electron wave functions (lattice with **quartic** anharmonicity):

$$\Phi_i(\xi) \approx \sqrt{\frac{\rho_0}{2D}} Sech\left(\kappa\left(\xi \pm \frac{l}{2}\right)\right)\sqrt{1+\gamma\rho_0{}^2 Sech^4\left(\kappa\left(\xi \pm \frac{l}{2}\right)\right)}$$

Here l is the **distance between the two maxima**. It is determined from the condition of the energy minimum for a bisolectron with account of the Coulomb repulsion. This gives:

$$l_0 \approx \frac{1}{2}\left(\frac{3De^2}{4\pi\varepsilon_0 \chi a^2 \rho_0{}^2 \kappa}\right)^{1/3}$$

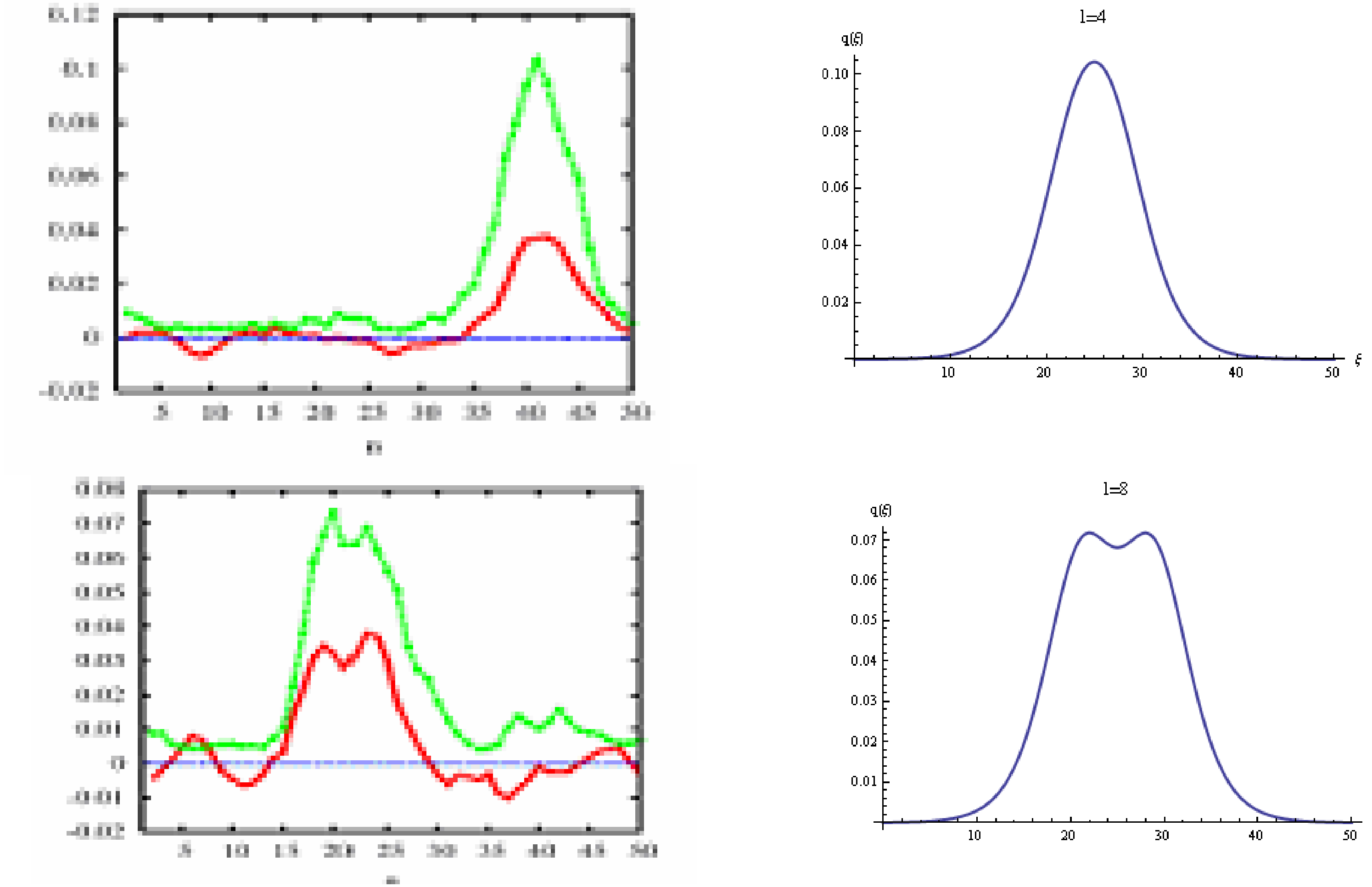
Account of the Coulomb repulsion



(a) (b)

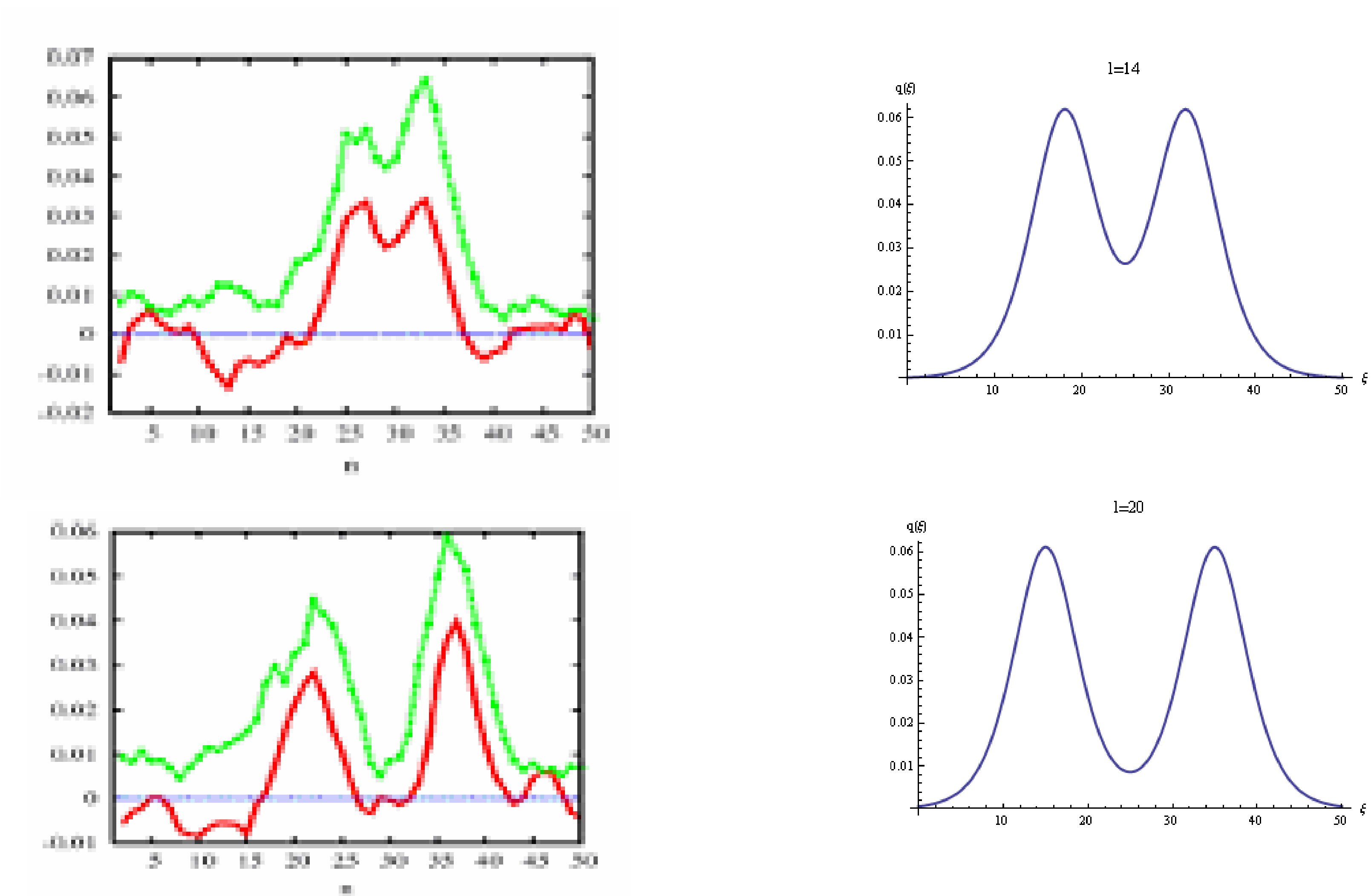
(a) *One-electron wave functions (thin lines) and bisolectron wave function (thick line) with account of the Coulomb repulsion, for* κ*=1 and l=1*. (b) *Charge distribution over the lattice sites in the bisolectron state for* κ *=1 for l=1 (thick line) and l=1.5 (thin line).*

Coulomb repulsion in bisoliton



Comparison of the charge distribution obtained in numerical simulation of the Morse lattice with Hubbard repulsion (left, ***green****) and analytical model (right) for two different values of Coulomb repulsion,* $U_1 < U_2$

Coulomb repulsion in bisoliton



Comparison of charge distribution obtained in numerical simulation of the Morse lattice with Hubbard repulsion (left, ***green****) and analytical model (right) for two different values of Coulomb repulsion,* $U_1 < U_2 < U_3 < U_4$

Supersonic bisoliton and bisolectron

- **Supersonic bisolitons** are possible in chains **when** $J > \frac{1}{2} M V_{ac}^2$
- In this regime **nonlinear dispersion of the lattice** is important. It's account leads to **improved Boussinesq equation**

$$\frac{\partial^2 \rho(\xi,\tau)}{\partial \tau^2} - \frac{\partial^2 u(\rho)}{\partial \xi^2} - \frac{1}{12}\frac{\partial^4 \rho(\xi,\tau)}{\partial \xi^2 \partial \tau^2} + 2\frac{\partial^2 \Phi^2(\xi,\tau)}{\partial \xi^2} = 0$$

corresponding to the **lattice dispersion**

$$\omega_1^{\ 2}(k) = \frac{k^2}{1 + k^2/12} \qquad k = Arc\cos\sqrt{1 - \frac{s^2}{4j^2}} \qquad j = \frac{J}{MV_{ac}^2}, \qquad u = \frac{U}{MV_{ac}^2},$$

or to the **ill-posed Boussinesq equ**ation

$$\frac{\partial^2 \rho(\xi,\tau)}{\partial \tau^2} - \frac{\partial^2 u(\rho)}{\partial \xi^2} - \frac{1}{12}\frac{\partial^4 \rho(\xi,\tau)}{\partial \xi^4} + 2\frac{\partial^2 \Phi^2(\xi,\tau)}{\partial \xi^2} = 0$$

corresponding to the **lattice dispersion**

$$\omega_2^{\ 2}(k) = k^2(1 - k^2/12)$$

Supersonic bisoliton

Electron energy dispersion:

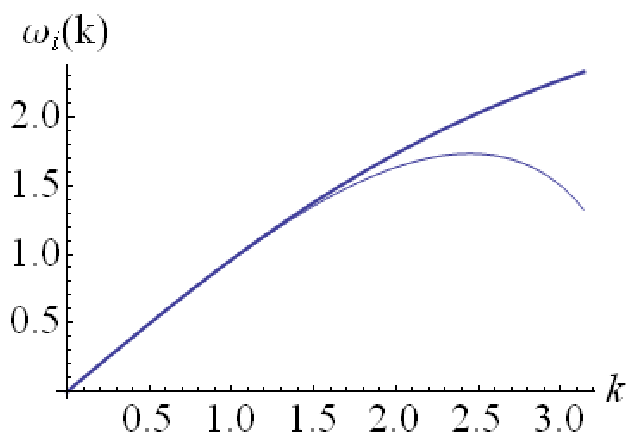
$$\varepsilon(k) = 4j\sin^2\frac{k}{2} \qquad k \in [-\pi, \pi]$$

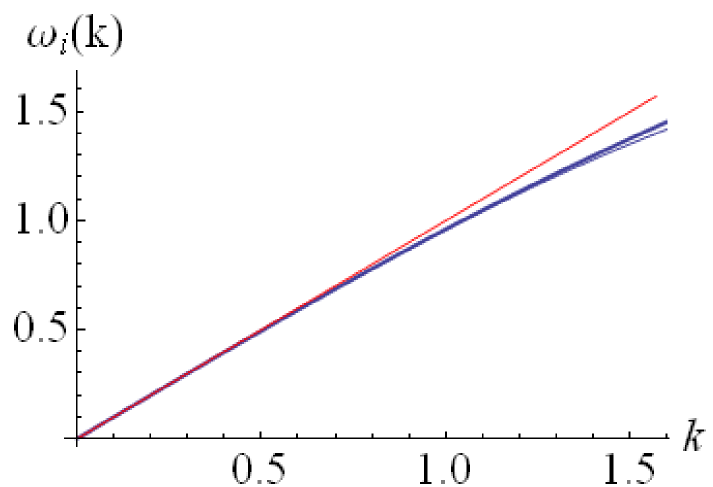
Dimensionless electron group velocity and its **maximum value**

$$s \equiv \frac{V_g}{V_{ac}} = \frac{d\varepsilon(k)}{dk} = 2j\sin k$$

$s_{max} = 2j$ at $k = \pi/2$.

In the physically relevant region both lattice dispersions are very close:





Phonon energy dispersions for the ***improved*** *(**thick** line) and* ***ill-posed*** *(thin line) Boussinesq equations. Red line is a linear dispersion.*

Supersonic bisolectron

The system of equations:

$$\lambda \frac{\partial^2 \Phi(\varsigma)}{\partial \varsigma^2} + 2h\rho(\varsigma)\Phi(\zeta) + \varepsilon_b(k)\Phi(\varsigma) = 0$$

$$\mu \frac{\partial^2 \rho(\varsigma)}{\partial \varsigma^2} + (1 - s^2)\rho(\varsigma) + \frac{du_{anh}(\rho)}{d\rho} = 2\sigma\Phi^2$$

Here

$$\lambda = j\cos k, \quad \varsigma = \xi - s\tau, \quad \tau = \frac{V_{ac}}{a}t, \quad h = \frac{\chi a}{\hbar V_{ac}}, \quad \mu_1 = s^2/12, \ \mu_2 = 1/12$$

It admits **three types of solutions**:

1. **Supesonic lattice soliton** and 2 free (delocalized) electrons
2. **Subsonic and supersonic bisoliton:** $\Phi^2(\rho) \propto \rho$
3. **Supersonic bisolectron** at faster decay of the wave-function:

$$2h\int_0^{\rho} \Phi^2(r)dr < u_{anh}(\rho)$$

Supersonic bisolectron

- The electron wavefunction:

$$\Phi^2(\rho) \cong C_p \rho^p$$

p=1 – **bisoliton** solution: $\varepsilon_b(k) = -j\kappa^2 \cos k,$ $\kappa^2 = \dfrac{2C_1\sigma - 1 + s^2}{4\mu}$

p>1 – **bisolectron** solution $\varepsilon_b(k) = -jp^2\nu^2 \cos k$ $\nu^2 = \dfrac{s^2 - 1}{4\mu}$

The parameter p can be found from the normalization condition.

Consider a lattice with cubic anharmonicity $u_{anh} = \alpha\rho^3/3$

Localized solution:

$$\Phi(\xi) = \sqrt{\frac{\rho_0}{2D}} Sech(\kappa\xi)\sqrt{1 + s^2 + \alpha\rho_0 Sech^2(\kappa\xi)}$$

$$\rho(\varsigma) = \rho_0 Sech^2(\kappa\varsigma)$$

$$\kappa \approx \kappa_0 = \sqrt{\frac{\sigma\rho_0}{2}} \frac{\sqrt{\frac{4}{3}\rho_0(\rho_0 + 2\delta) + \delta^2}}{2\rho_0 + \delta} \approx \frac{1}{2}\sqrt{\sigma\rho_0} \qquad \delta = \frac{1 - s^2}{\alpha}$$

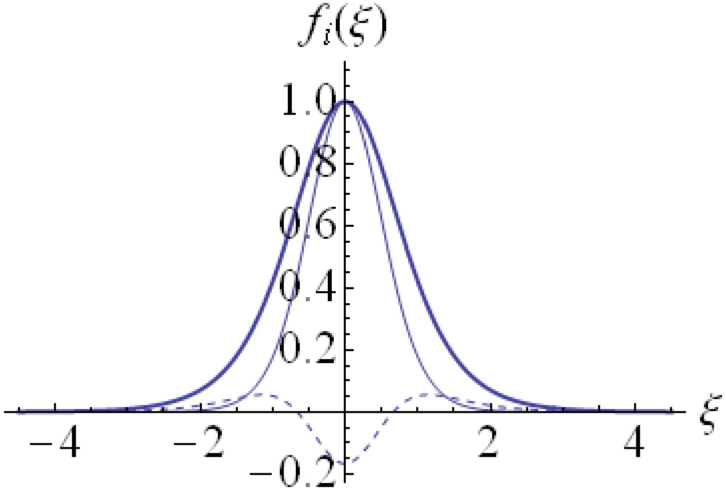
Supersonic bisolectron

- Boussinesq equation:

$$\mu \frac{\partial^2 \rho(\varsigma)}{\partial \varsigma^2} + \alpha\rho^2 + (1 - s^2)\rho(\varsigma) = 2h\Phi^2$$

Three terms in it's l.h.s.:

$$f_1 = \tilde{\rho} \equiv \frac{\rho}{\rho_0} \qquad f_2 = \tilde{\rho}^2 \qquad f_3 = \mu \frac{d^2\tilde{\rho}}{d\xi^2} \qquad \xi = \kappa\varsigma$$



Three terms in the Boussinesq eq. for the bisoliton type solution. Solid line - f_1, thin – f_2, dashed – f_3

Hence, f_1 and f_2 are the leading terms, f_3 : $(1 - s^2)\rho \to (1 - s^2 + \mu\rho''/\rho)\rho$

(equiv. to **increase of the allowed effective soliton velocity**)

Supersonic bisolectron

- **Exact solution at fixed velocity**:

$$s^2/\sqrt{1-s^2/4j^2} = 2j\alpha/h$$ - for the **improved** Boussinesq equation

$$\sqrt{1-s^2/4j^2} = h/2j\alpha$$ - for the **ill-posed** Boussinesq equation

Solution at p=1:

$$\Phi_{bs}(\varsigma) = \sqrt{\frac{\kappa}{2}} Sech(\kappa\varsigma)$$

$$\kappa\left(\kappa^2 - \frac{s^2-1}{4\mu}\right) = \frac{h^2}{4\mu j\cos k}$$

$$\rho_{bs}(\varsigma) = \frac{\lambda}{\sigma}\kappa^2 Sech^2(\kappa\varsigma)$$

It transforms to the **bisoliton** solution at $\alpha \to 0, \quad \mu \to 0$

Supersonic bisolectron

Exact supersonic bisolectron solution at *p*=2:

$$\Phi_{bs(\sup)}(\varsigma) = \frac{3}{h}\sqrt{\lambda\left(\frac{p\alpha}{2h} - \mu\right)}\kappa^2 Sech^2(\kappa\varsigma)$$

$$\rho_{bs(\sup)}(\varsigma) = \frac{3\lambda}{h}\kappa^2 Sech^2(\kappa\varsigma)$$

at fixed value of the velocity

$$s^2 = 1 + 4\mu\kappa^2\left[1 - 3(\gamma - 1)\right] \qquad \gamma = \frac{\lambda\alpha}{2\mu h}$$

Numerical results at 'arbitrary' value of the velocity:

Velarde, Ebeling, Chetverikov. Int. J. Bifurc. Chaos, 18 (2010) 885-890.

Ebeling, Velarde, Chetverikov. Cond.Matter Phys. 12 (2009) 633-645

Cisneros-Ake, Minzoni. Phys. Rev. E **85,** 021925 (2012)

Cisneros, Minzoni, Velarde: Variational Approximation to electron trapping by soliton-like localized excitations in one-dimensional anharmonic lattices. Springer Series on Wave Phenomena. ISSN 0931-7252. (in press)

Conclusions

- Anharmonicity in the lattice interactions facilitates binding of two electrons in a **singlet spin bisoliton state**, extended over a few lattice sites.

- Such a bisoliton can move along the lattice with finite effective mass and constant velocity in the **subsonic** and **supersonic** regimes and can be a **hyperconducting charge carrier** in LD systems.

- Due to the Coulomb repulsion between the electrons the two-electron wave function may have a **one-hump** envelope at relatively strong electron-lattice coupling or **two-hump** envelope at relatively weak coupling.

Conclusions

- **Capture** of one or two electrons by a lattice soliton **does not destroy or decelerate** the latter (comp. **quodons**).

- The results here reported complement and confirm earlier fragmentary results obtained by **computer simulations**:

  i) using the Gaussian approximation to the soliton excitation:

  Velarde, Neissner, Int J Bifurcation Chaos 2008, 18, 885

  ii) for lattices with the harmonic and Morse potentials:

  Cruzeiro, Eilbeck, Marín, Russell, Eur Phys J B 2004, 42, 95.

  Hennig, et al., Phys Rev E 2008, 78, 066606.

  Velarde, et al., Int J Bifurcation Chaos 2011, 21, 546

- What happens if *N*>2? The **charge density wave** is formed in harmonic lattices at density of electrons **below the critical value**. Preliminary results: it can be formed also in anharmonic lattices.

THANK YOU, ALL!

Дякую! **¡Gracias!**

Solitary wave recreated in the Union Canal near Edinburgh in 1995
“The great solitary wave” or “Soliton community in a boat”

Experimental data for proteins

- *H.-B.Kraatz, I.Bediako-Amoa, S.H.Gyepi-Garbah, T.C. Sutherland*, Electron transfer through H-bonded peptide assemblies, J.Phys.Chem, **108,** 2004,20164-20172.

- *R.H. Austin, et al*, PRL **84** (2000) 5435; PRL **88** ('02) 018102; J.Phys.:Cond.Matt. **15** ('03) S1693

Experimental measurements of Amid-I vibration lifetime:

- in **L-alanine** molecules *t= 2.7 ps*

- in photoactive **yellow protein** (β sheets): *t =15 ps*

- in **myoglobine** (α-helix): *t=400 – 500 ps*

Explanation: soliton formation in alpha-helix *(Brizhik,Eremko, Zakrzewski, Piette, PRE **70** (2004) 031914*; Chem. Phys. **324** (2006) 259 *)*