Coherent charge transport mediated by solitonic excitations

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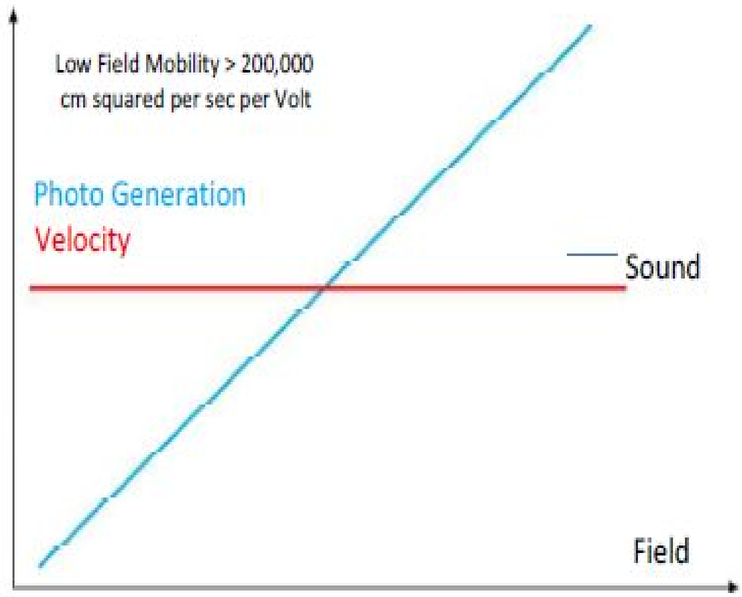
CONTENTS of this talk

1. Evidence of nonlinear excitations as solitons and solectrons in molecular systems (solectrons = supersonic polarons) .
2. Localized supersonic excitations in the Toda/Morse chains and in 2d systems interacting with electrons, control of charges
3. “Tight-binding” model, solve simult Langevin and Schrödinger equations, Pauli’s master equations, solve kinetic eqs.
4. Soliton-mediated electron control and transfer
5. Momentum distr and Fokker-Planck eqs.

- Conclusions

Exp on conductivity of photo-electrons in pure polydiacetylen crystals (Wilson 81-86): Coherent fast electrons (up to 5 km/s) indep. of electr field



Qualitative sketch of results, combining data from of Donovan & Wilson (1981a) and Donovan & Wilson (1981b), of photo-generation efficiency, and photoelectron velocity PDATS crystals, as a function of electric field. The field varies over four decades.

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Chemistry

Femtosecond dynamics of DNA-mediated electron transfer

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Nobel price 1999

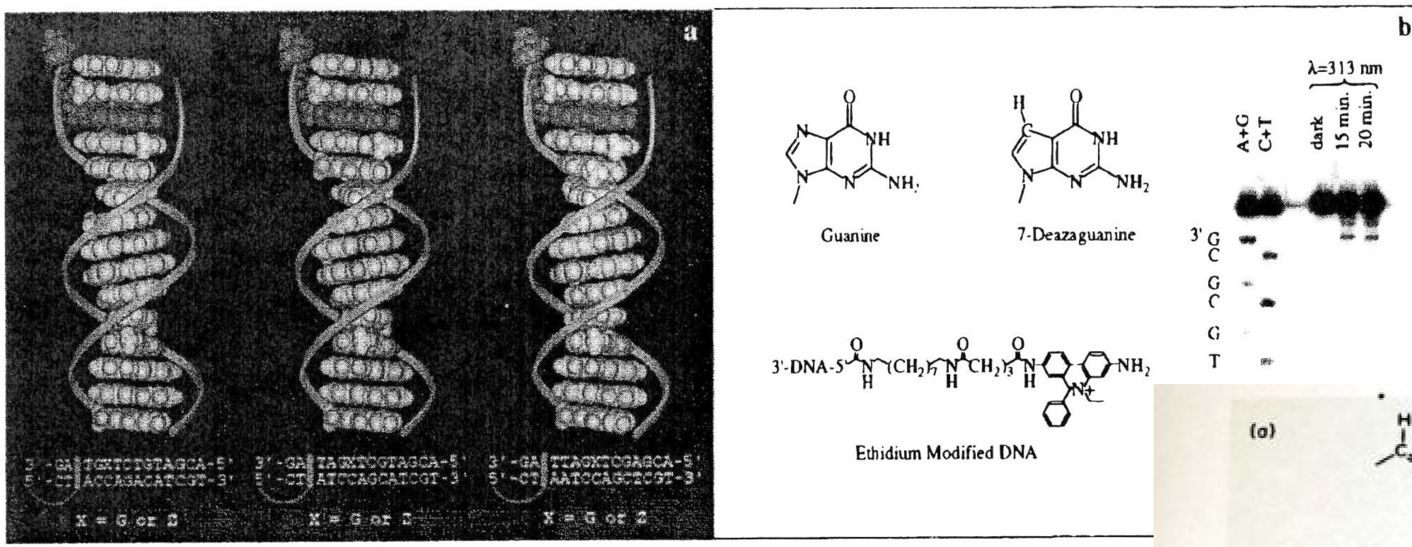


FIG. 1. The DNA assemblies. (*a*) Molecular models (Insight II) illustrating the E-tethered (red) DNA assembl
7Z. The Z base is shown in yellow. Sequences are given below. (*b*) Structures of guanine (G), Z, and the E-m
autoradiogram (right) after denaturing 18% PAGE, showing photoinduced damage of an E-modified duplex gener
of the duplex (10 μM) in 5 mM phosphate/50 mM NaCl, pH 7, 5′ ^{32}P-labeled on the strand complementary to that cont
occurs at the first two base steps on the 3′ side (near E); see *The DNA Assemblies* and ref. 35. The sequence 3′-CGCGC

Barton et al. measure in artif DNA velocities in range Angstrom/picosec; see also Solitons in

conducting polymers by Heeger et al. --------->

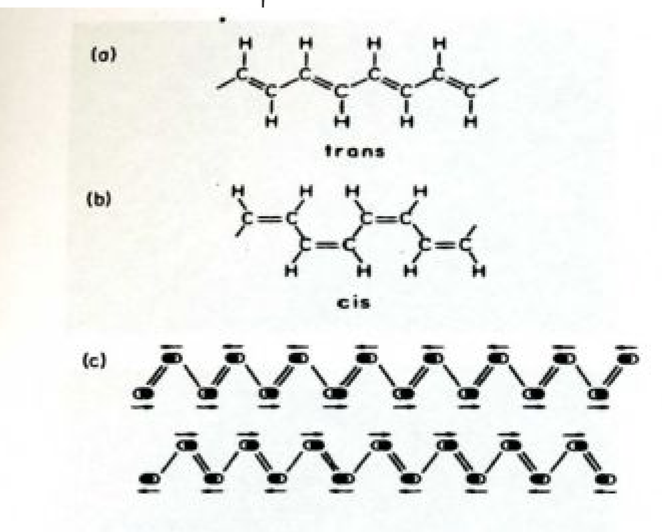
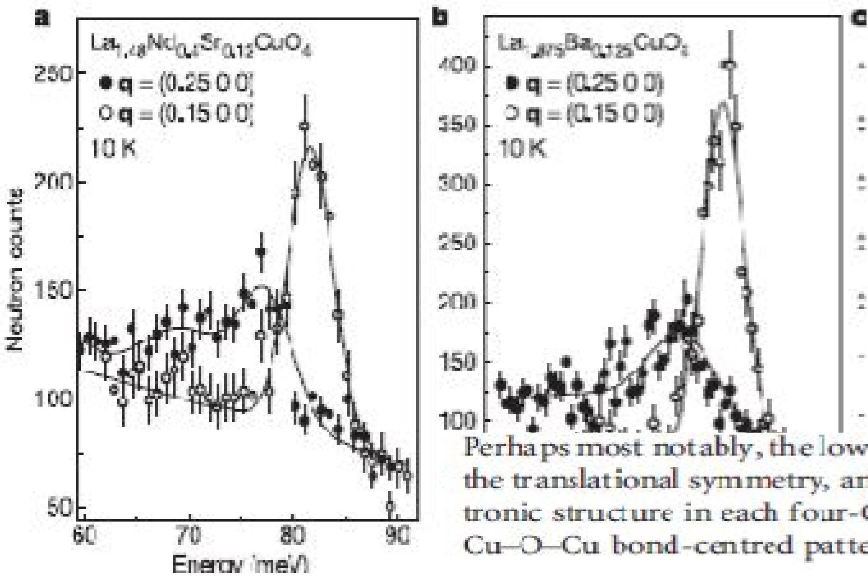
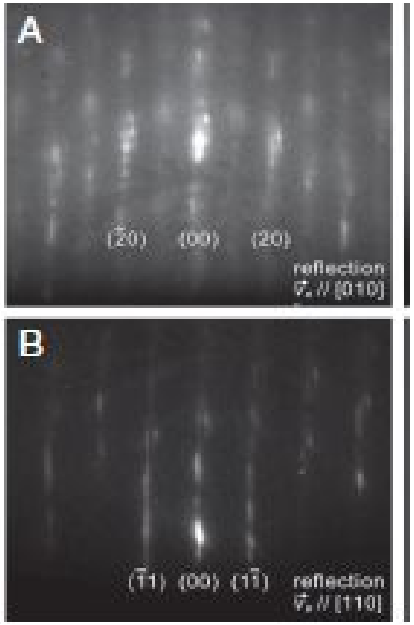


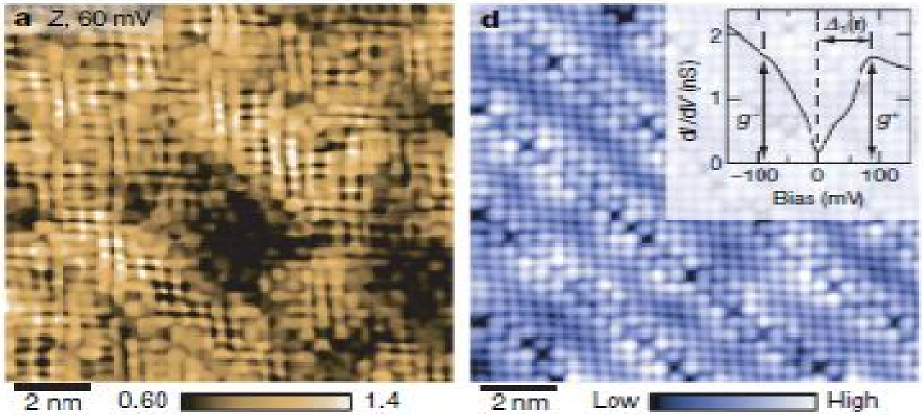
FIG. 1. Structural diagrams for polyacetylene: (a) *cis*-(CH)$_x$; (b) *trans*-(CH)$_x$; (c) the two degenerate ground states of *trans*-(CH)$_x$.

Exp results: Nonl exc.-charge inhomogeneity in cuprates (Reznik 07,Kohsaka 08, Zewail 08)

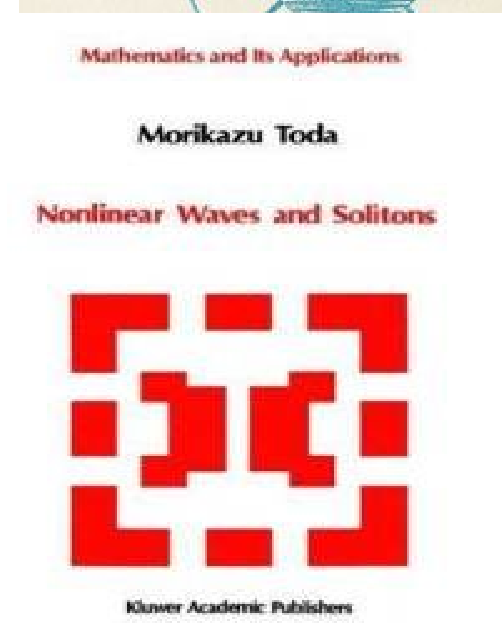




Perhaps most notably, the low-p pseudogap excitations locally break the translational symmetry, and reduce the C_4 symmetry of the electronic structure in each four-Cu-atom plaquette to C_2 symmetry in Cu–O–Cu bond-centred patterns without long-range order[20].



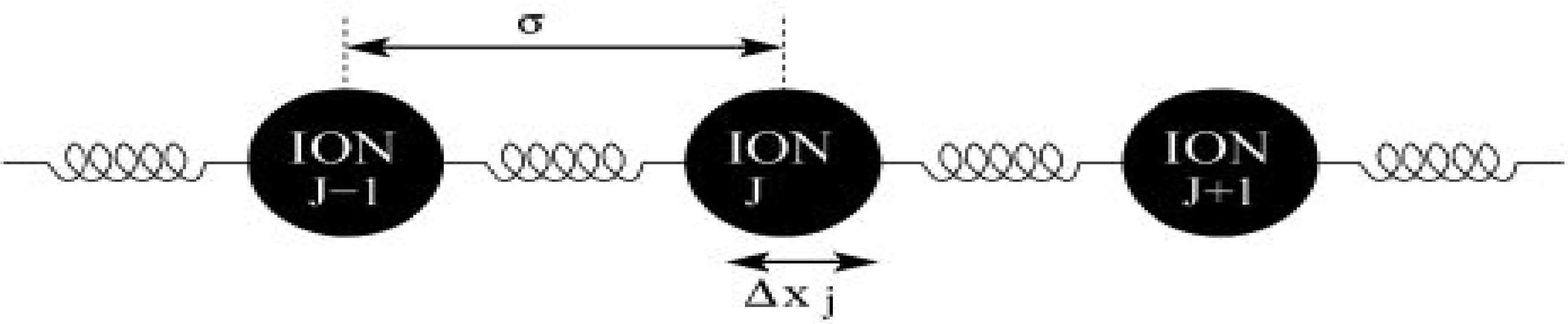
А.С. ДАВЫДОВ
СОЛИТОНЫ
В МОЛЕКУЛЯРНЫХ СИСТЕМАХ
To Prof. Werner Ebeling
with best wishes



Mathematics and Its Applications
Morikazu Toda
Nonlinear Waves and Solitons
Kluwer Academic Publishers

Studies of excitations in molecular 1d chains with Toda – Morse interactions

$$H = \sum_j \left[\frac{p_j^2}{2} + \frac{w^2}{b} e^{b(x_{j-1} - x_j - \sigma)} \right].$$



We will discuss: How to excite solitons, role of interactions, noise-heat, riding, control

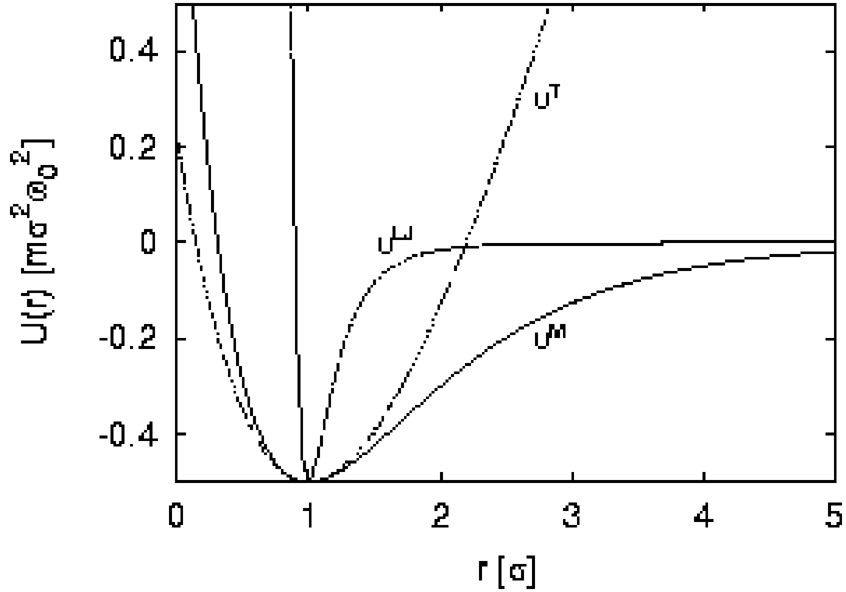
Langevin dynamics of atoms in chains/layers

The Langevin equation

$$\frac{d\mathbf{x}_i}{dt} = \mathbf{v}_i; \qquad \boldsymbol{x}_{i+N} = \boldsymbol{x}_i$$

$$\frac{d\,\mathbf{v}_i}{dt} = -\frac{\partial U}{\partial \mathbf{x}_i} - \gamma \mathbf{v}_i + \sqrt{2D}\,\xi(t)$$

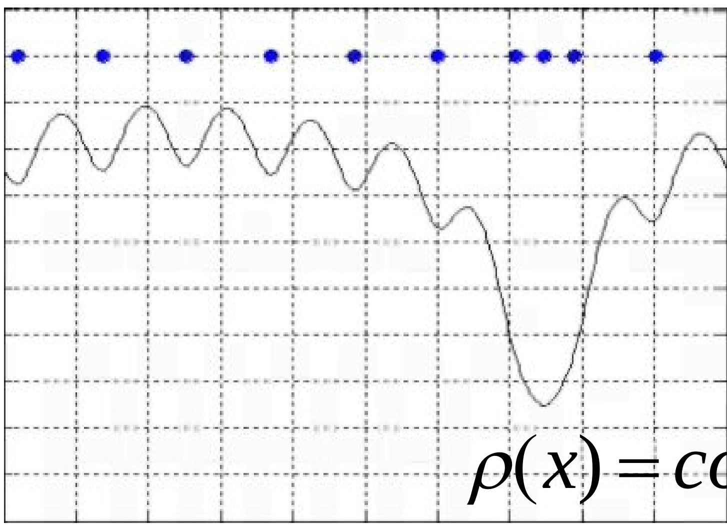
The Toda, Morse and L-J potentials



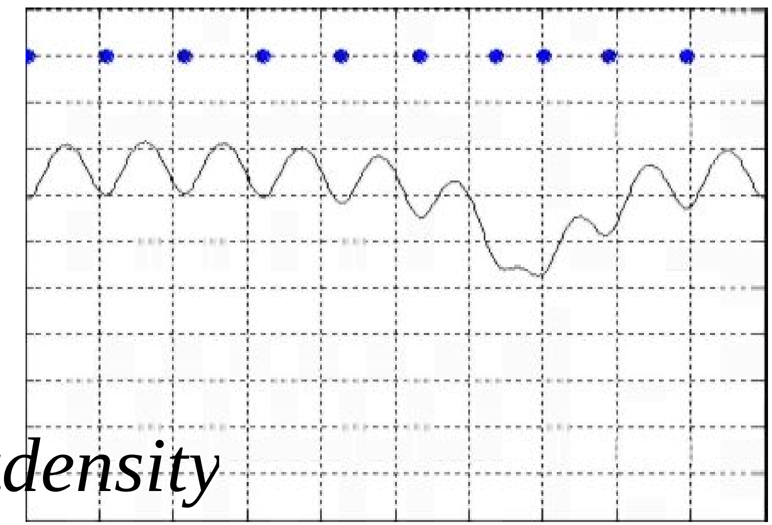
$$U^M(r) = D\left[e^{-2B(r-\sigma)} - 2e^{-B(r-\sigma)}\right]$$

T=0 study mechanical excitations in Morse chains which create moving local fields

Dynamics of the effective potential acting on electrons



B=2

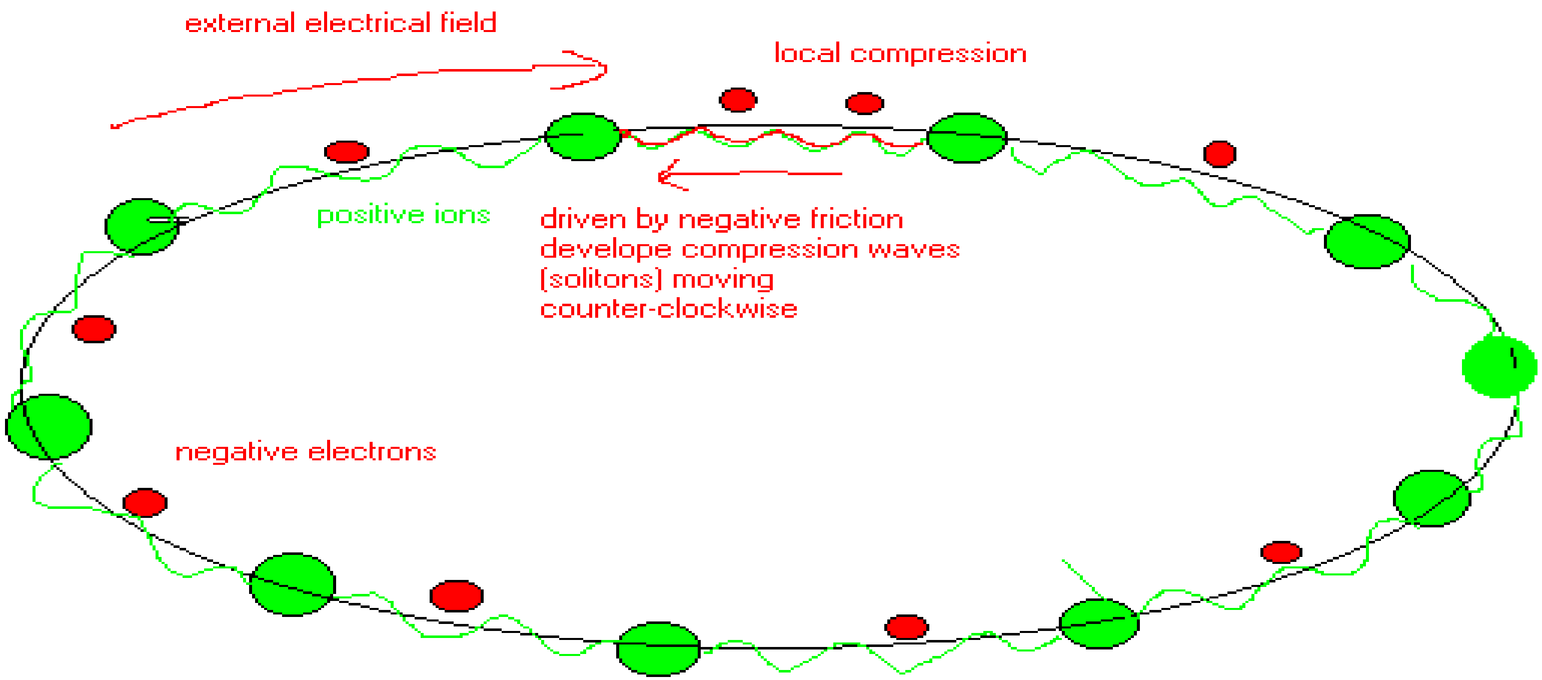


B=10

$$\rho(x) = compr.density$$

A deep minimum corresponding to the soliton
(local compression) propagates "upstream" COMPRESSION WAVE attracts charges

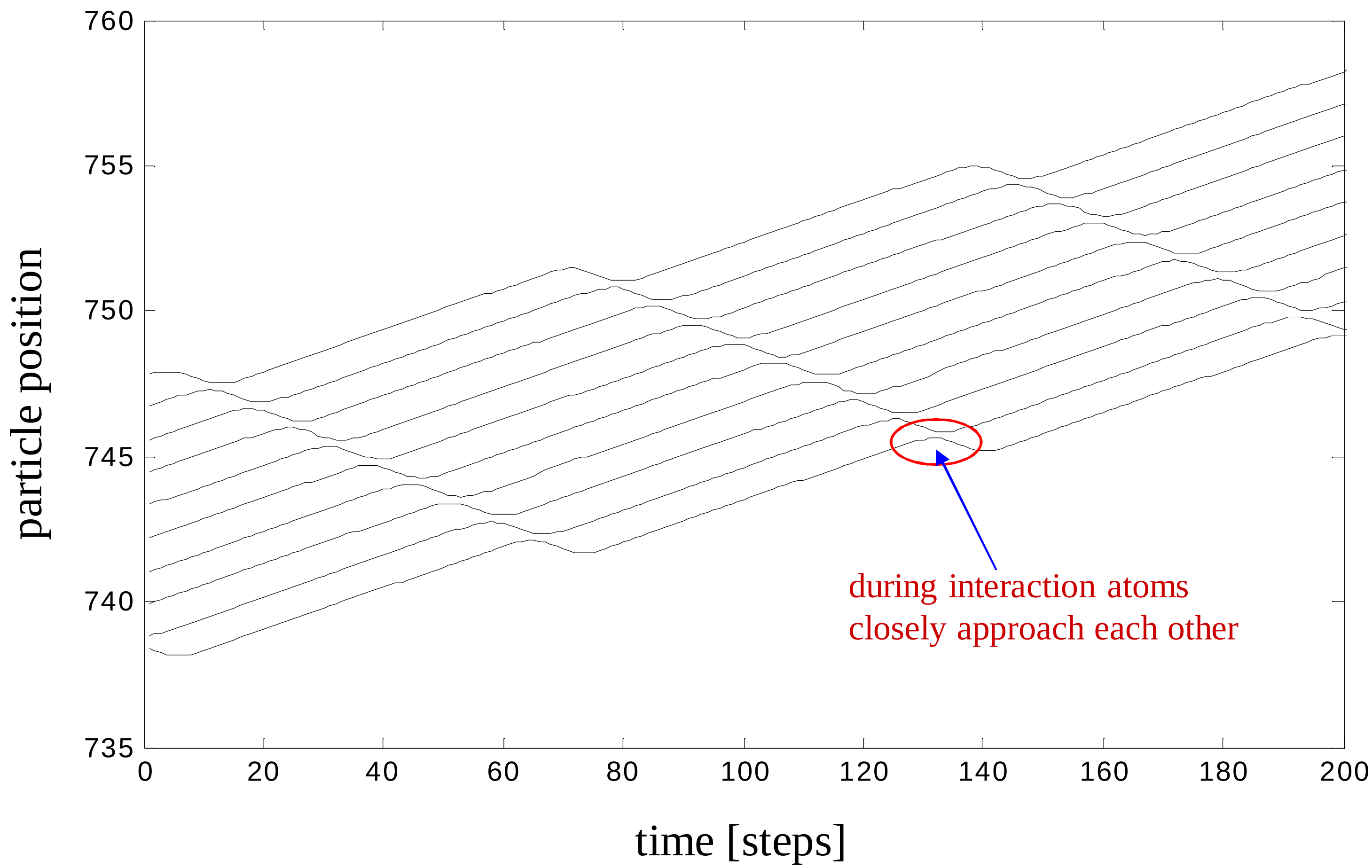
The Morse chains including interaction with free charges:
Electrons are attracted by compressions: $\rho(x,t) = \max$



Polarons: Landau/Pekar/Bolyubov/Tyablikov/
Gogolin/Zolotaryuk etal/Lakhno - HERE SUPERSONIC CASE

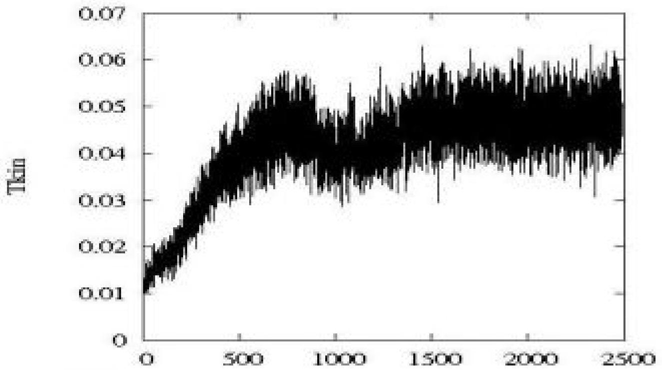
T=0 mechanical excitations = running compressions = soliton-like modes in Morse chains

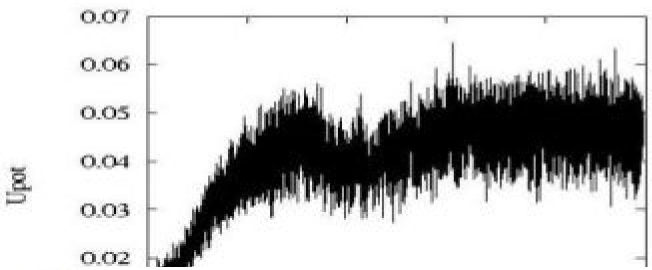
(Bσ=2) $U^M(r) = D\left[e^{-2B(r-\sigma)} - 2e^{-B(r-\sigma)}\right], \ \rho(x,t) = comdens$



step = 0.1

Heated Morse chain (without electrons)





Temperature

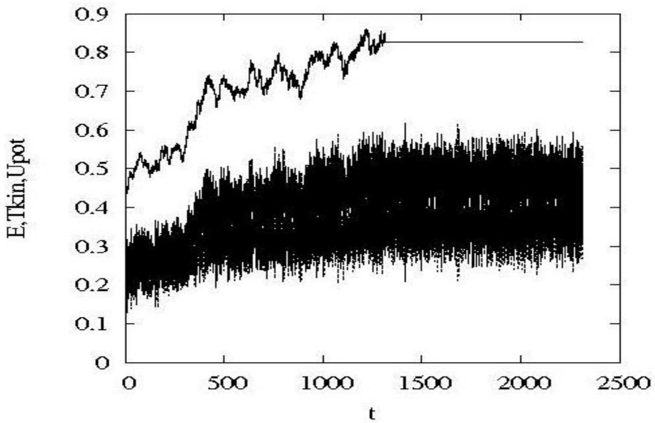
$$T = D / \gamma$$

Kin. energy

(1D case)

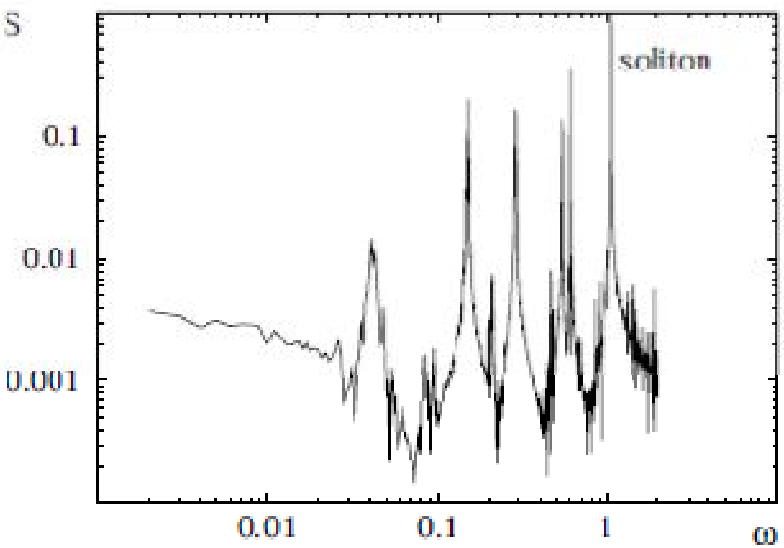
$$T_{kin} = T / 2$$

$$E = T_{kin} + U\_pot$$



Optimal T~0.1

unit 2D ~ 0.5 eV.



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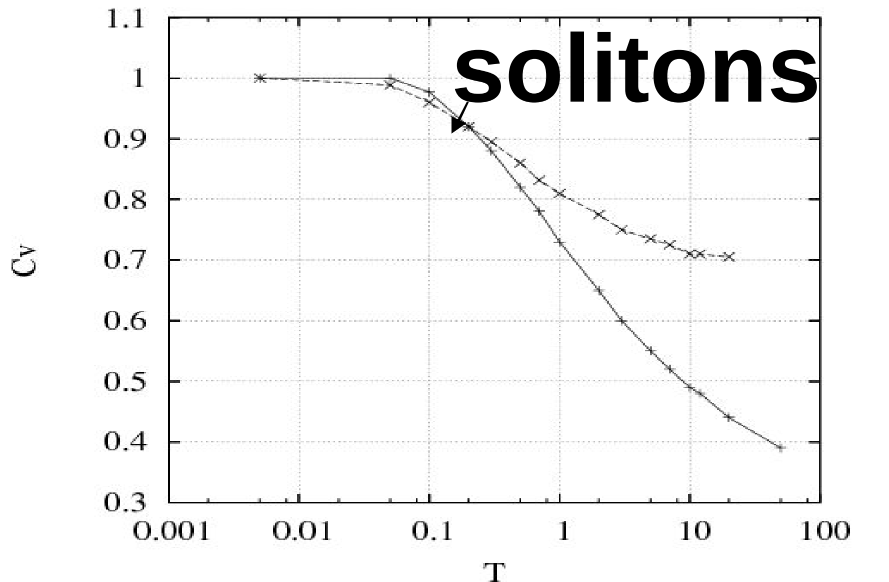
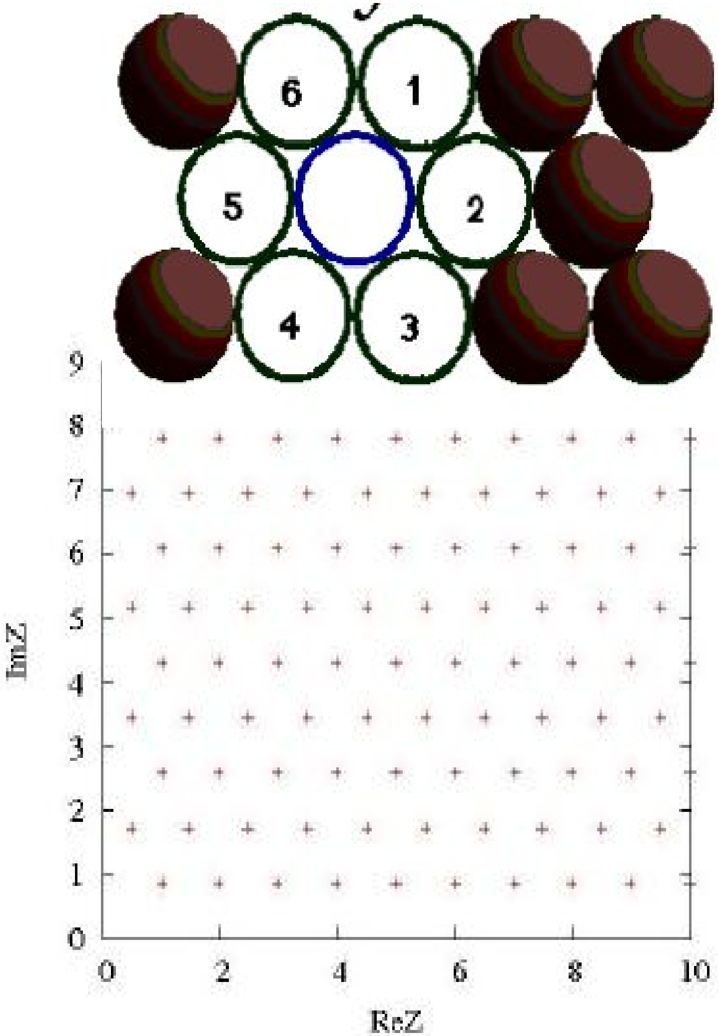
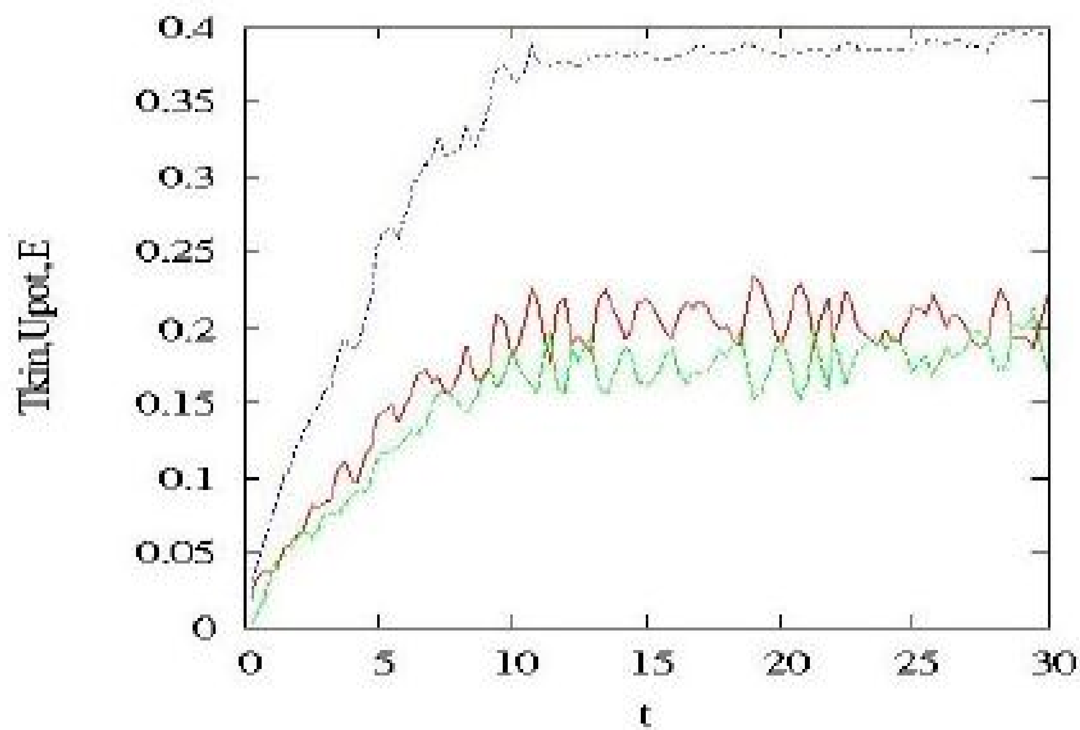


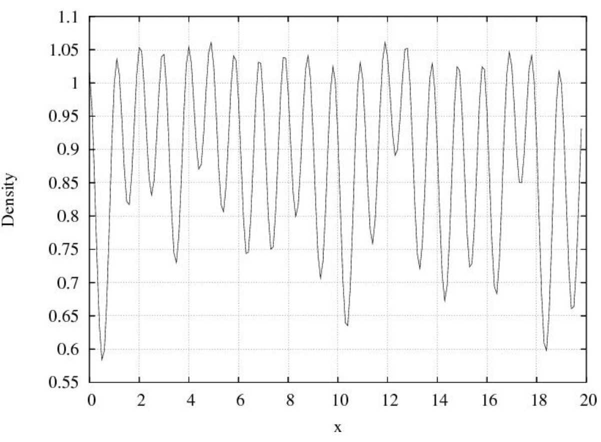
Simulations of 100 Morse particles 2d equilateral triangular lattices

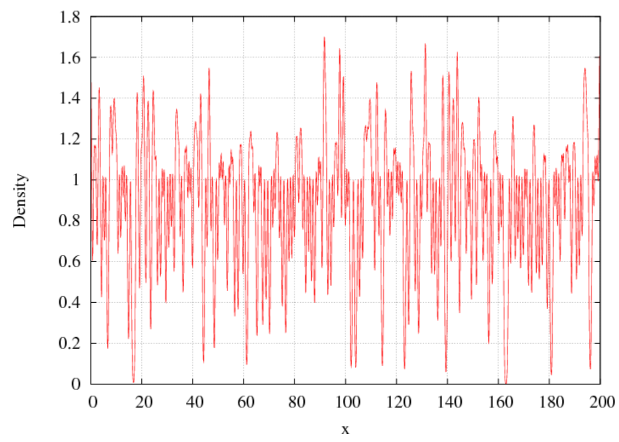


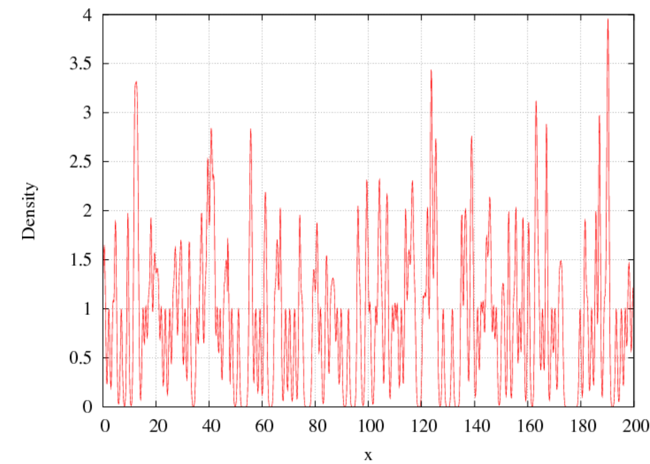


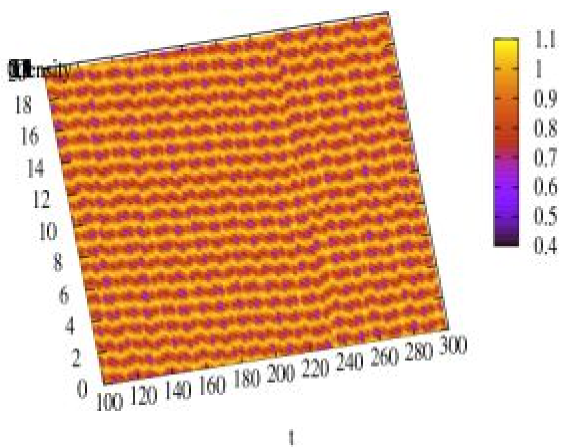
Compression density in 1d-chains T > 0

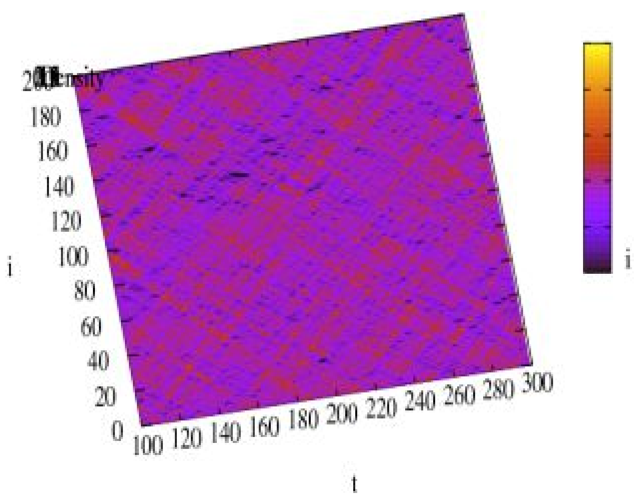
$$\rho(x,t)$$

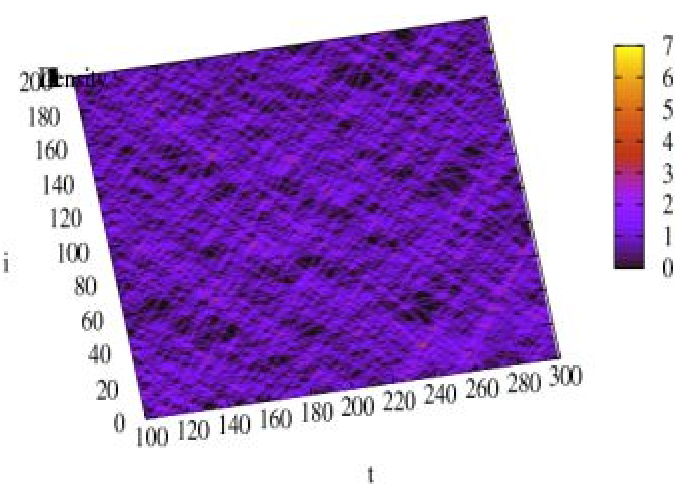








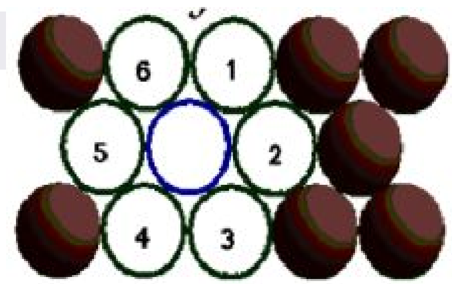




T=0.005 T=0.1 T=1

Compression density for 2d-atomic systems (snapshots)

$$\rho(x,y,t)$$



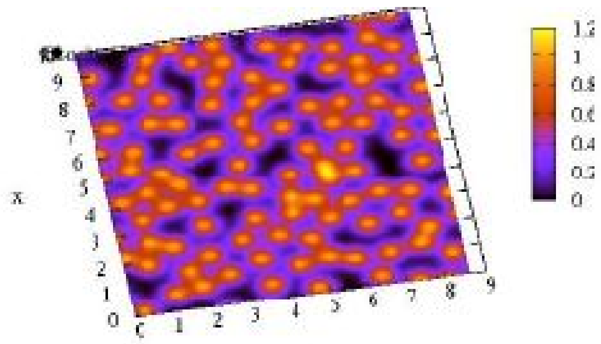


Fig1a ($t=t_0$)

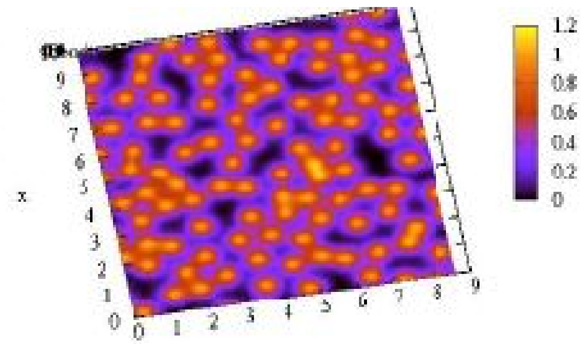


Fig2a ($t=t_0+0.2$)

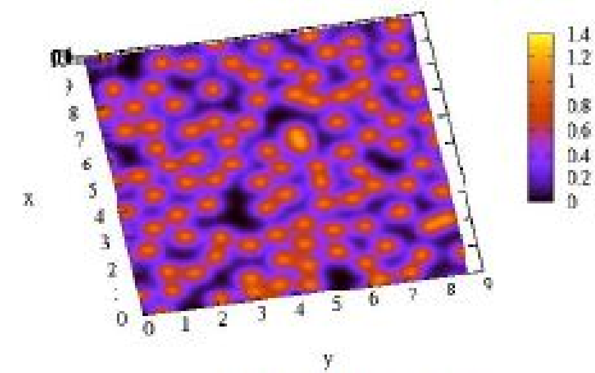
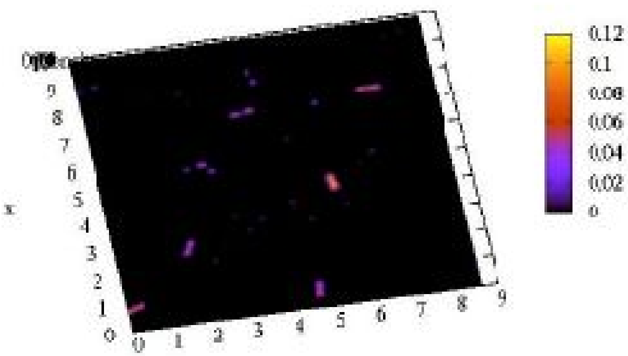
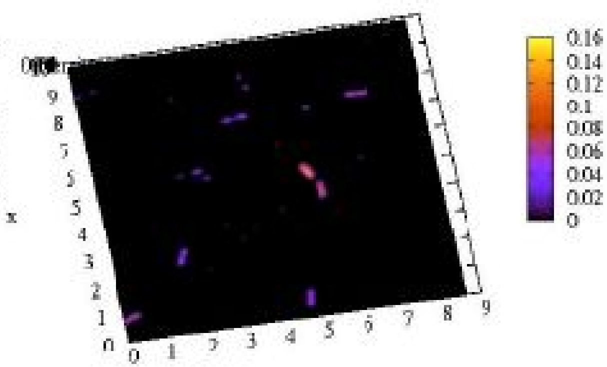
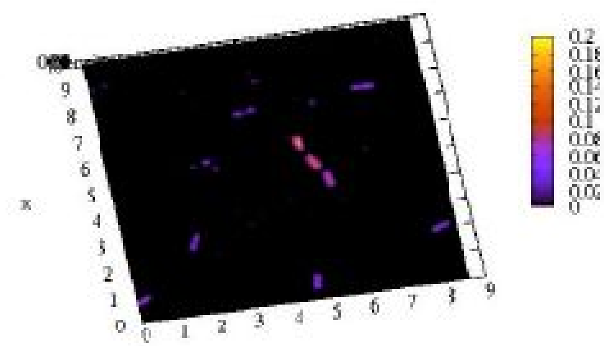


Fig3a ($t=t_0+1.$)







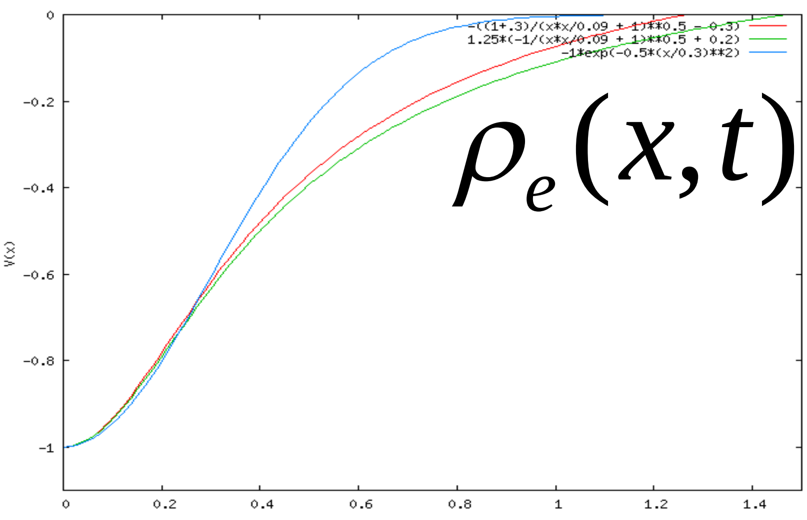
moving strong compressions

Interaction electron-atom and adiabatic electron dynamics: e-density follows compress.

We study now the local fields created by thelattice particles acting on the free electrons.

$$cont \quad \rho_e(x,t) \sim \rho(x,t) = \rho_0 \operatorname{sech}^2(x - vt),$$

$$discr \quad U(\mathbf{x},t) = \sum_i U_i(\mathbf{x} - \mathbf{x}_i); \quad \mathrm{U}_i(\mathbf{r}) = -\frac{U_e r_0^4}{[\mathbf{r}^2 + r_0^2]}$$



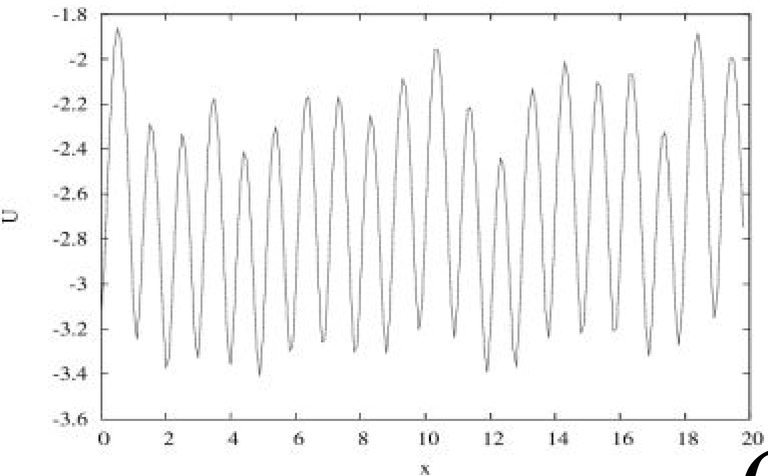
$$\rho_e(x,t) \approx \exp(-U(x,t)/k_B T)$$

$U_i(r)/U_e$ in comparison with a Gaussian(blue)

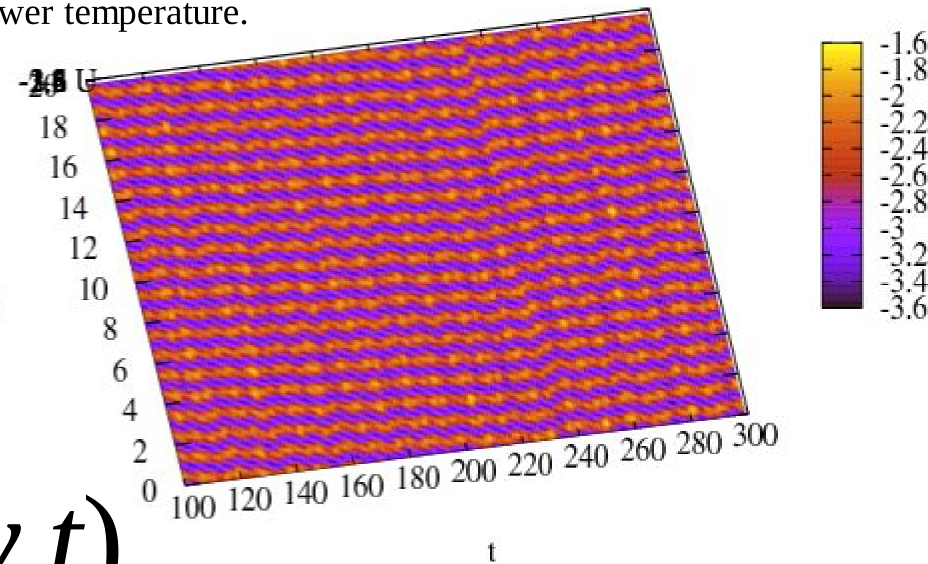
We assume : Ue ~ 0.1-1D.

electron density in heated 1d-lattices - Boltzm appr

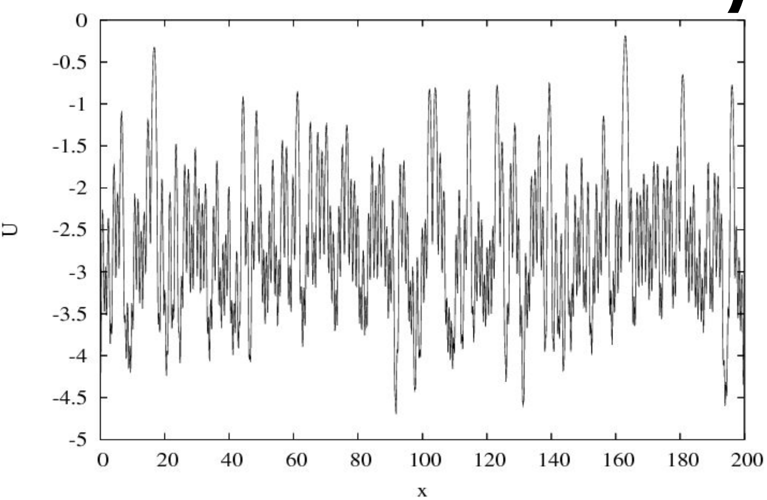
A landscape of local fields and local density in a chain at lower temperature.



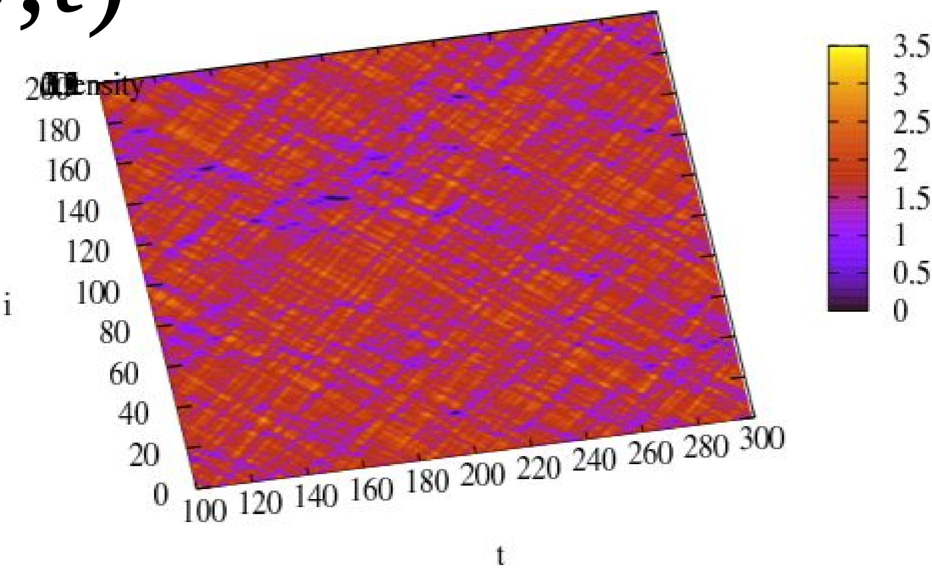
T=0.005



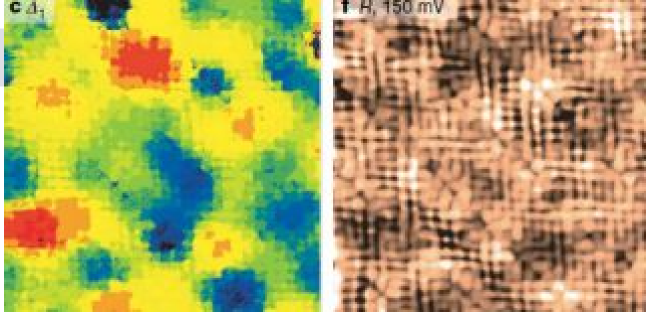
$$\rho_e(x, y, t)$$



T=0.1

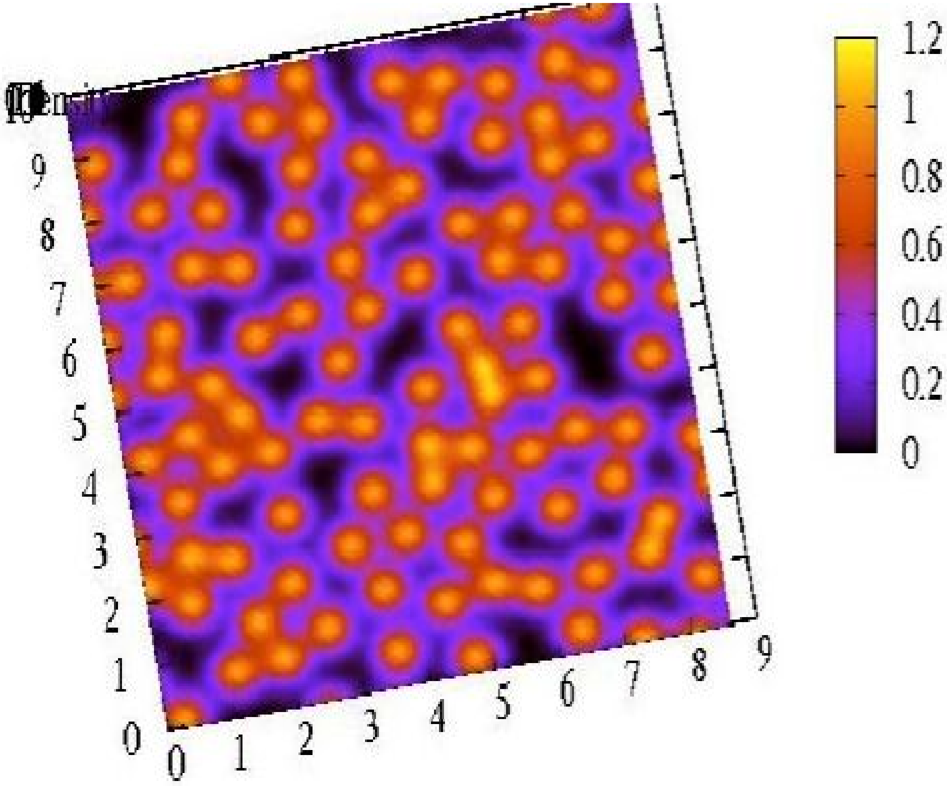


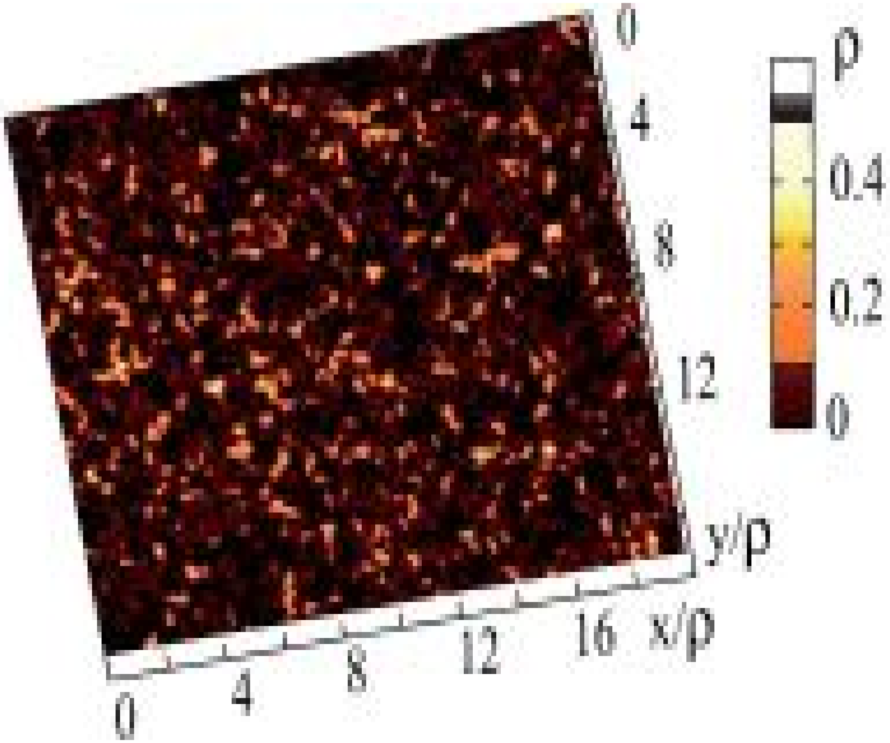
Two-dim systems: Snapshots of distr of electrons



Kohsaka et Nature 08 CuO

$$\rho_e(x,y,t)$$





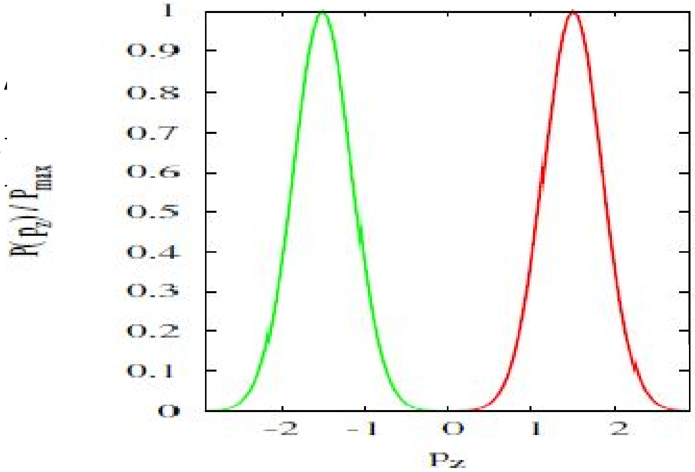
Cont QM description (Davydov)

$$\mathrm{H}\phi = -a\chi\rho(x,y,t)\phi$$

$$\rho(x,t) = \rho_0 \mathrm{sech}^2(\kappa\xi), \qquad \xi(t) = [x(t) - x(0) - v_s t]$$

$$\phi_0(x,t) = C\mathrm{sech}(\kappa\xi), \qquad \xi'(t) = [x(t) - x(0) - v_{se} t$$

$$P_0(p,t) = |\phi_0(p,t)|^2 \sim C\exp\left[-\frac{(p \pm p_{se})^2}{(h\kappa/\sigma)^2}\right]$$



- quasiparticles (solectrons) first described by Davydov = localized fastly moving charges (several km / sec in solid)

Discrete quantum mechanics:

Tight binding-model for hopping electrons

Hamiltonian of electrons on 1d-Morse latts

$$H = H_{lattice} + H_{electron} + H_{\text{int}}$$

$$V(r) = D\left[\left(e^{-B(r-\sigma)} - 1\right)^2 - 1\right] \qquad H_{lattice} = \sum_i \frac{p_i^2}{2m} + \sum V(r_{ij})$$

$$H_{electron} + H_{\text{int}} = \sum_n \left(E_n c_n c_n^* + V_{nn-1}\left(c_n^* c_{n-1} + c_n c_{n-1}^*\right) \right)$$

- "tight binding" Hamiltonian for "electrons",

$|C_n|^2$ gives the probability of finding the "electron" residing at n-th site

$$V_{nn-1} = V_0 \exp\left[-\alpha(q_n - q_{n-1})\right] \sim V_0\left[1 - \alpha(q_n - q_{n-1})\right],$$

$\tau \sim V_0$

cont.appr $\quad H_{\text{int}} \sim a\chi\rho(x)$

Discrete eqs of motion for Morse lattice +tight binding electrons

$$\frac{d^2 q_n}{dt^2} = \left[1 - e^{(q_n - q_{n+1})}\right] e^{(q_n - q_{n+1})} - \left[1 - e^{(q_{n-1} - q_n)}\right] e^{(q_{n-1} - q_n)} -$$

$$-2i\alpha V_0 \,\mathrm{Im}\left[C_{n+1}^* C_n e^{\alpha(q_n - q_{n+1})} - C_n^* C_{n-1} e^{\alpha(q_{n-1} - q_n)}\right]$$

$$\frac{dC_n}{dt} = -i\varepsilon_n C_n + i\tau \left[e^{\alpha(q_n - q_{n+1})} C_{n+1} - e^{\alpha(q_{n-1} - q_n)} C_{n-1}\right]$$

Here q_n is displacements from equilibrium positions, no energy shifts

$|C_n|^2$ gives the probability of finding the "electron" residing at n-th site

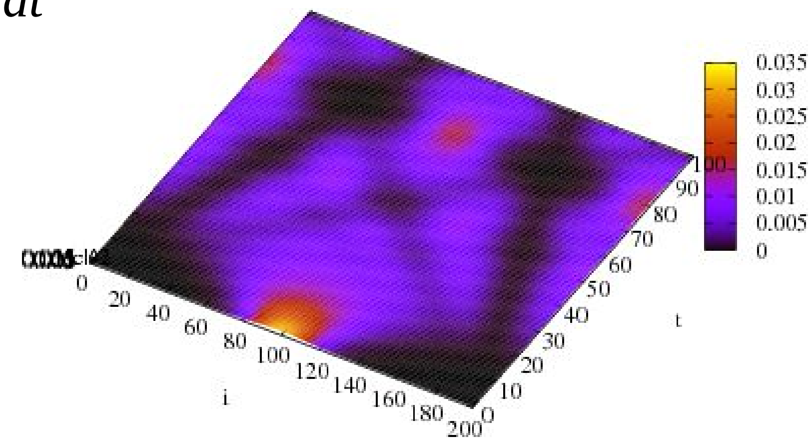
and tau is the adiabaticity parameter separating the time scales.

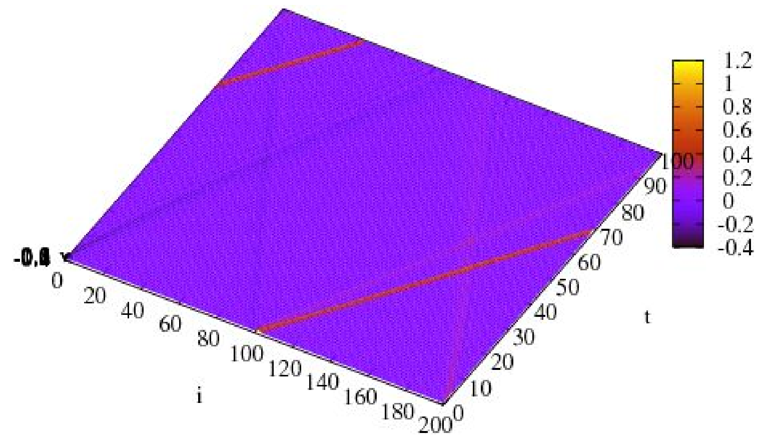
$V_{nn-1} = V_0 \exp\left[-\alpha\left(q_n - q_{n-1}\right)\right] \quad \tau \sim V_0$, α accounts for the strength of the coupling

Cold lattice:Localization of electrons interacting with a soliton

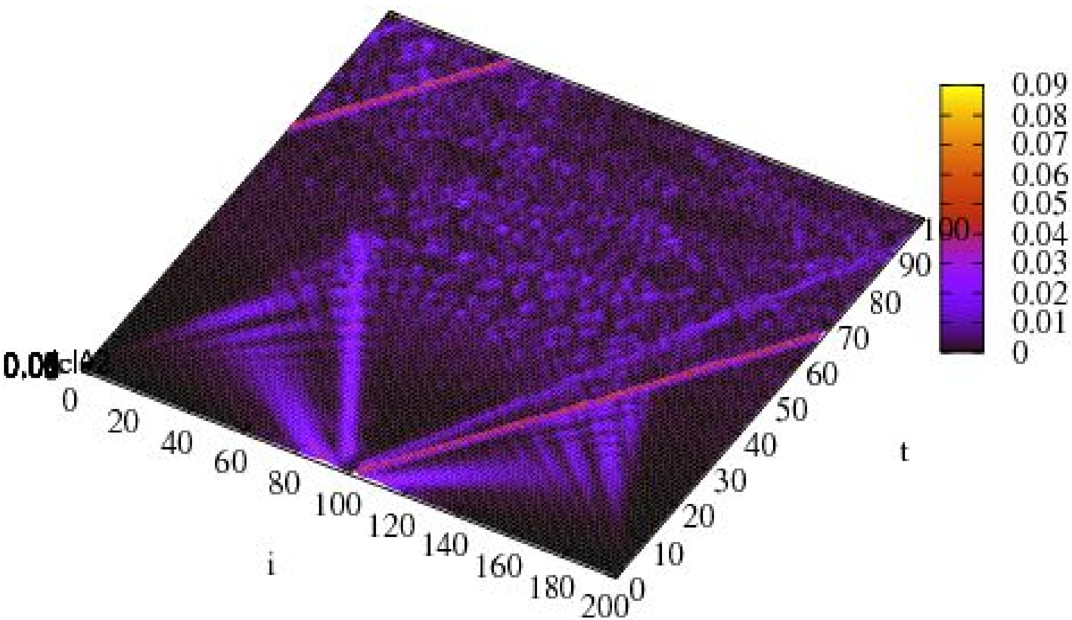
$$\frac{dC_n}{dt} = i\tau\ [C_{n+1} - C_{n-1}],$$

α=1.75,   V=0.1-0.5,   τ=20.





Left: free electron density   below with INTERACTION   Right Moving soliton.

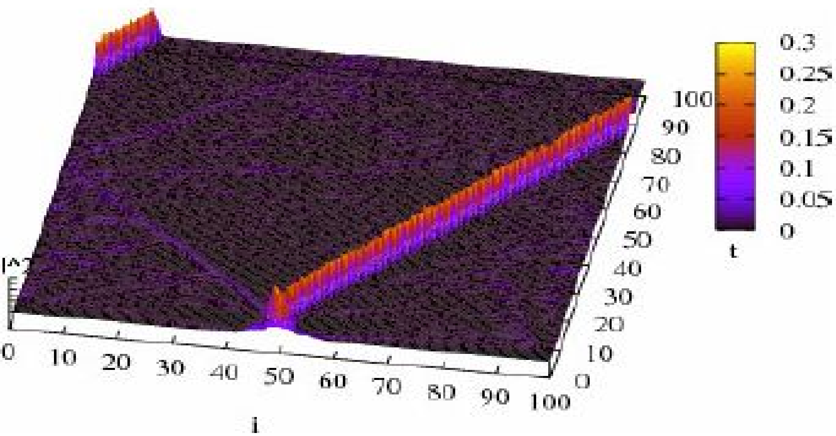


Electron density including interaction electron - solitont:

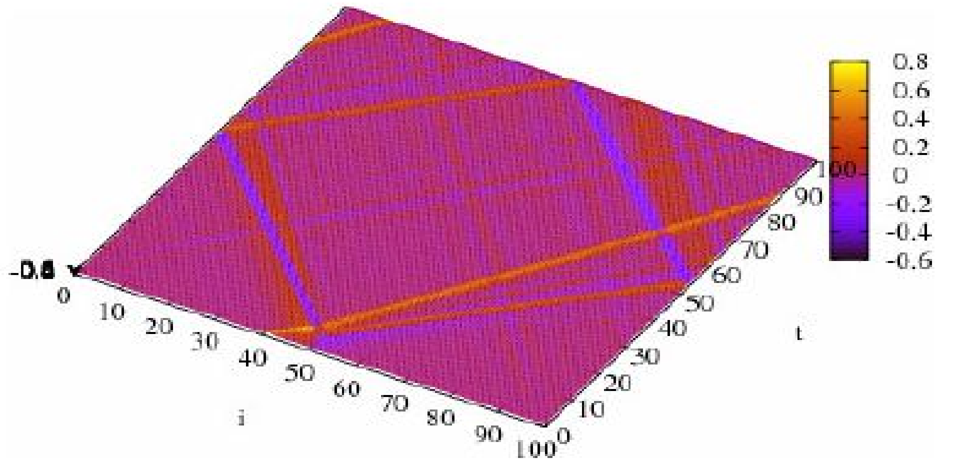
The electron basically follows the soliton, riding on it

Vacuum-cleaning: Electron (starting at site 50) catched by soliton (started at site 40). Below: Extract bound elec out of wells

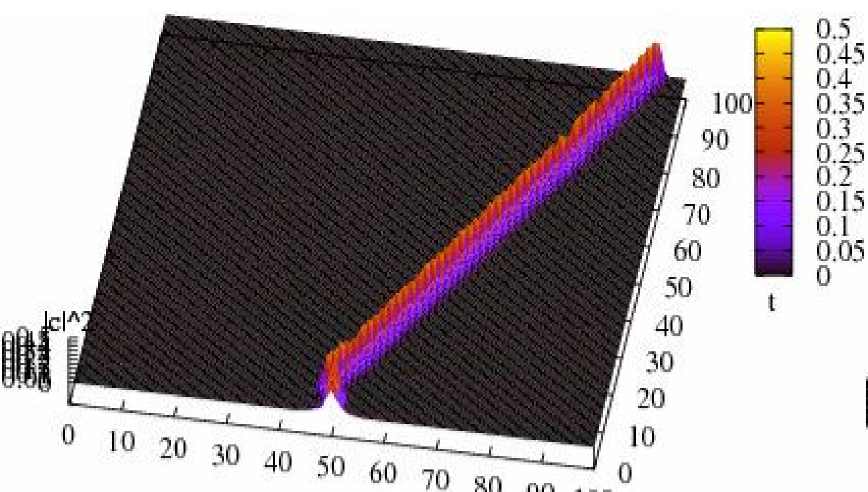
α=1.75,   V=.6,   τ=10, T = 0

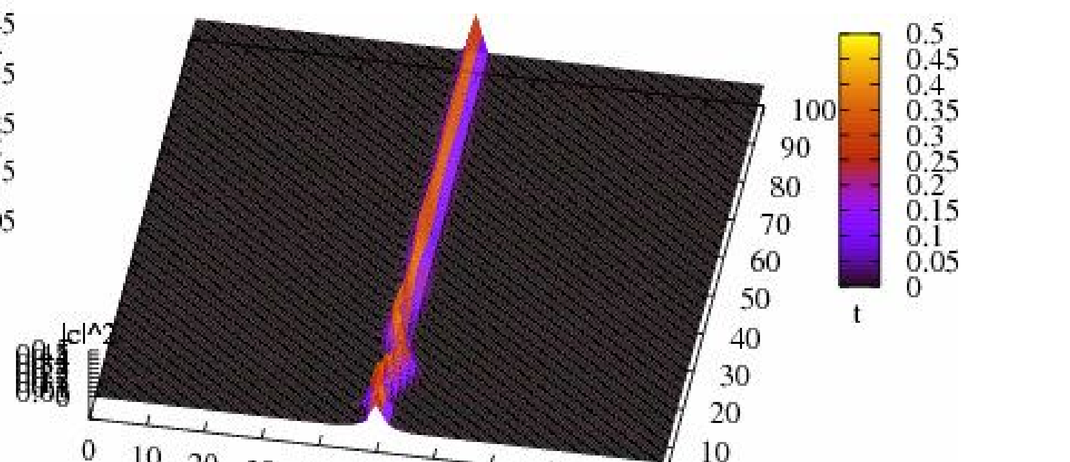


a)

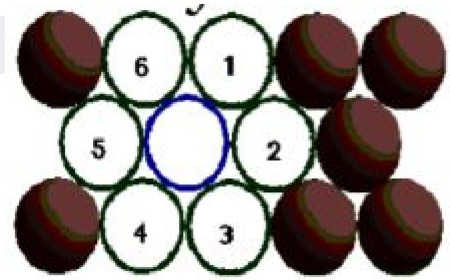


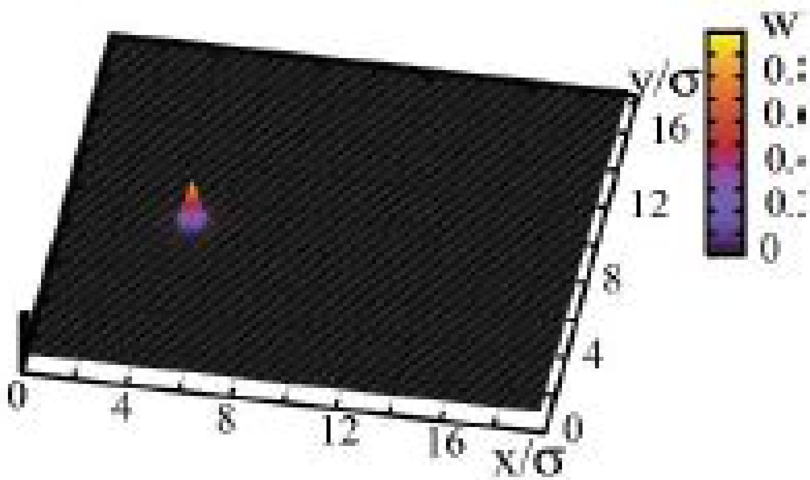
b)



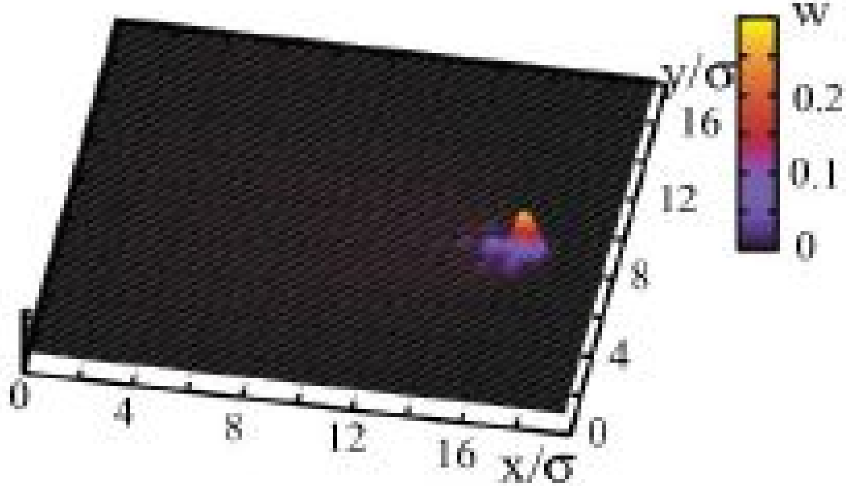


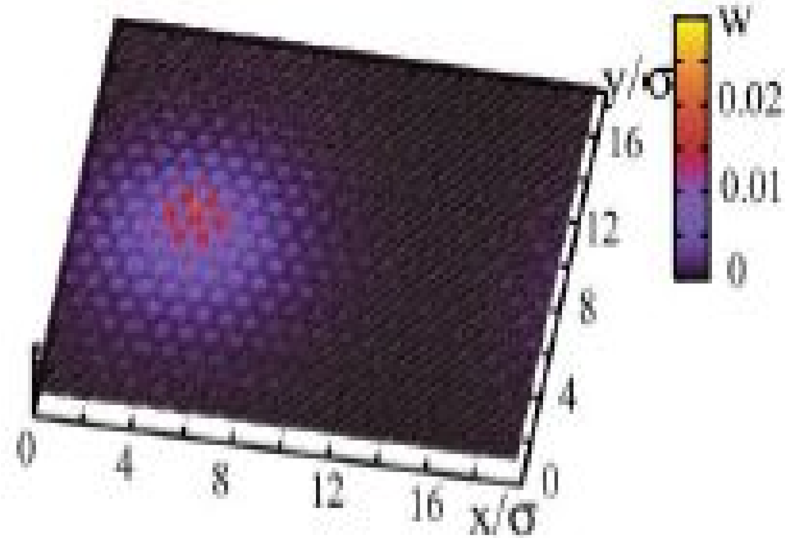
2d tr lattice along cryst ax

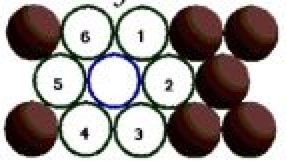




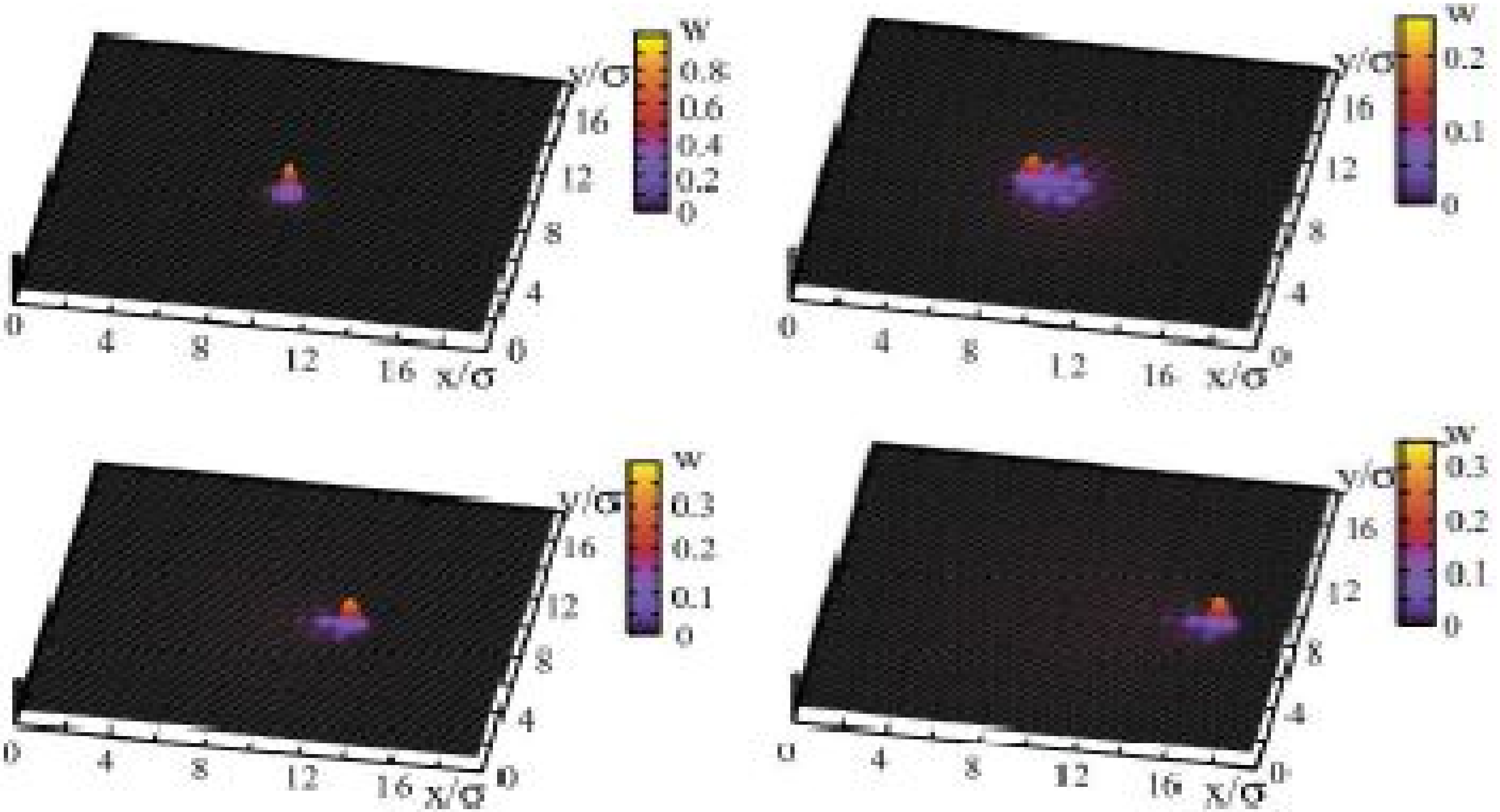
- Switch off interaction electron - soliton
- --> electron dispersion







Electron and soliton start in different rows of 2d triangular lattice - vacuum cleaner effect



Experiments on control of electrons by acoust exc/ solitons on surfaces :
V. Nayanov (Saratov) since 1982, monogr. 2005
New papers 2011 in Nature:

doi:10.1038/nature10444

On-demand single-electron transfer between distant quantum dots

R. P. G. McNeil[1], M. Kataoka[1,2], C. J. B. Ford[1], C. H. W. Barnes[1], D. Anderson[1], G. A. C. Jones[1], I. Farrer[1] & D. A. Ritchie[1]

doi:10.1038/nature10416

Electrons surfing on a sound wave as a platform for quantum optics with flying electrons

Sylvain Hermelin[1], Shintaro Takada[2], Michihisa Yamamoto[2,3], Seigo Tarucha[2,4], Andreas D. Wieck[5], Laurent Saminadayar[1,6], Christopher Bäuerle[1] & Tristan Meunier[1]

First conclusions:

- The effects of dispersion / incoherence of electron wave functions may be supressed by nonlinear compression waves (solitons = nonlinear sound waves)
- New quasiparticles (solectrons) first described by Davydov => localized fastly moving charges (supersonic polarons, several km / sec in solid)
- Possible applications to control of electrons

Finite T: Electron distr from Pauli equations

$$H_e = \sum_n (E_n^0 + \delta E_n) c_n * c_n - V_0 \exp[-\alpha(q_n - q_{n-1})](c_n^+ c_{n-1} + c_n c_{n-1}^+)$$

$$E_n = E_n^0 + \delta E_n, \delta E_n \approx U \ (x;...q_{n-1}, q_{n+1},...)$$

$$W_{nn'} \sim \exp(-2\alpha(q_n - q_{n'}) \circ \exp(-\delta E_{nn'} / k_B T) \ \text{uphill}$$

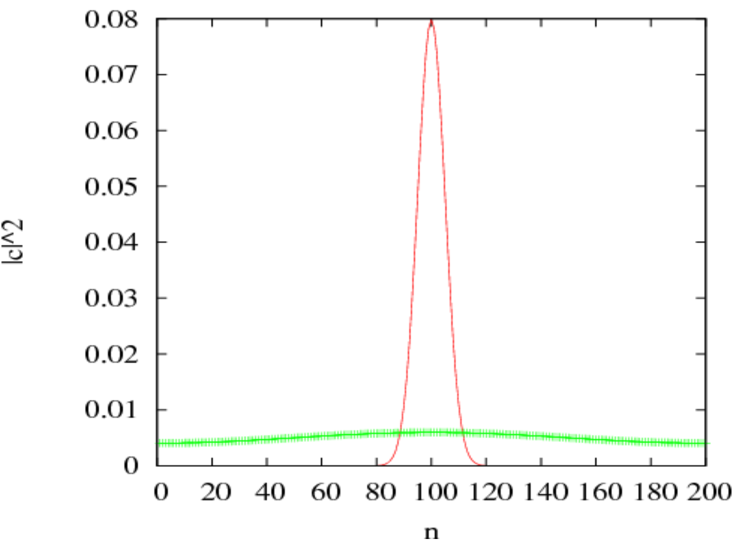
$$W_{nn'} \sim \exp(-2\alpha(q_n - q_{n'}) \quad \text{downhill}$$

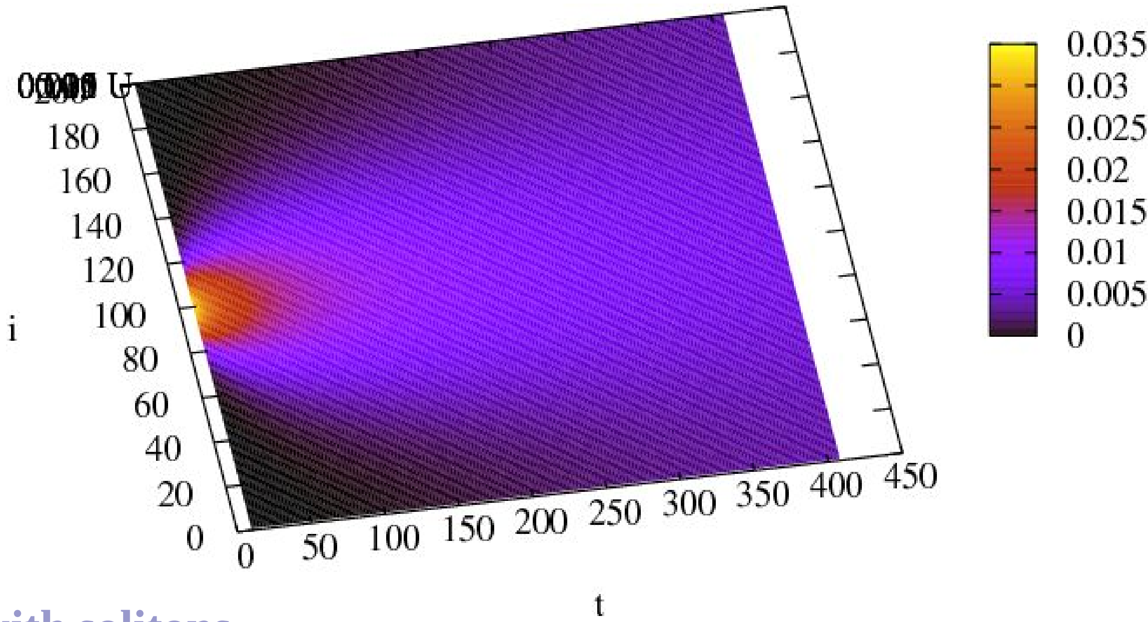
(according to Miller/Abr ahams/Mott et al.)

master eq.

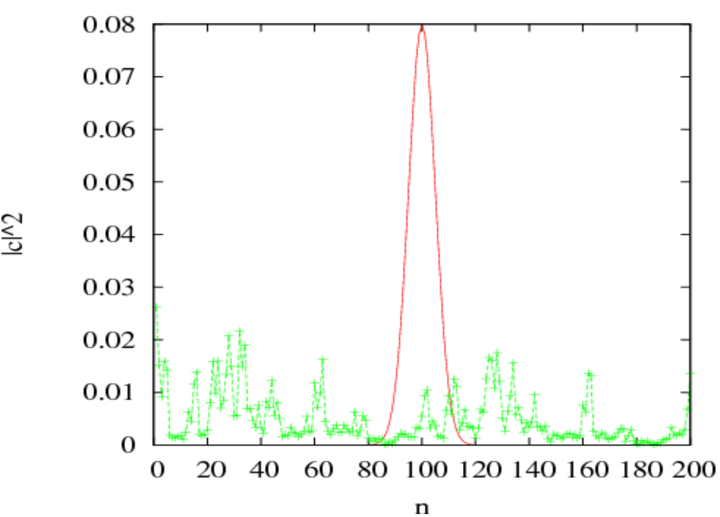
$$\frac{dp_n}{dt} = \sum_{n'} (W_{nn'} p_{n'} - W_{n'n} p_n)$$

Cold lattice T=0: dispersion of wave function

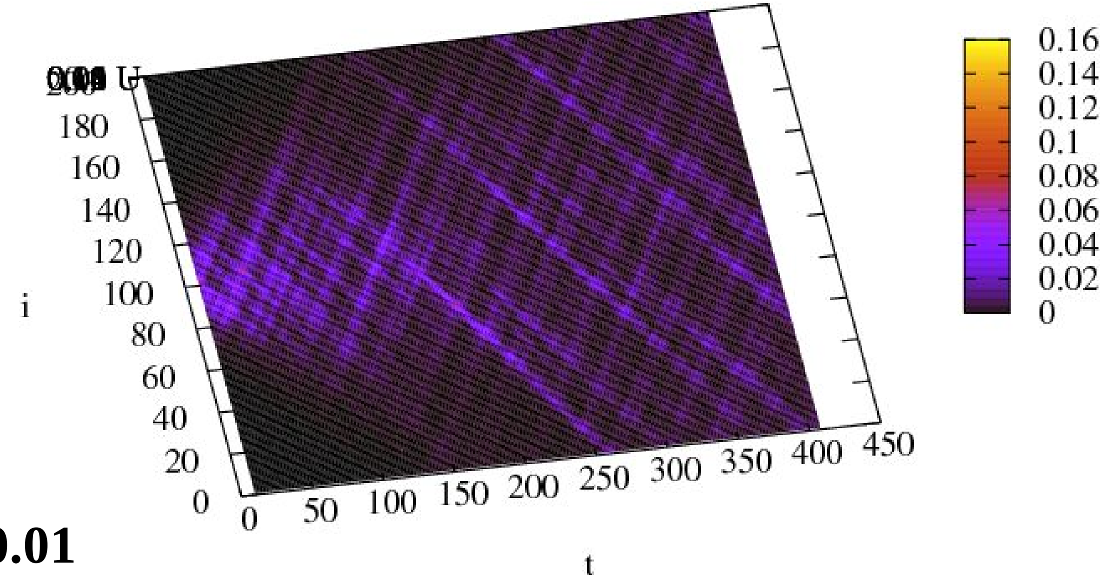




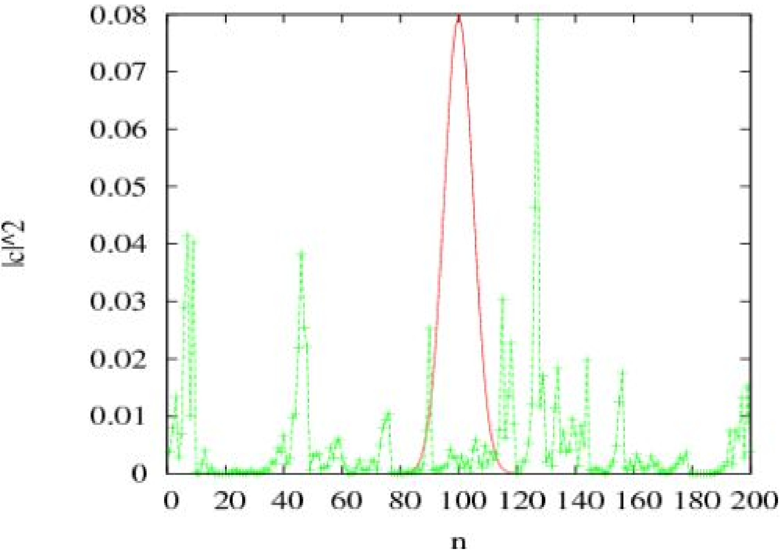
Heated lattice: effects of coherence with solitons

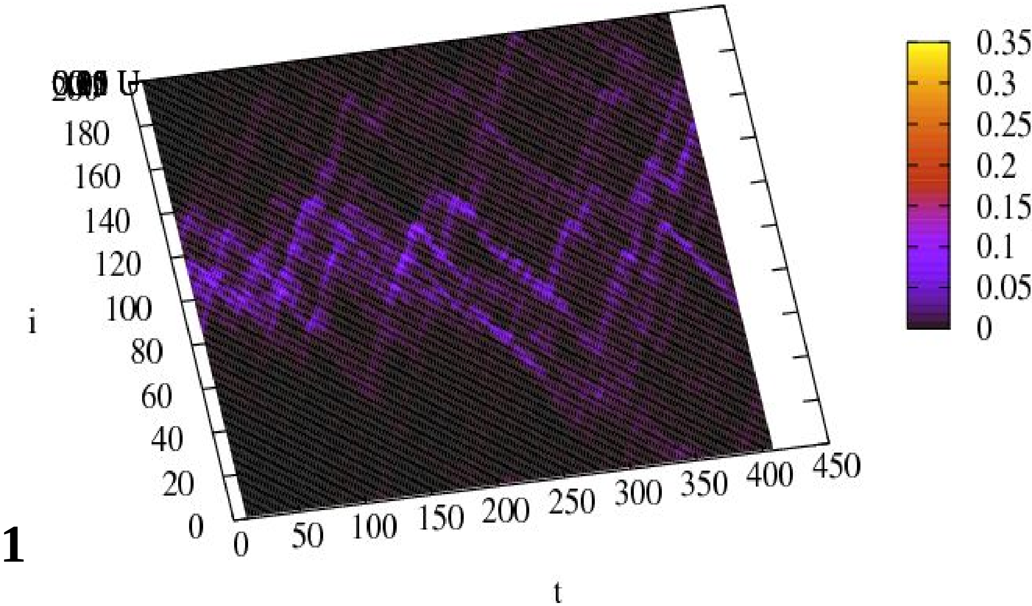


T=0.01

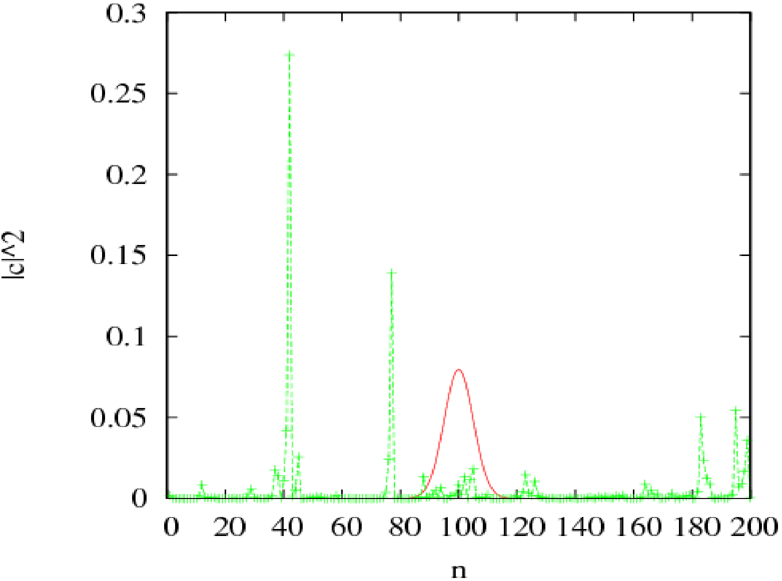


Heated lattice in soliton regime

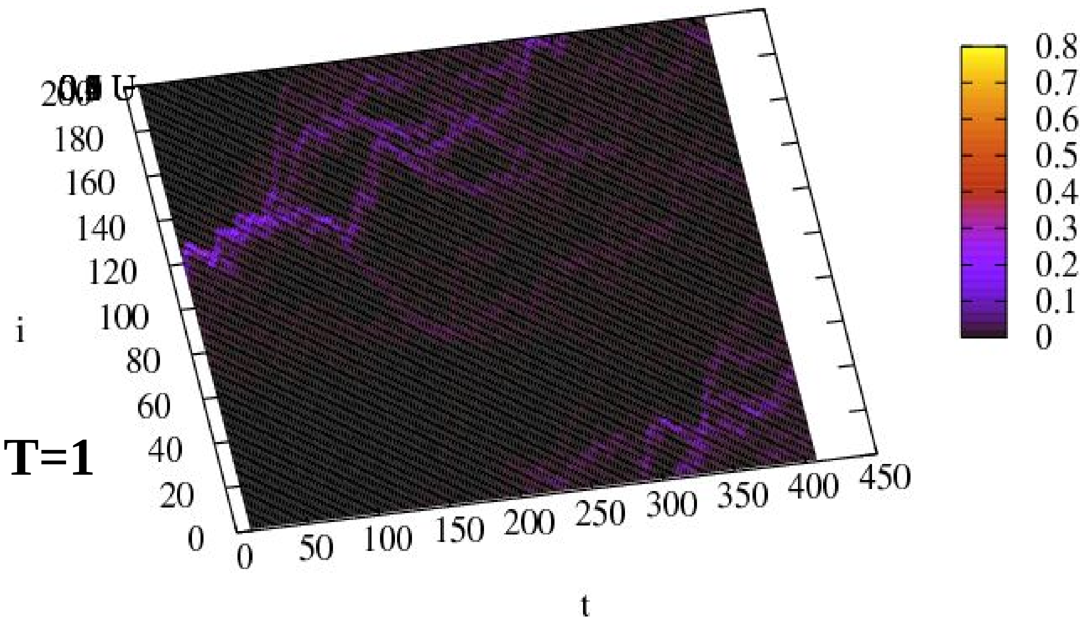




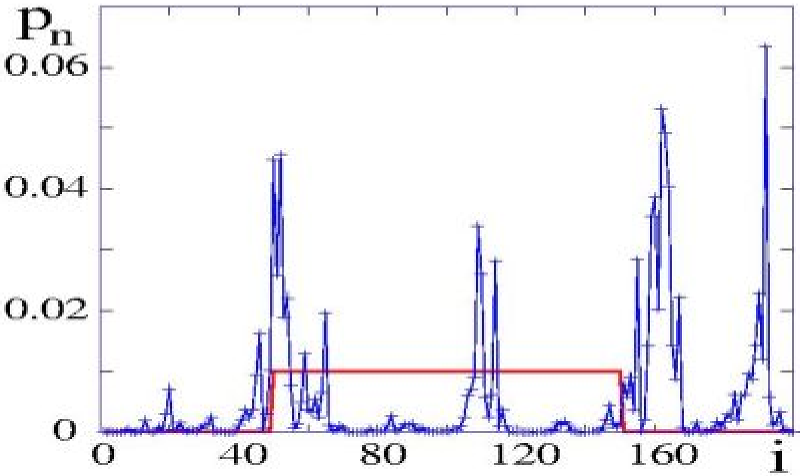
T=0.1

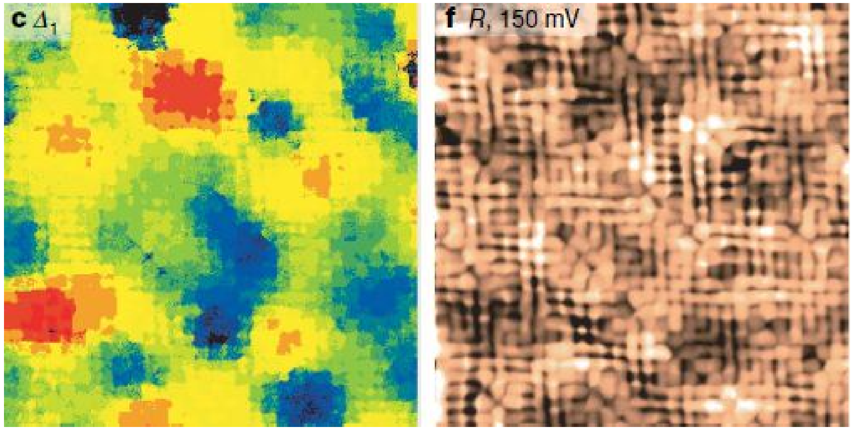


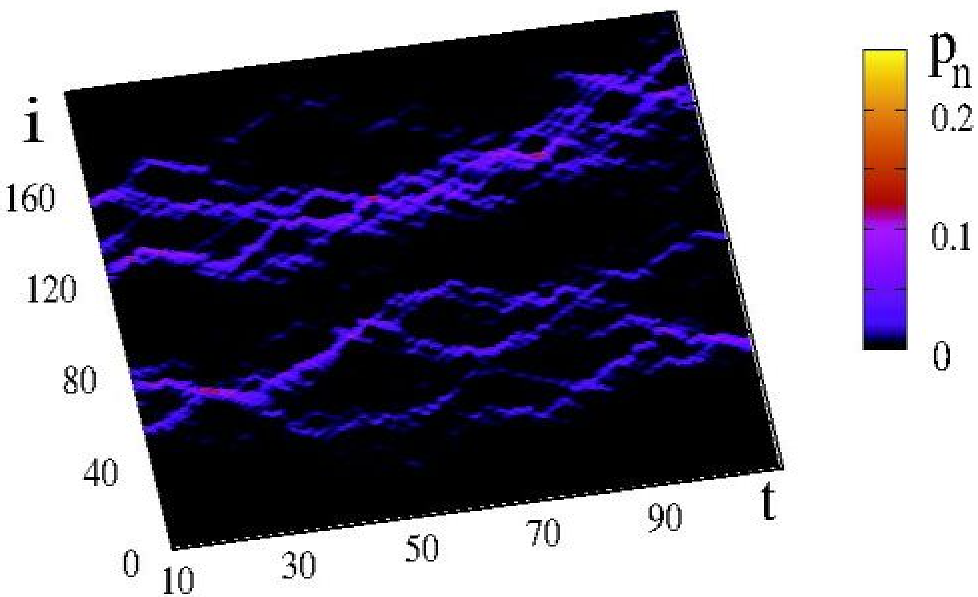
T=1

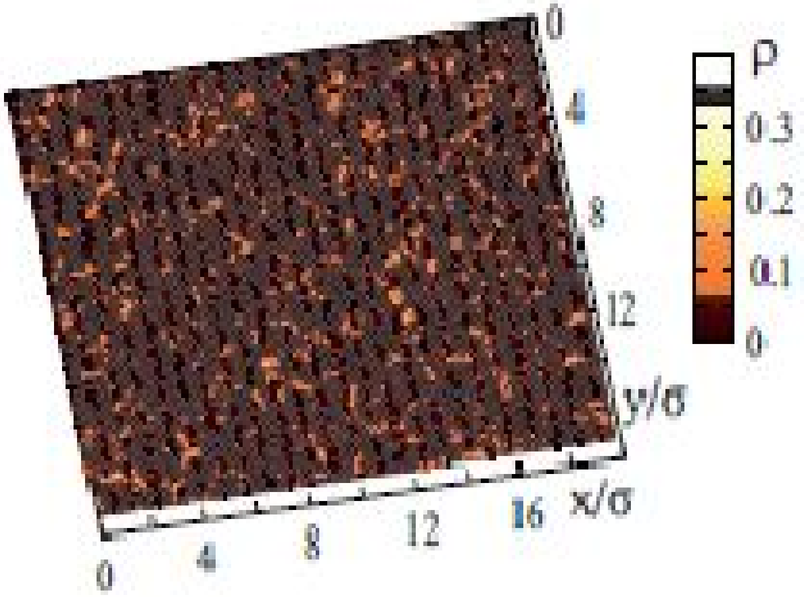


Example for the structure of the electron density in a therm soliton system:Electrons ride on thermal solitons; Kohsaka-exp CuO !



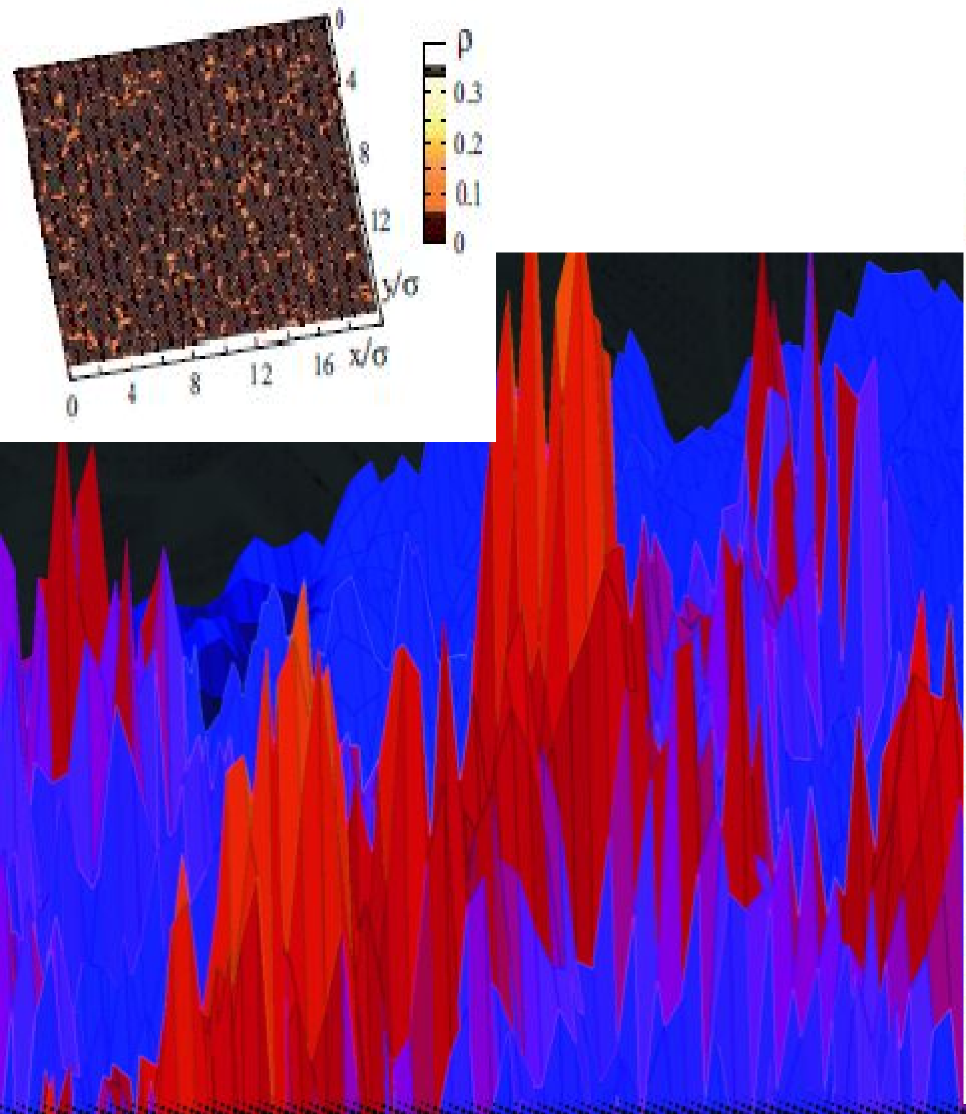


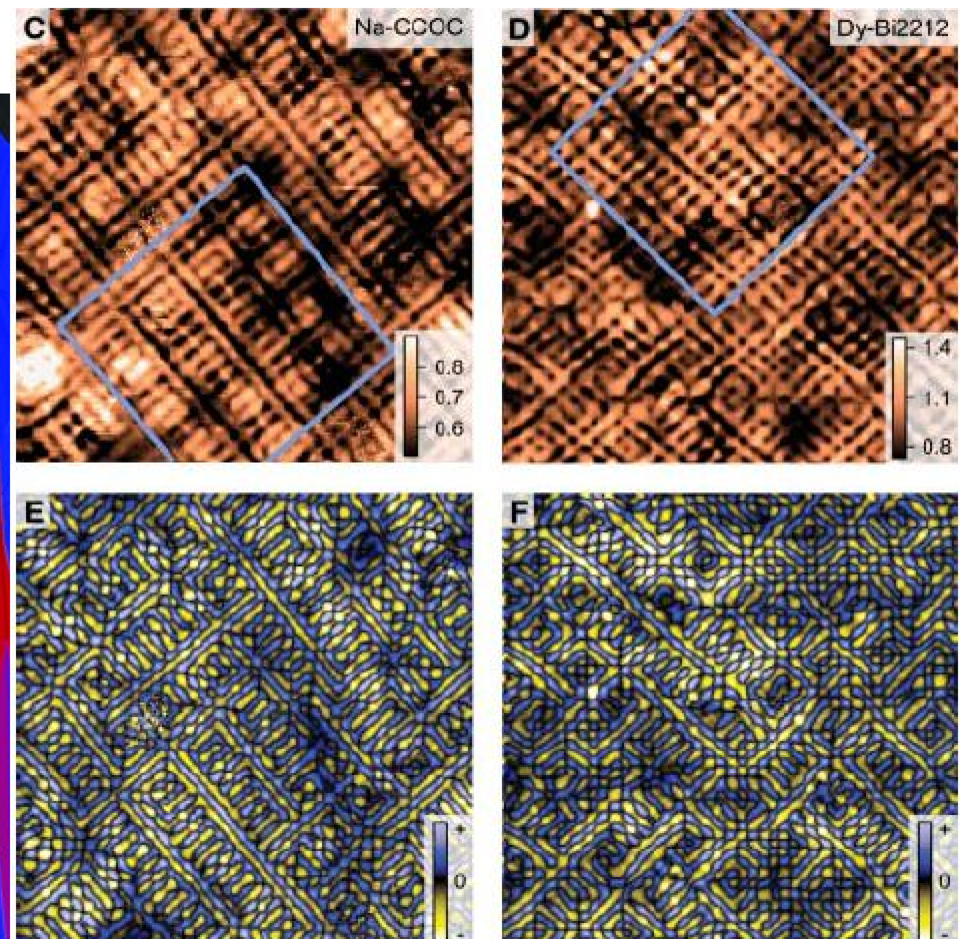




Example for the electron density in a therm soliton-bearing system:l.h.s. simulation of electrons on th. Sol.

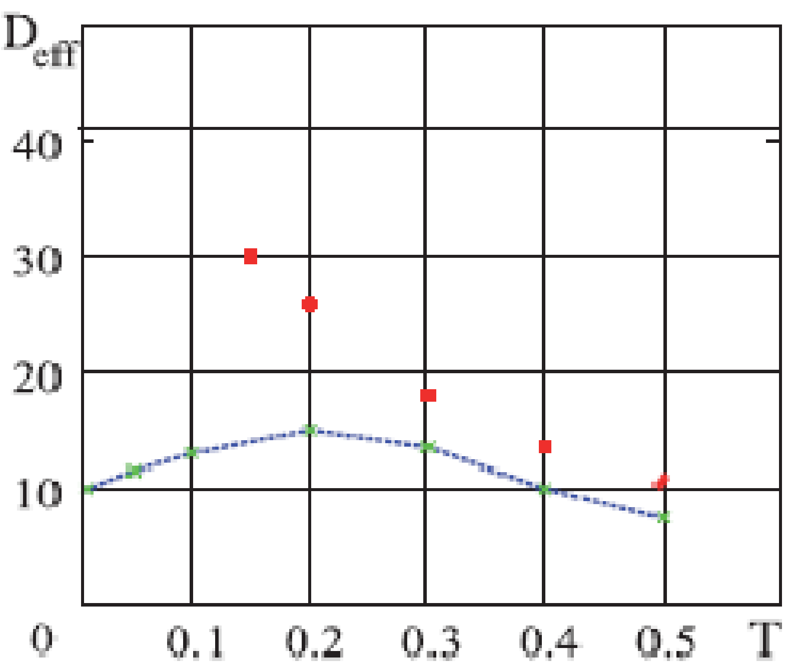
r.h.s Kohsaka: topogr curr dens in underdoped cuprates

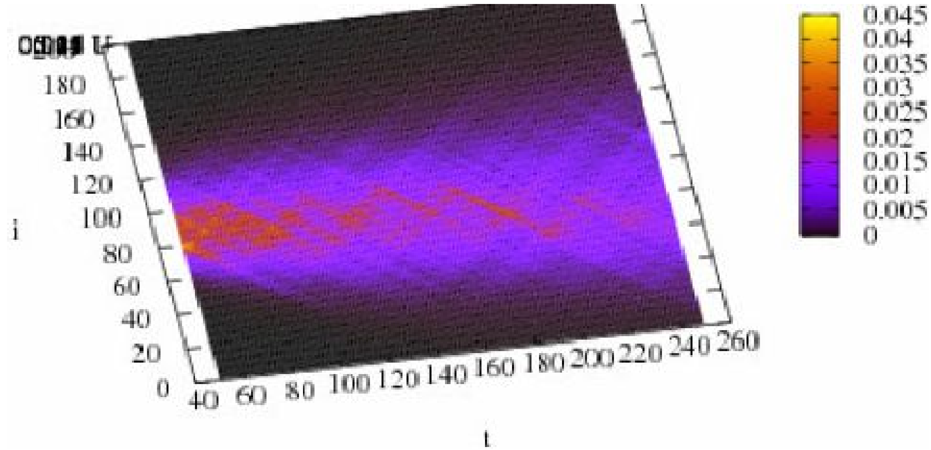




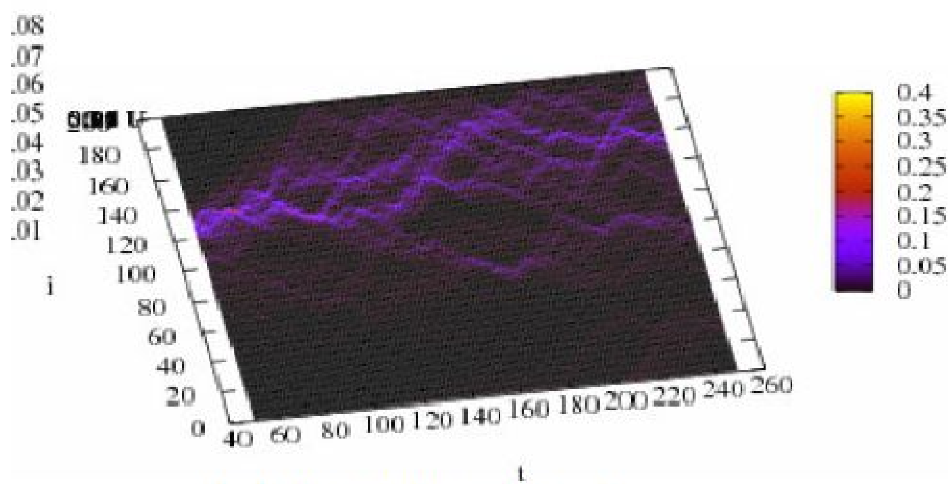
Diffusion and transport is modified by the new coherent electron dyn. riding - hopping

- D ~ <v v>
- increase of correlation times - incr of diffus





b) $T=0.01$ $\alpha=1$ $U_e=0.01$ $\tau=2$



d) $T=1$ $\alpha=1$ $U_e=0.01$ $\tau=2$

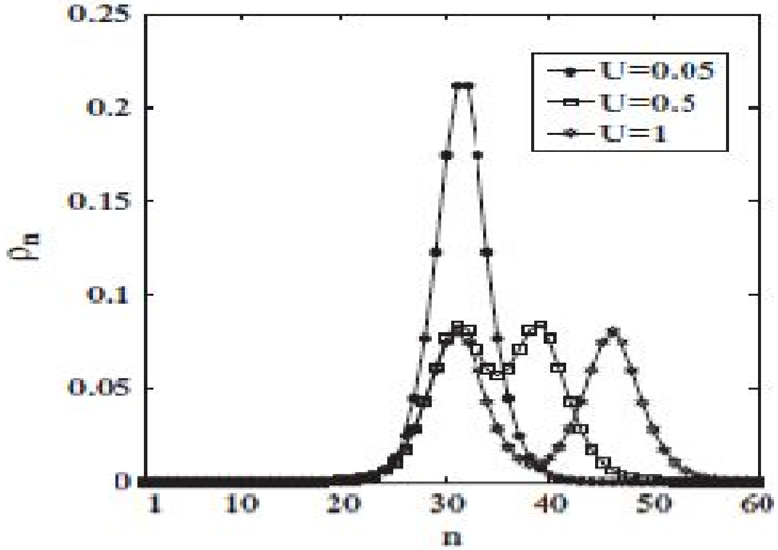
Solitons interacting with Hubbard pairs

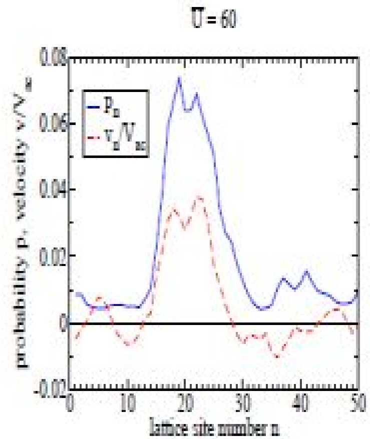
$$|\psi(t)\rangle = \sum_{m,n} \phi_{mn}(\{p_m\},\{q_m\})\,\hat{a}^+_{m\uparrow}\hat{a}^+_{n\downarrow}\,|0\rangle\ ,$$

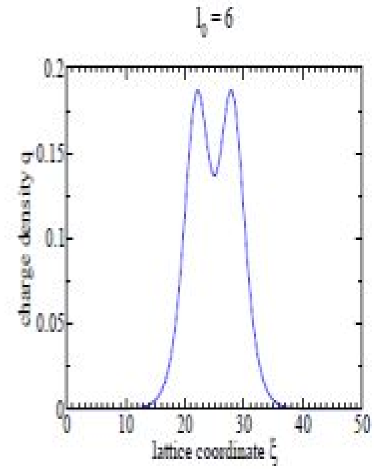
$$\begin{aligned} i\,\frac{d\phi_{mn}}{dt} = & -\tau\,\{\exp[-\alpha\,(q_{m+1}-q_m)]\,\phi_{m+1n} + \exp[-\alpha\,(q_m-q_{m-1})]\,\phi_{m-1n} \\ & + \exp[-\alpha\,(q_{n+1}-q_n)]\,\phi_{mn+1} + \exp[-\alpha\,(q_n-q_{n-1})]\,\phi_{mn-1}\} \\ & + \bar{U}\,\phi_{mn}\delta_{mn}, \end{aligned} \tag{45}$$

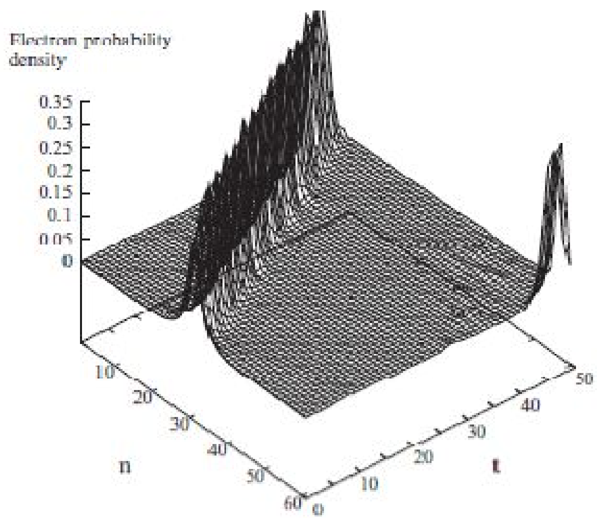
$$\begin{aligned} \frac{d^2q_n}{dt^2} = & \ [1-\exp\{-(q_{n+1}-q_n)\}]\exp[-(q_{n+1}-q_n)] \\ & -[1-\exp\{-(q_n-q_{n-1})\}]\exp[-(q_n-q_{n-1})] \\ & +\alpha V\exp[-\alpha\,(q_{n+1}-q_n)] \\ & \sum_m\{[\phi^*_{mn+1}\phi_{mn}+\phi^*_{mn}\phi_{mn+1}]+[\phi^*_{n+1m}\phi_{nm}+\phi^*_{nm}\phi_{n+1m}]\} \\ & -\alpha V\exp[-\alpha\,(q_n-q_{n-1})] \\ & \sum\{[\phi^*_{mn}\phi_{mn-1}+\phi^*_{mn-1}\phi_{mn}]+[\phi^*_{nm}\phi_{n-1m}+\phi^*_{n-1m}\phi_{nm}]\}\ . \end{aligned} \tag{46}$$

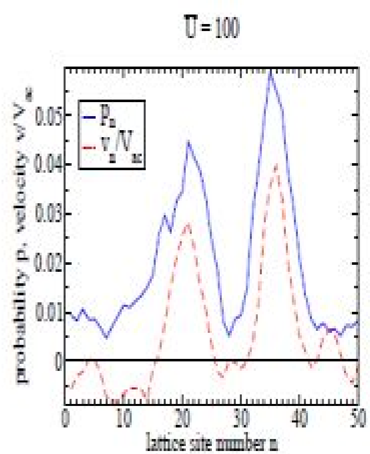
The pdf of electron pairs: depend on Hubb repulsion U + left below time evol alpha=1.75, V=.1, U=0.05

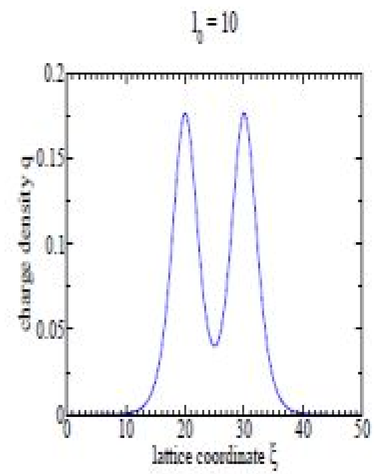






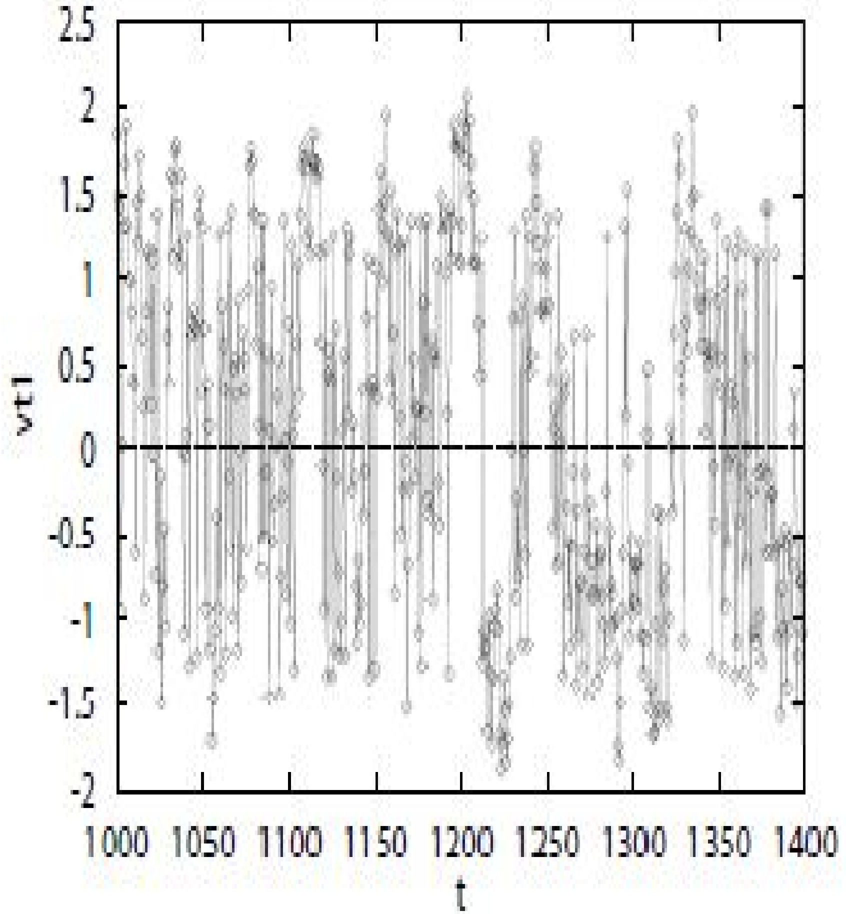




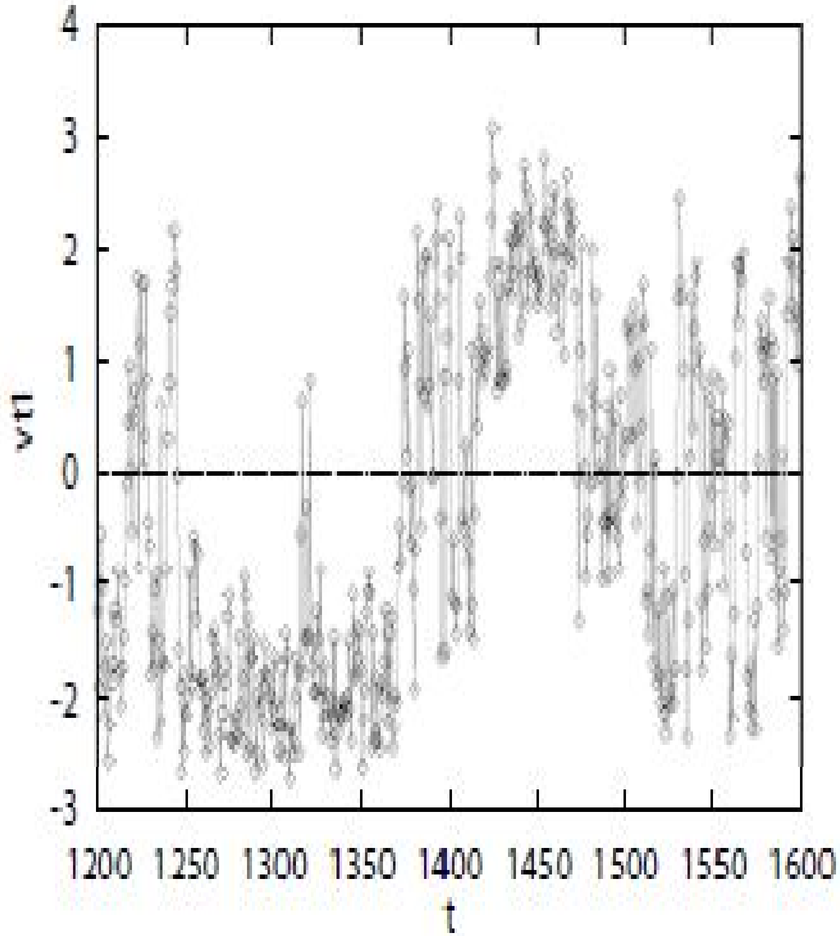


Momentum distributions FPE:
Study trajectories of velocity of thermal solectrons
in a 1d noise-heated lattice → velocity distributions

T=0.005



T=0.075.



Kinetic potential of quasi-classical solectrons = like driven Brownons

$$E(v) = \frac{M}{2}[v^2 - q\ln(1 - a|v| + dv^2)]$$

$$\frac{\partial P(v,t)}{\partial t} + eE\frac{\partial P}{\partial v} = B\left[\frac{\partial E(v)}{\partial v}P + kT\frac{\partial P}{\partial v}\right]$$

$$P_0(v) = C\exp[-\beta E(v)]$$

like driven Brownian particles, like ?

В жидком гелии закон дисперсии элементарных возбуждений имеет форму, изображенную на рис. 2: после начального линейного возрастания функция $\varepsilon(p)$ достигает максимума, затем

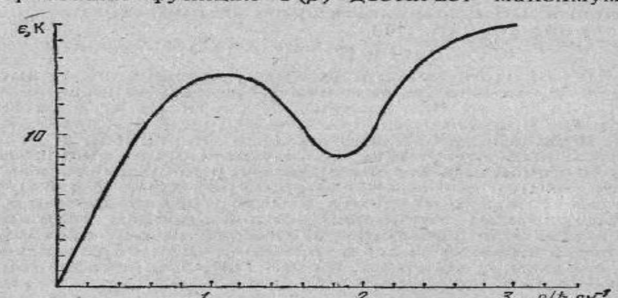
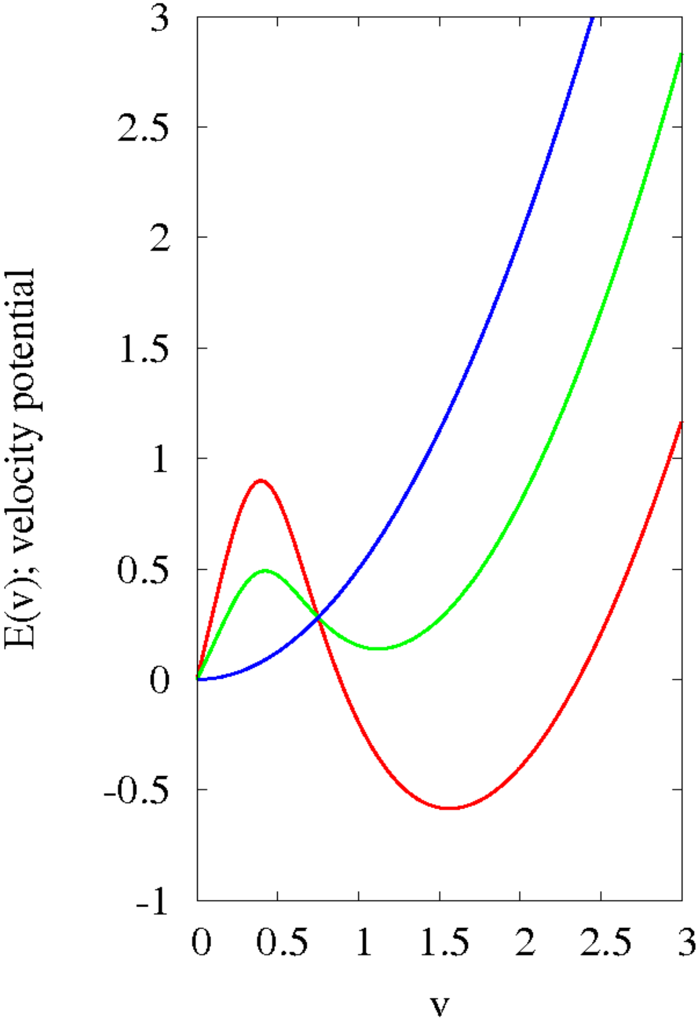


Рис. 2.

убывает и при определенном значении импульса p_0 проходит через минимум [1]). В тепловом равновесии большинство элементарных возбуждений в жидкости имеет энергии в областях вблизи минимумов функции $\varepsilon(p)$, т. е. в области малых ε (область вблизи $\varepsilon = 0$), и в области значения $\varepsilon(p_0)$. Поэтому именно эти области особенно существенны. Вблизи точки $p = p_0$ функция $\varepsilon(p)$



Fokker-Planck equations for qumech solectron-quasiparticles (Gogolin 88)

$$\frac{\partial f(p)}{\partial t} + eE\frac{\partial f(p)}{\partial p} =$$

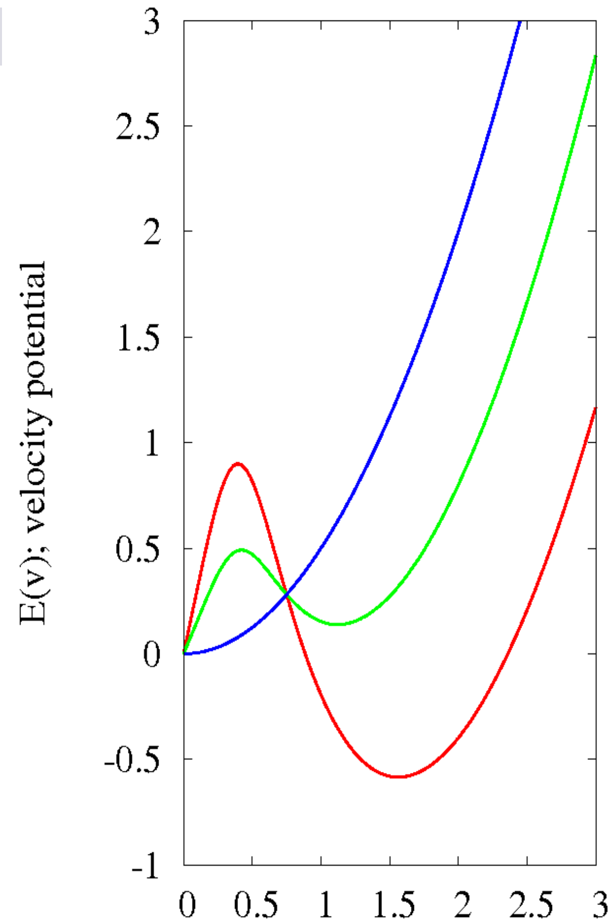
$$\frac{\partial}{\partial p}B(p)\left[\frac{\partial \varepsilon(p)}{\partial p} + \frac{1}{T}\frac{\partial f(p)}{\partial p}\right]$$

$$\varepsilon(p) = \frac{1}{2M}[p^2 - q\ln(1 - a|p| + dp^2)]$$

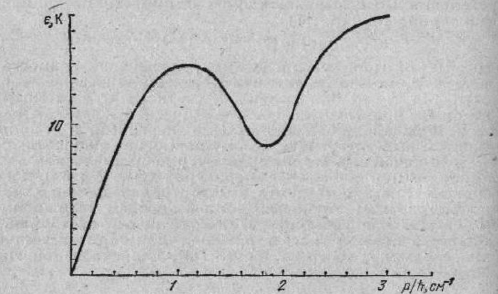
$$P_0(p) = C\exp[-\beta\varepsilon(p)]$$

like driven Brownian particles

or Landau rotons ?



В жидком гелии закон дисперсии элементарных возбуждений имеет форму, изображенную на рис. 2: после начального линейного возрастания функция $\varepsilon(p)$ достигает максимума, затем



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Ref on e-transfer, TBA, Hubbard pairs

- Chetverikov/Eb/Ve: Euro Phys J B, (2009-2012)
- Eb/Velarde/Ebeling/Chetverikov/Hennig: Anharmonicity and soliton-mediated transp In: Russo/Antonchenko/Kryachko Springer (2009)
- Brizhik et al., PRE (2012)
- Hennig et al.Phys.Rev B 73(2006) 024306, Phys.Rev. E 76(2007)046602;78(2008)066606
- Velarde et al.: Int.J. Bifurc.&Chaos 18(2008) 19(2009), Int.J.Quant.Chem.(2009-2011)

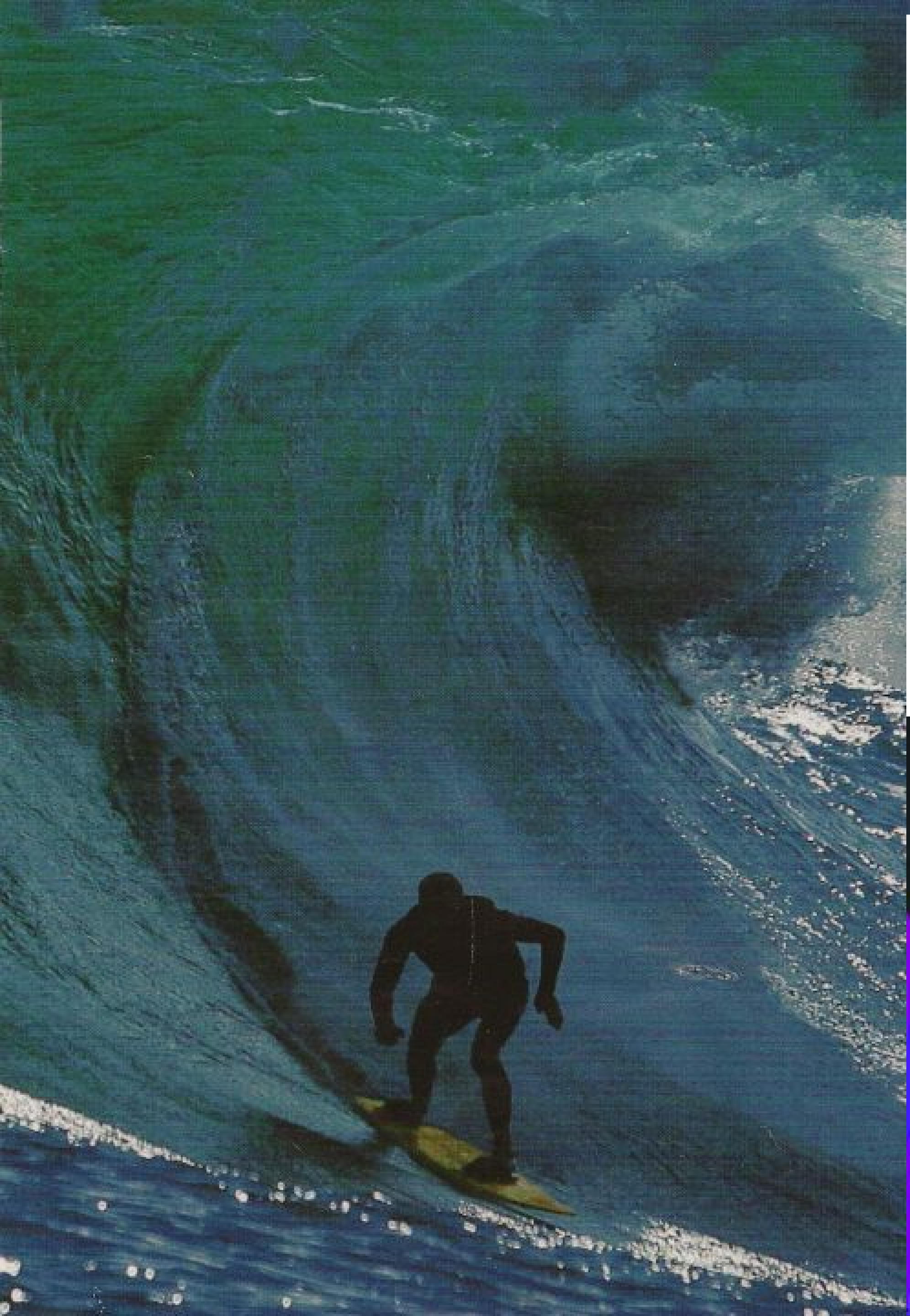
Conclusion:

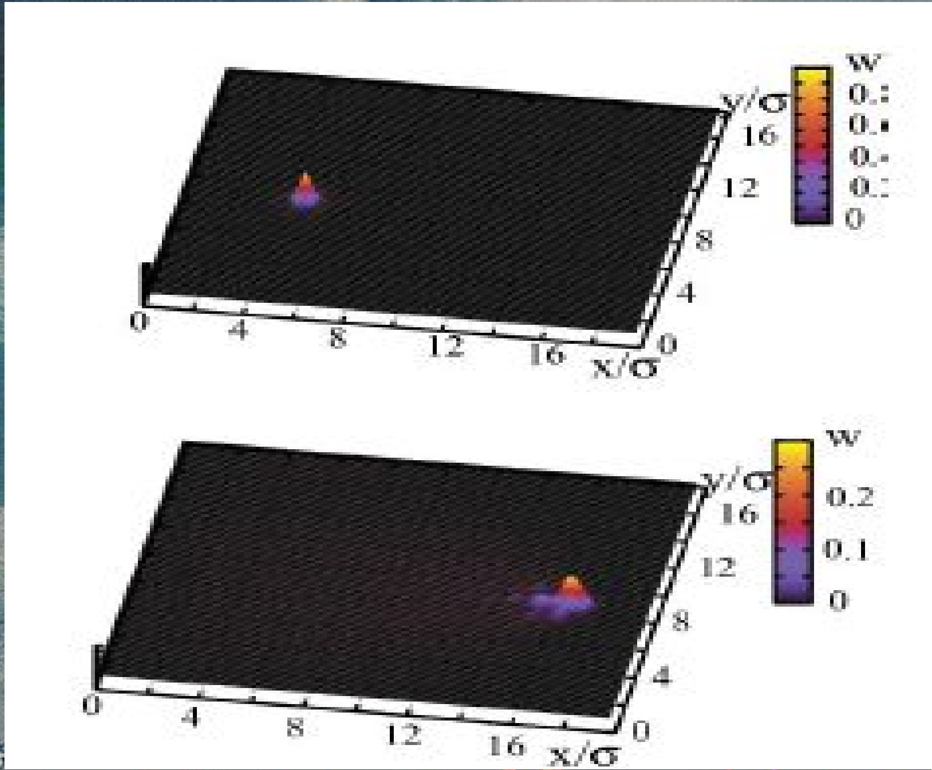
- Not only at T=0 but also at moderate T the effects of dispersion / incoherence of electron wave functions can be suppressed by nonlinear compression waves (electron is guided by solitons or loc nonlin sound waves)
- New quasiparticles (solectrons) first described by Davydov = localized fastly moving charges (supersonic ~several km / sec in solid)
- Electrons coupled to the lattice/fluid excitations may ride coherently several ps on the solitons like surfers. Electron diff/transport=enhanced.

Thank you for attention!

Thanks to L. Brizhik, L. Cruzeiro, D. Hennig, C.Neissner, G.Vinogradov, G. Wilson for discussions and collaboration

to the EU-project SPARK II FP 7-ICT and to the Spanish project EXPLORA FIS09 MAT11 for support

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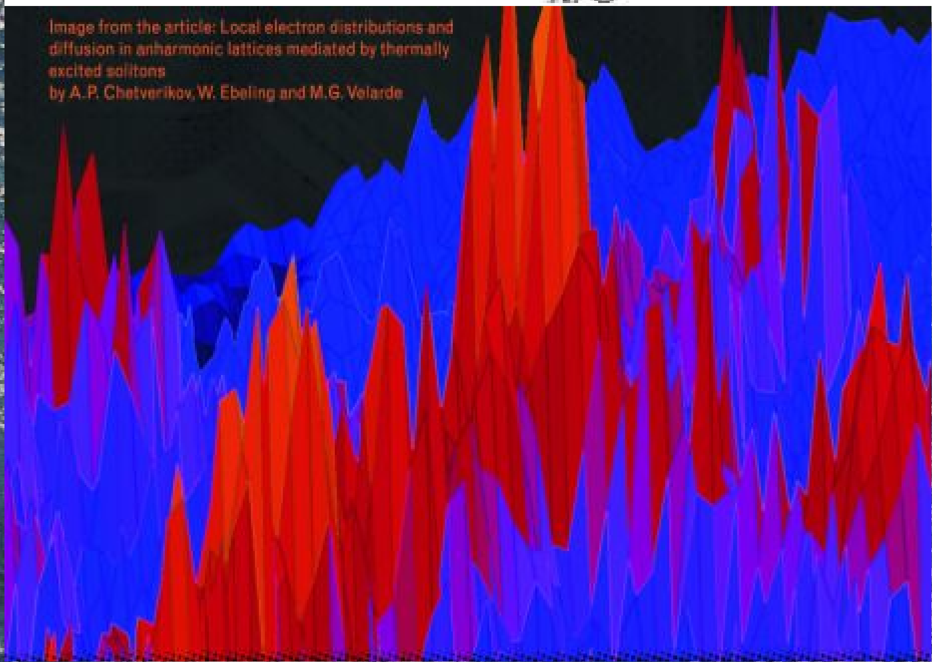
Image from the article: Local electron distributions and diffusion in anharmonic lattices mediated by thermally excited solitons
by A.P. Chetverikov, W. Ebeling and M.G. Velarde