Wigner thermoelectricity and interactions

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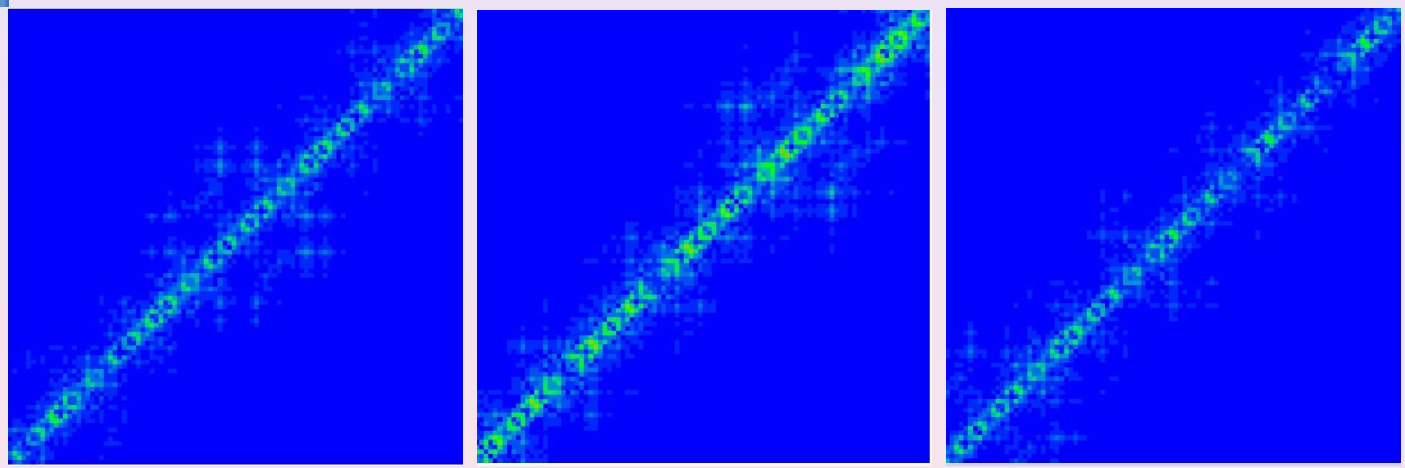
- meeting with JLP: Varenna School on Quantum chaos (1991); visit to SPEC CEA (1992)
- Two-interacting particles (TIP): from (1995) discussions at SPEC with JLP group K.Frahm, A.Muller-Groeling, D.Weinmann; discussions with Y.Imry; continued at SPEC, Toulouse ... till March 2015 Luchon Superbagneres
- TIP in the Harper model (with Klaus Frahm)
- Thermoelectricity of Wigner crystal in a periodic potential (with O.Zhirov, I.Garcia-Mata, J.Lages)

Support: LABEX NEXT THETRACOM project (disruptive)

Can two walk together, except they be agreed? (Amos 3:3) as questioned by Y.Imry

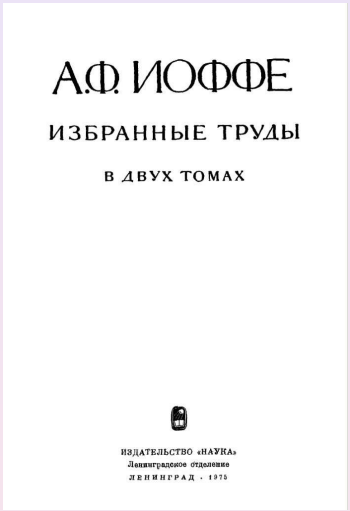
$H\psi_n = \lambda \cos(\alpha n + \beta)\psi_n + (\psi_{n-1} + \psi_{n+1}) = E\psi_n$;
Aubry-Andre (1980) $\rightarrow$ only localized states at $\lambda > 2$,
1d,2d Harper model for TIP
with Hubbard interaction U, $\lambda = 2.5$ (instead of disorder):
$\rightarrow$ delocalized TIP, $U = 4.5$, $E = -3.09$

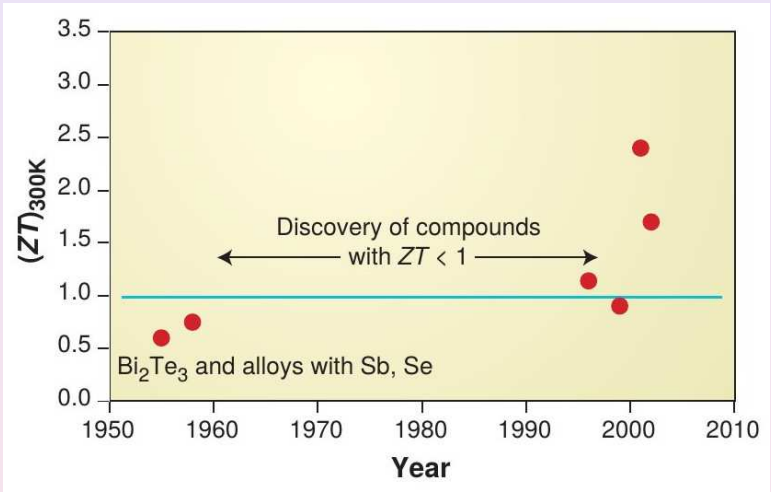


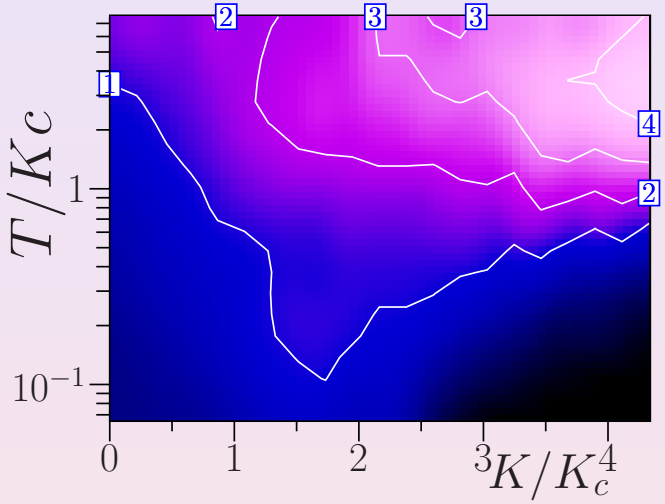
density snapshots at $n = 0, 5000, 10000$, zoom 100×100 sites
quasi-ballistic states Frahm, DS EPJB (2015)
(also $\rightarrow$ model DS PRB (1994), TIP delocalization Flach et al. EPL (2012))
TIP in 2d $\rightarrow$ subdiffusive spreading $(\Delta n)^2 \propto t^{0.5}$ (Frahm, DS EPJB (2016))
Chaons $\rightarrow$ delocalization and diffusion of classical TIP due to chaos 1d, 2d (DS EPJB (2016)); Bloch group cold atoms exp Science **349**, 842 (2015)

Thermoelectricity at nanoscale: theoretical models

main scentific interest of Jean-Louis Pichard in last years

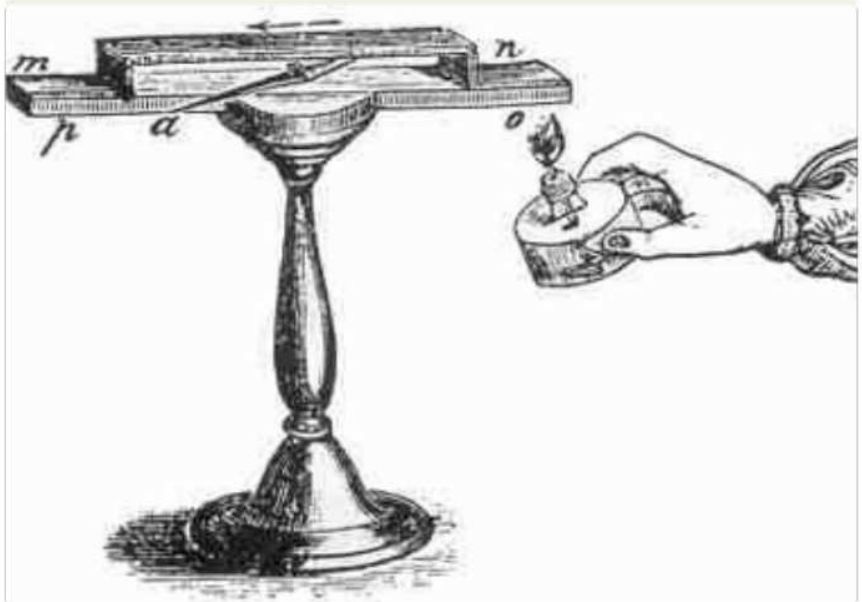






Left: A.F.Ioffe book (1956)
Center: figure of merit *ZT* with time (A.Majumdar Science **303**, 777 (2004))
Right panel: ZT diagram (Zhirov, DS EPL **103**, 68008 (2013))

Early works



T. Seebeck-deflection of a compass needle (circa 1823)

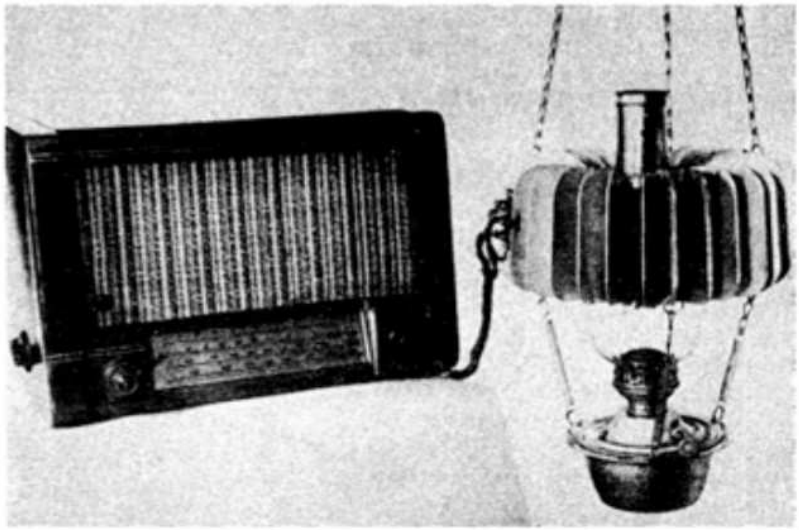
from Y.Imry (Weizmann Inst) talk at Inst. H. Poincaré, Paris (2012)

Early works

A. F. Ioffe

semiconductors

and figure of merit



Oil burning lamp powering a radio using the first commercial thermoelectric generator containing ZnSb built in USSR, circa 1948

from Y.Imry (Weizmann Inst) talk at Inst. H. Poincaré, Paris (2012)

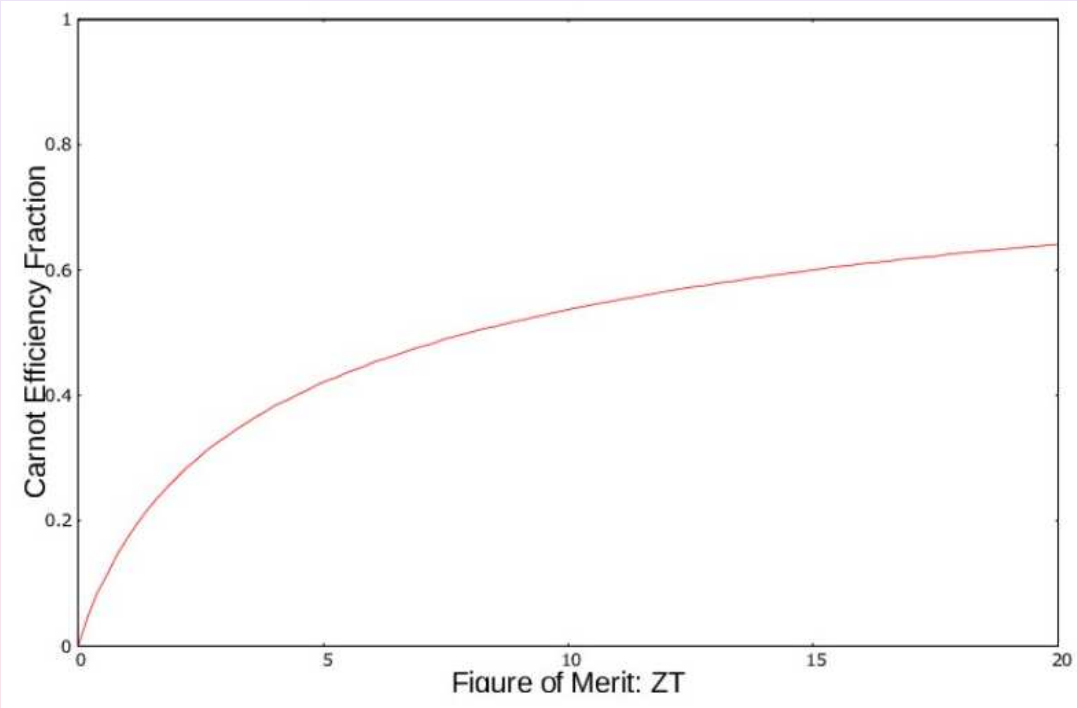
Main characteristics

Seebeck coefficient:

$S = \Delta V/\Delta T = \pi^2 {k_B}^2 T[(d \ln \sigma/dE)]|_{E_F}/e$ (Mott relation (1958))

For 2DEG with Wiedemann-Franz law: $S = 2\pi {k_B}^2 Tm/(3eh^2 n_e)$;

typical value $S \approx 10\mu V/K$ at $T = 0.3K$, $n_e = 4 \cdot 10^{10} cm^{-2}$



Thermoelectric figure of merit $ZT = \sigma S^2 T/\kappa$,

thermoefficiency $\eta_{max} = \eta_{Carnot}(\sqrt{ZT+1}-1)/(\sqrt{ZT+1}+1)$

thermal conductivity $\kappa = \kappa_{el} + \kappa_{phonon}$ (heat flux $Q = -\kappa \bigtriangledown T$)

Experiments on Seebeck coefficient for 2DEG

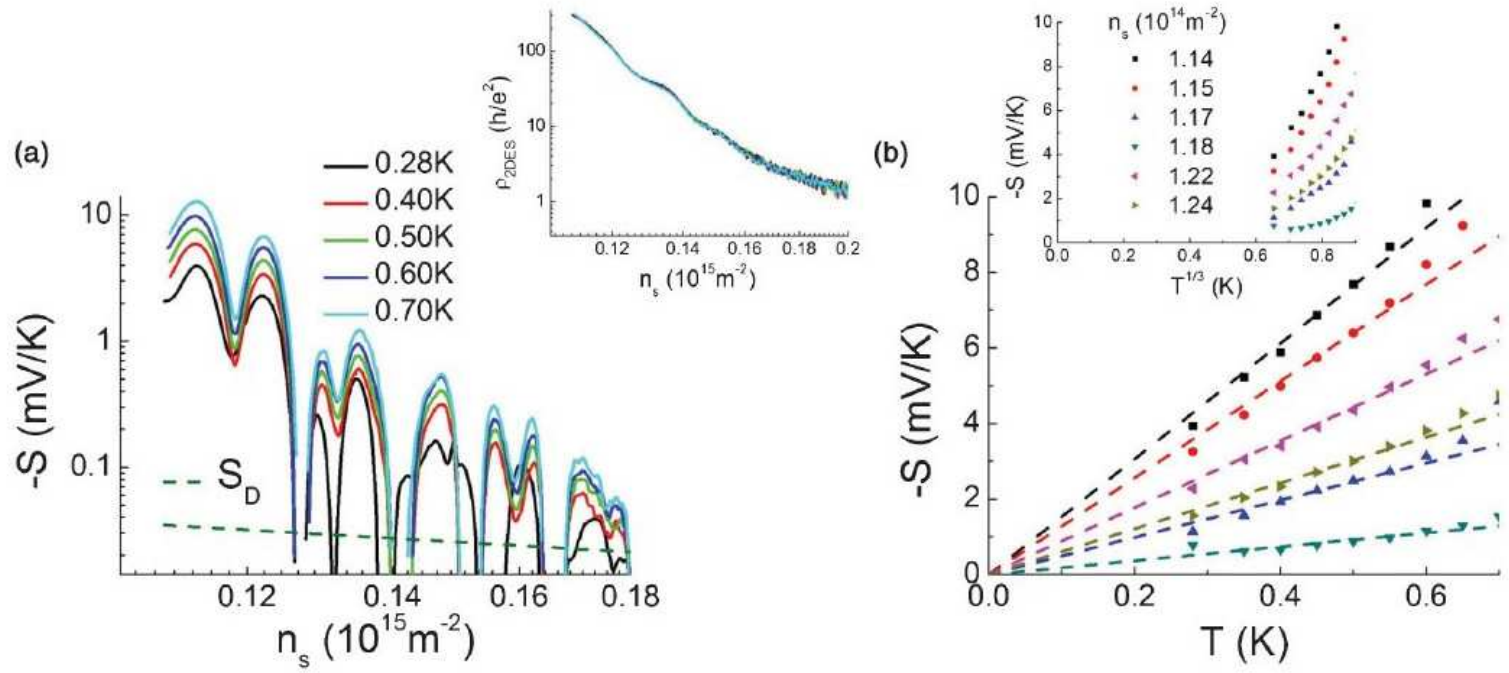
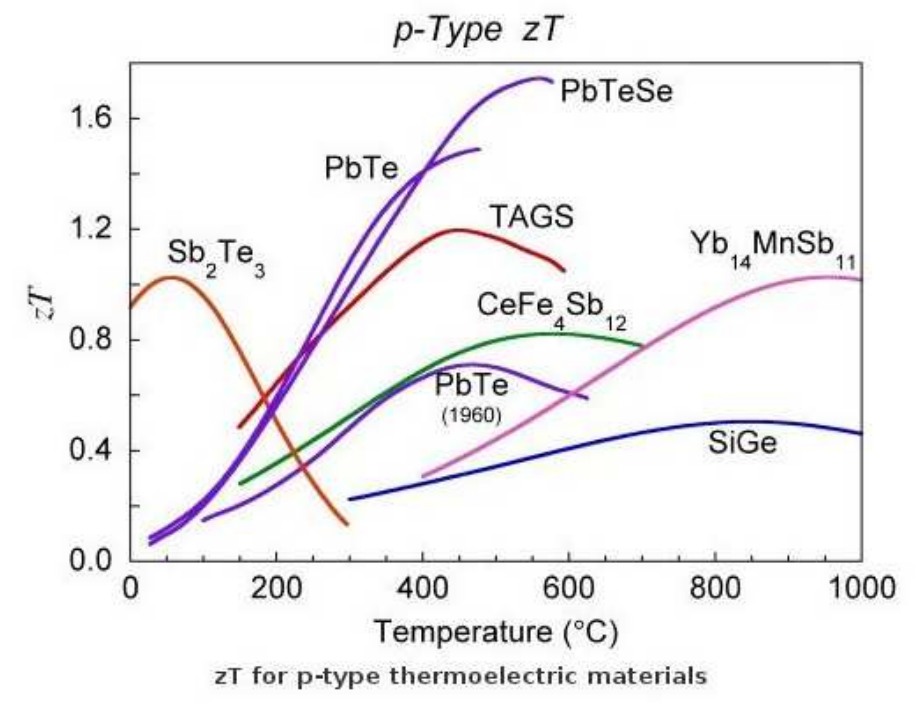


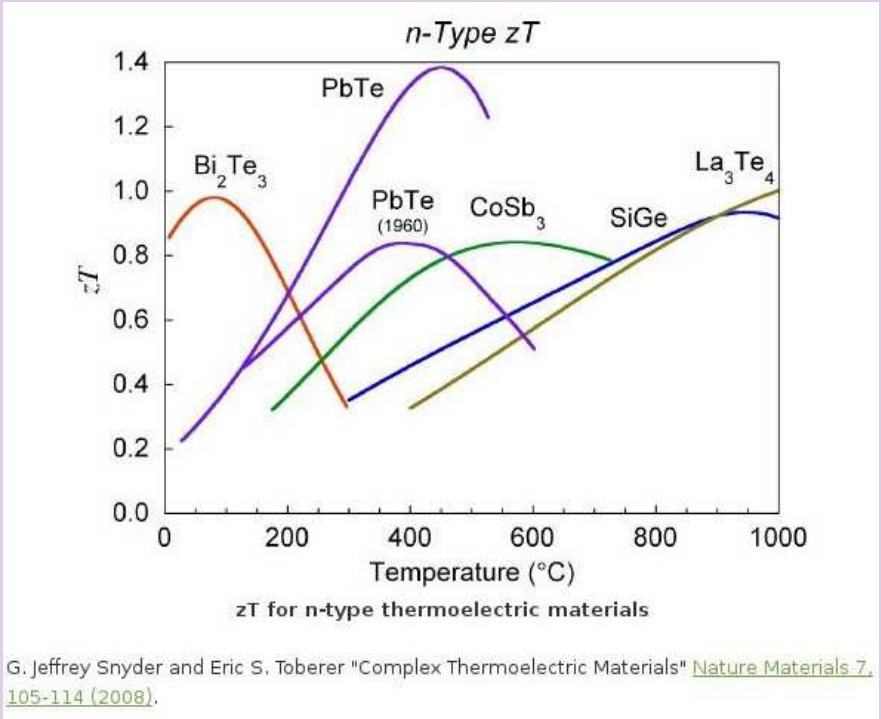
FIG. 5. (Color online) (a) S vs n_s for 0.28 K $< T <$ 0.7 K. The broken green line shows S_d [Eq. (2)] at 0.28 K. Inset: ρ_{2DES} vs n_s at the same T values; there is little T dependence in this range. (b) Low-T linear variation of S. Inset: Descriptions based on variable-ranged hopping, where S is expected to decay to zero as $T^{1/3}$, do not adequately describe the observed data.

V.Narayan, S.Goswami, M.Pepper et al. PRB **85**, 125406 (2012)

In dimensionless units $S = 10mV/K \approx 100 \gg 1$ ($e = k_B = 1$)

ZT in various materials





from http://www.thermoelectrics.caltech.edu/thermoelectrics/

ZT in *SnSe*

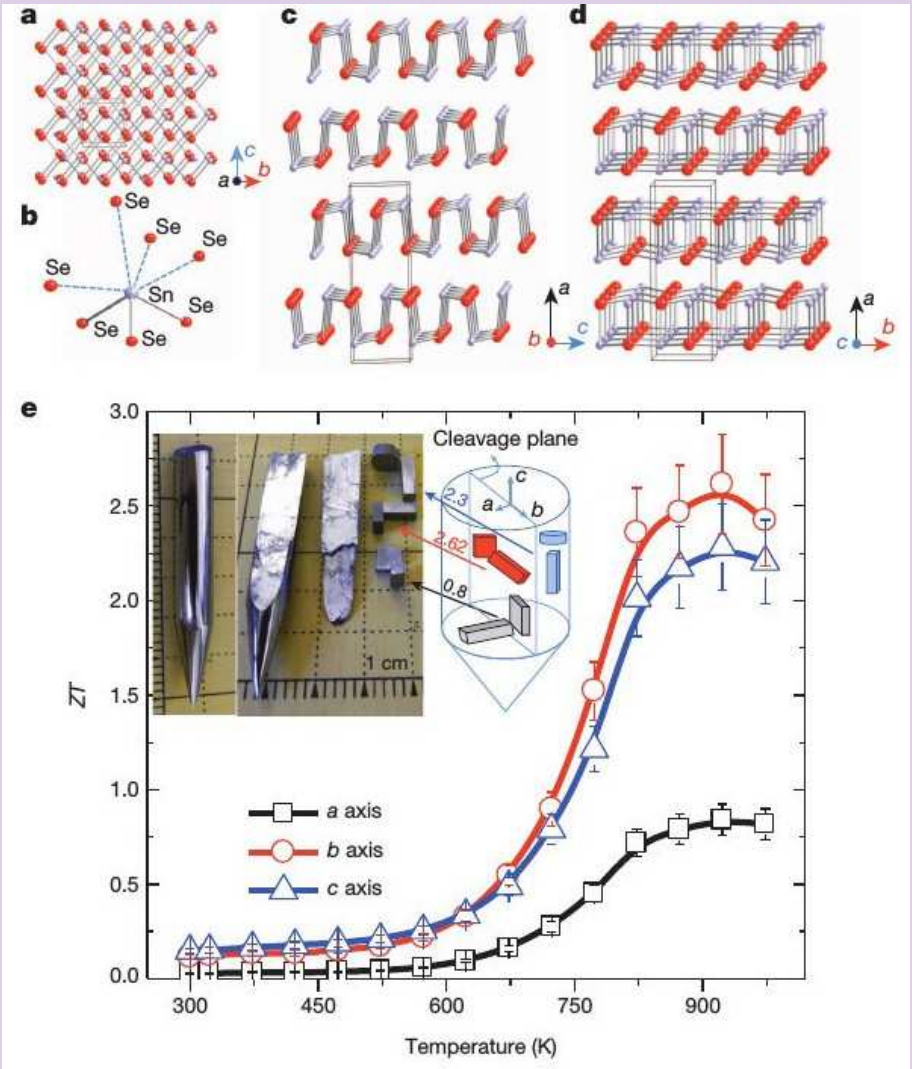


Figure 1 | SnSe crystal structure *Pnma* and *ZT* values. **a**, Crystal structure along the *a* axis: grey, Sn atoms; red, Se atoms. **b**, Highly distorted $SnSe_7$ coordination polyhedron with three short and four long Sn–Se bonds. **c**, Structure along the *b* axis. **d**, Structure along the *c* axis. **e**, Main panel, *ZT* values along different axial directions; the *ZT* measurement uncertainty is about 15% (error bars). Inset images: left, a typical crystal; right, a crystal cleaved along the (l00) plane, and specimens cut along the three axes and corresponding measurement directions. Inset diagram, how crystals were cut for directional measurements; *ZT* values are shown on the blue, red and grey arrows; colours represent specimens oriented in different directions.

Li-Dong Zhao et al. (Illinois) Nature **508**, 373 (2014)

Applications

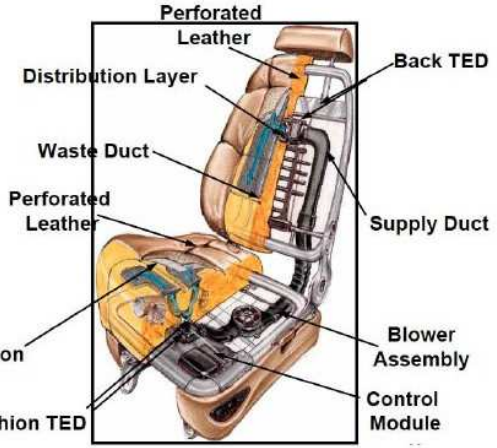
from Thermoelectric Workshop, Cargese (2012) organized by Jean-Louis

TE Applications are mostly 'Niche' Applications

-Laser, PCR

CITIZEN
Eco-Drive Thermo
Watch

Production CCS
Assembly



today…

POWER SOURCE
- Batteries

CLIMATE CONTROL
- None

Enabled by
Thermoelectrics (TE)

…tomorrow

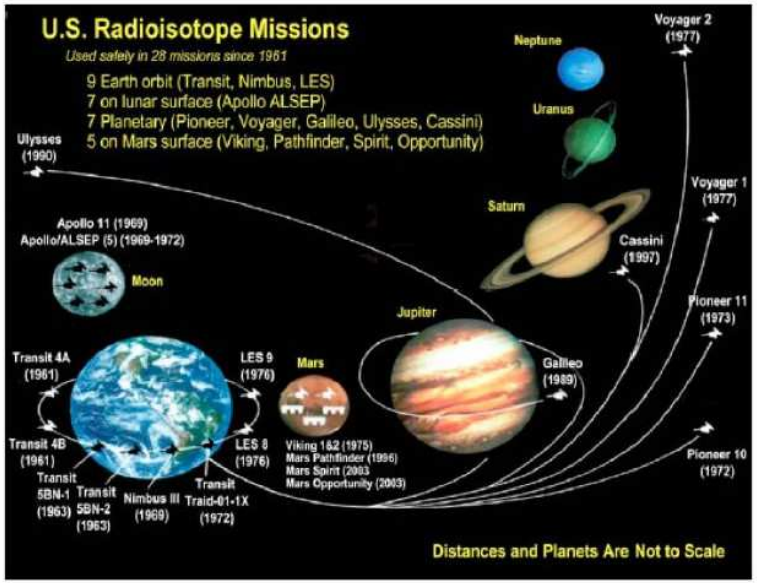
POWER SOURCE
- Logistic fuel based system

CLIMATE CONTROL
- Thermoelectric based cooling/heating
- On-demand

IMPACT
- >30% weight savings over existing systems

Assumptions
12 hour mission @ 110°F ambient temperature

DARPA TTO Program Manager: Ed van Reuth



Frenkel-Kontorova model (ZhETF 1938)

Chirikov standard map (1969-1979); Aubry transition $K > K_c = 0.9716$ (1983)

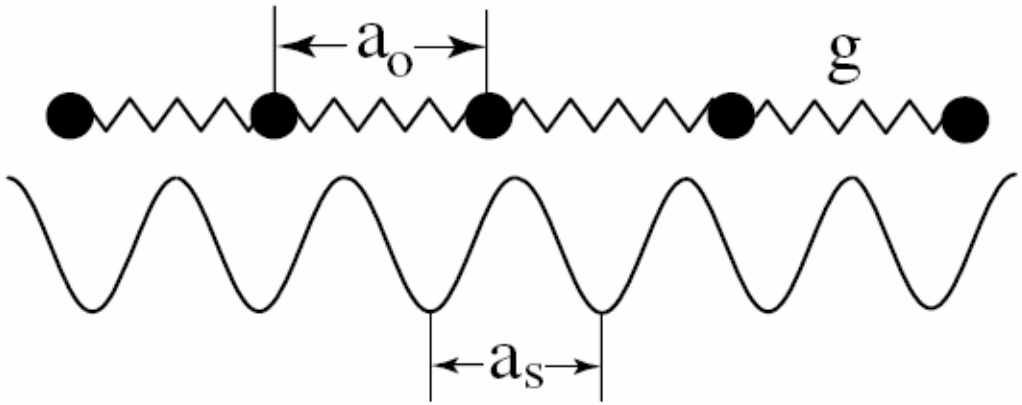


Fig. 1.1. Schematic presentation of the Frenkel-Kontorova model: A chain of particles interacting via harmonic springs with elastic coupling g is subjected to the action of an external periodic potential with period a_s.

Introducing the dimensionless variables, we re-write the Hamiltonian (1.1)–(1.5) in the conventional form ($H = 2\mathcal{H}/\varepsilon_s$)

$$H = \sum_n \left\{ \frac{1}{2}\left(\frac{dx_n}{dt}\right)^2 + (1 - \cos x_n) + \frac{g}{2}\left(x_{n+1} - x_n - a_0\right)^2 \right\}, \qquad (1.8)$$

fixed particle density $\nu = 0.618...$ $\rightarrow$ golden KAM curve

O.M.Braun and Yu.S.Kivshar, *The Frenkel-Kontorova model ...* Spriner (2004)

Wigner crystal in a periodic potential

The dimensionless Hamiltonian has the form:

$$H = \sum_{i=1}^{N} \left(\frac{P_i^2}{2} - K \cos x_i \right) + \sum_{i>j} \frac{1}{|x_i - x_j|} \qquad (1)$$

where P_i, x_i are ion momentum and position, K gives the strength of optical lattice potential and all N ions are placed in a harmonic potential with frequency ω. To make a transfer from (1) to dimensional physical units one should note that the lattice constant d in $K \cos(x_i/d)$ is taken to be unity, the energy $E = H$ is measured in units of ion charge energy e^2/d. In the quantum case $P_i = -i\hbar\partial/\partial x_i$ with dimensionless $\hbar$ measured in units $\hbar \to \hbar/(e\sqrt{md})$, m is charge mass.

Related map:

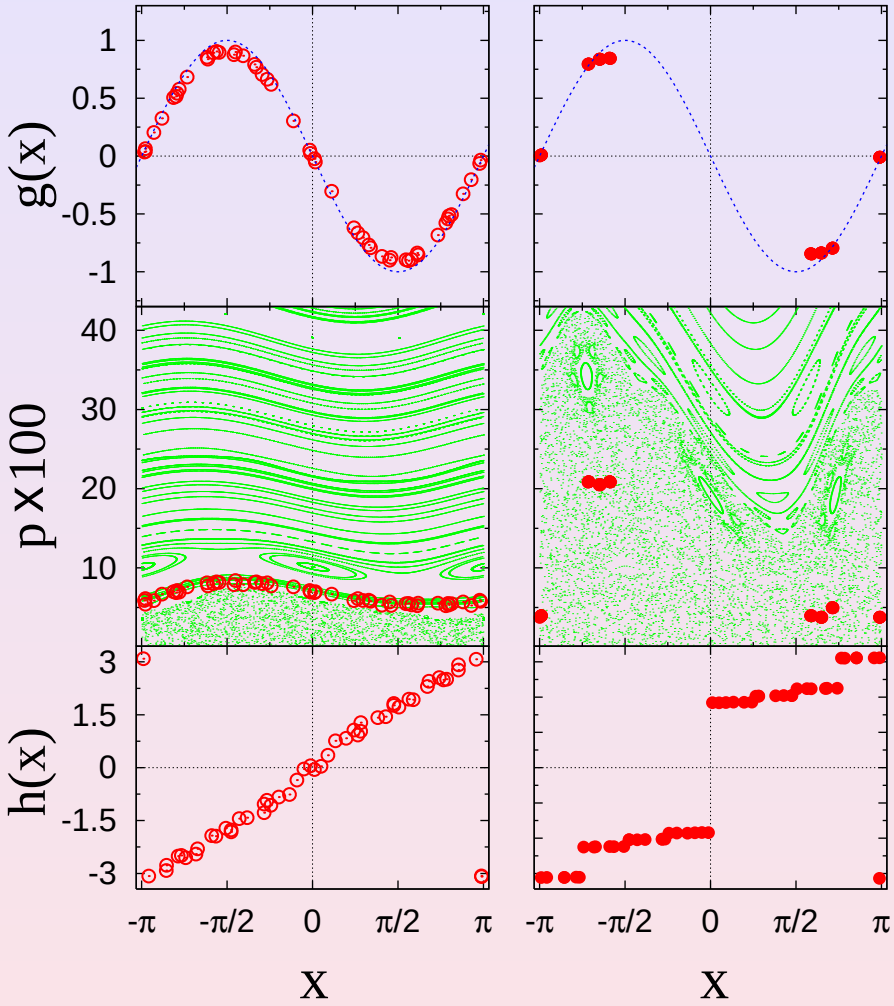
$$p_{i+1} = p_i + Kg(x_i) \ , \quad x_{i+1} = x_i + 1/\sqrt{p_{i+1}} \ , \qquad (2)$$

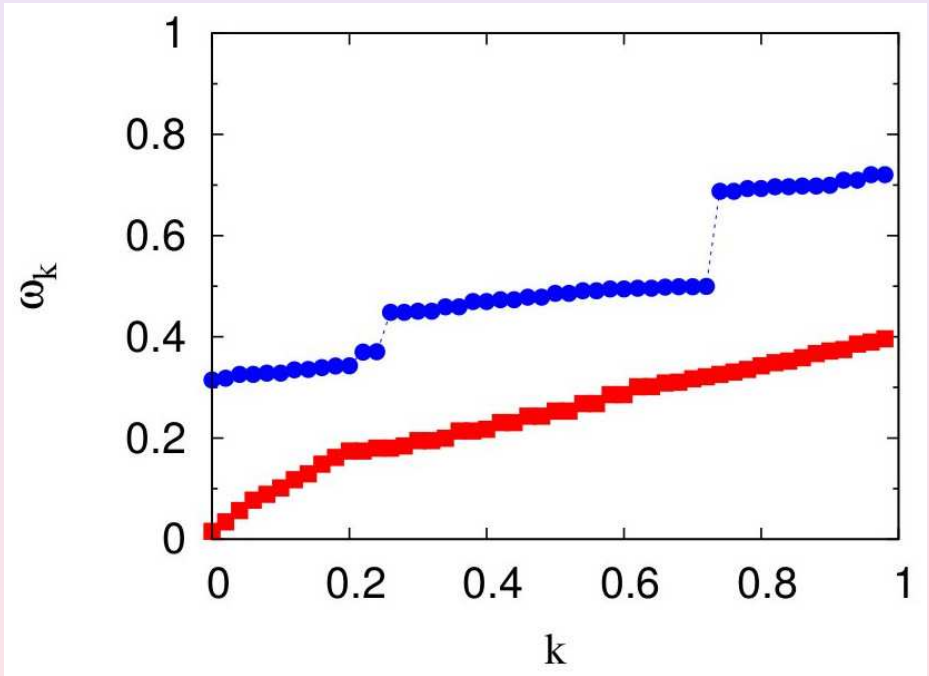
where the effective momentum conjugated to x_i is $p_i = 1/(x_i - x_{i-1})^2$ and the kick function is $Kg(x) = -K \sin x$.

For the Frenkel-Kontorova model the equilibrium positions are described by the Chirikov standard map (1969-1979): $p_{i+1} = p_i + K \sin x_i, \ x_{i+1} = x_i + p_{i+1}$ with $K_c = 0.971635...$ for the golden mean density $\nu = (\sqrt{5}+1)/2$.

I.Garcia-Mata, O.V.Zhirov, D.S. EPJB **41**, 325 (2007) $\to K_c = 0.046$ *vs.* 0.034

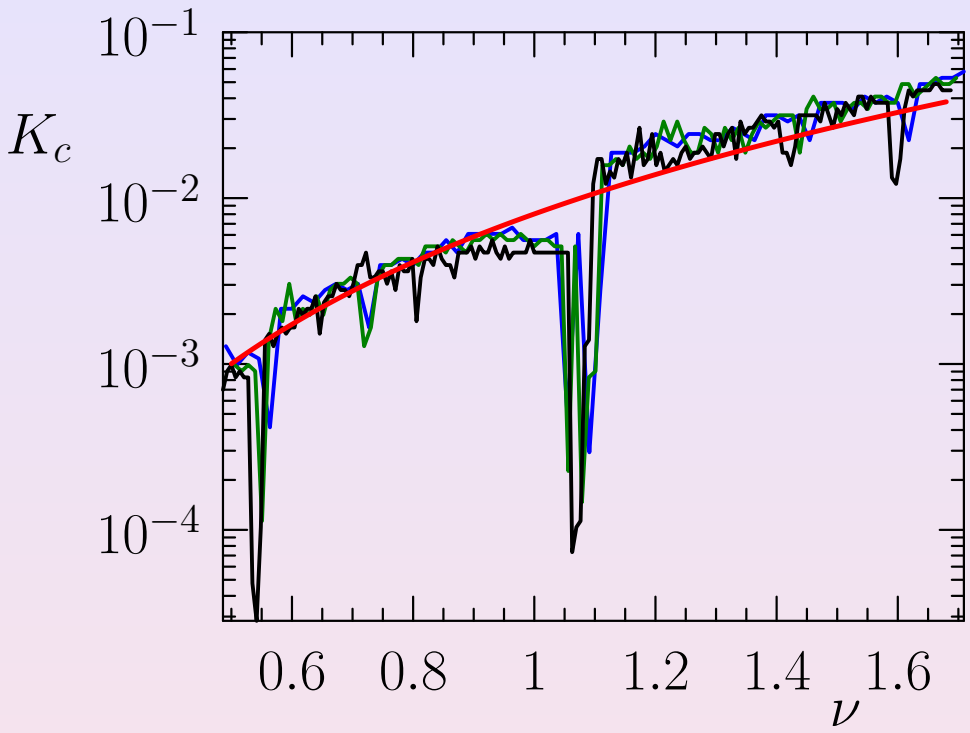
Classical Wigner crystal: map, spectrum





$N = 150$ ions in oscillator potential (central part) at $K = 0.03$ (left/red), $K = 0.2$ (right/blue); $\nu \approx 1.618$

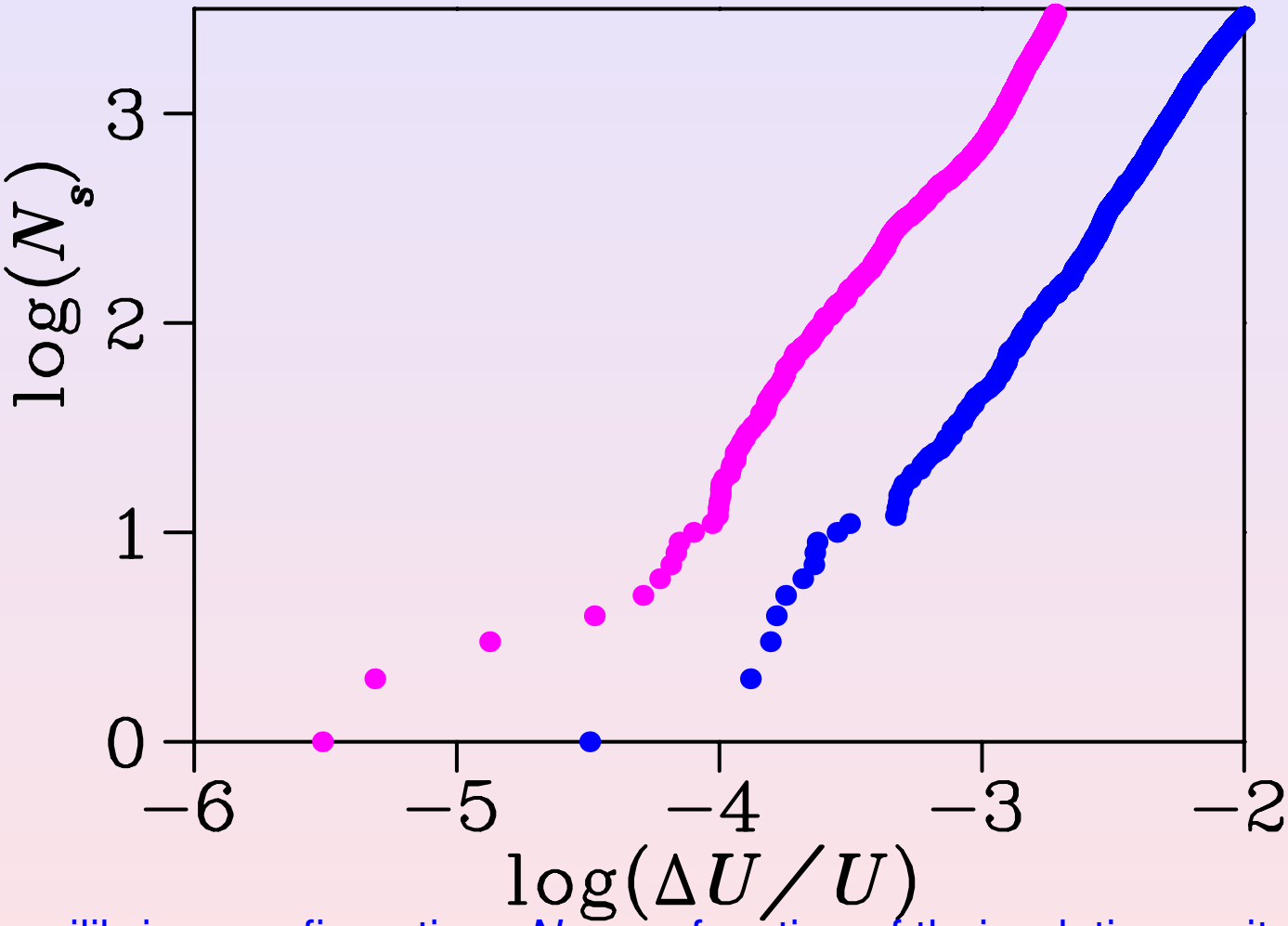
Density dependence of Aubry transition



Linearized approximation by the Chirikov standard map gives
$K_c = 0.034(\nu/1.618)^3$
Numerical data for number of wells $N_w = 55, 89, 144$ and varied number of ions N_{ions} with $\nu = N_{ions}/N_w$;
red curve is from the Chirikov standard map approximation
Zhirov, Lages, DS (in progress 2018)

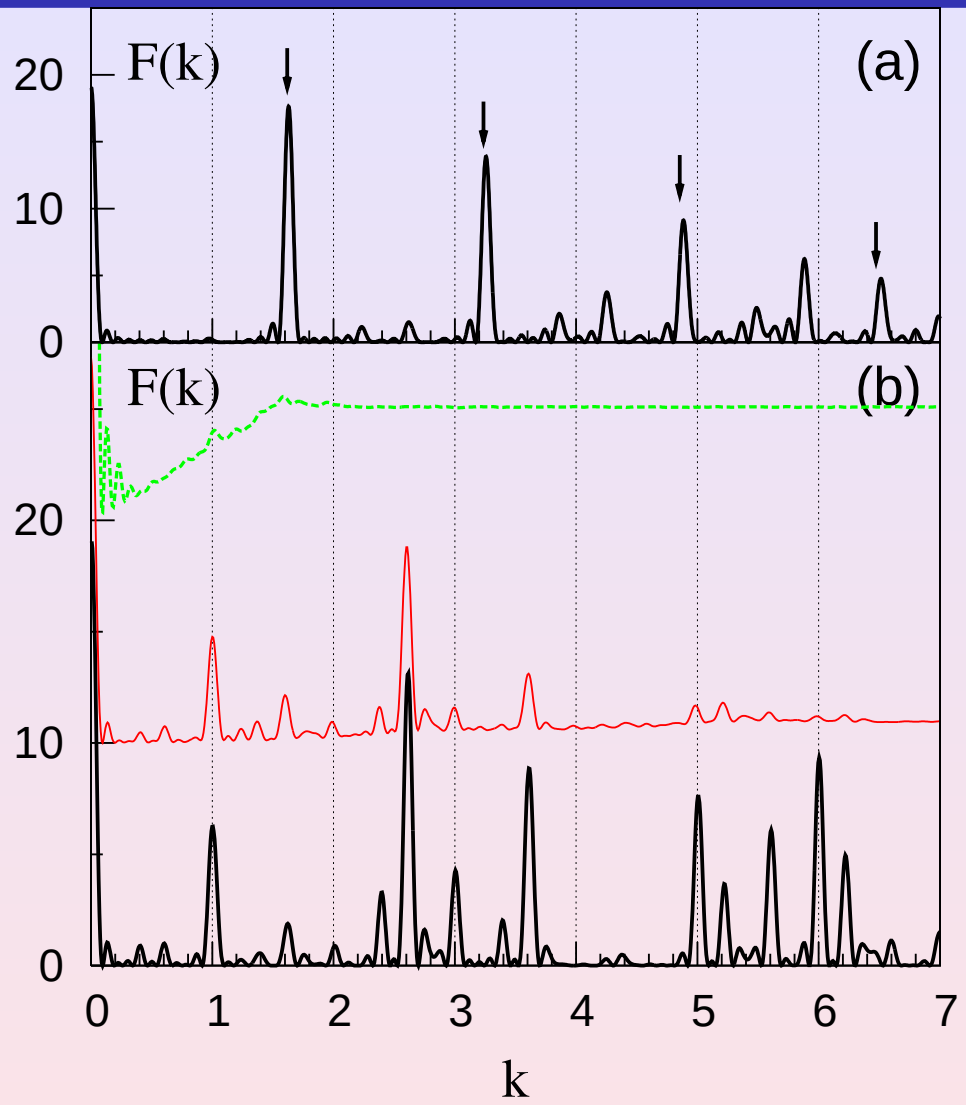
Dynamical spin-glass in Aubry pinned phase

Quantum Monte Carlo computations



Number of equilibrium configurations N_s as a function of their relative excitation energy $\Delta U/U$ above the ground state for 50 (blue) and 150 (magenta) ions at $K = 0.2$ (logarithms are decimal).

Quantum melting of Wigner crystal



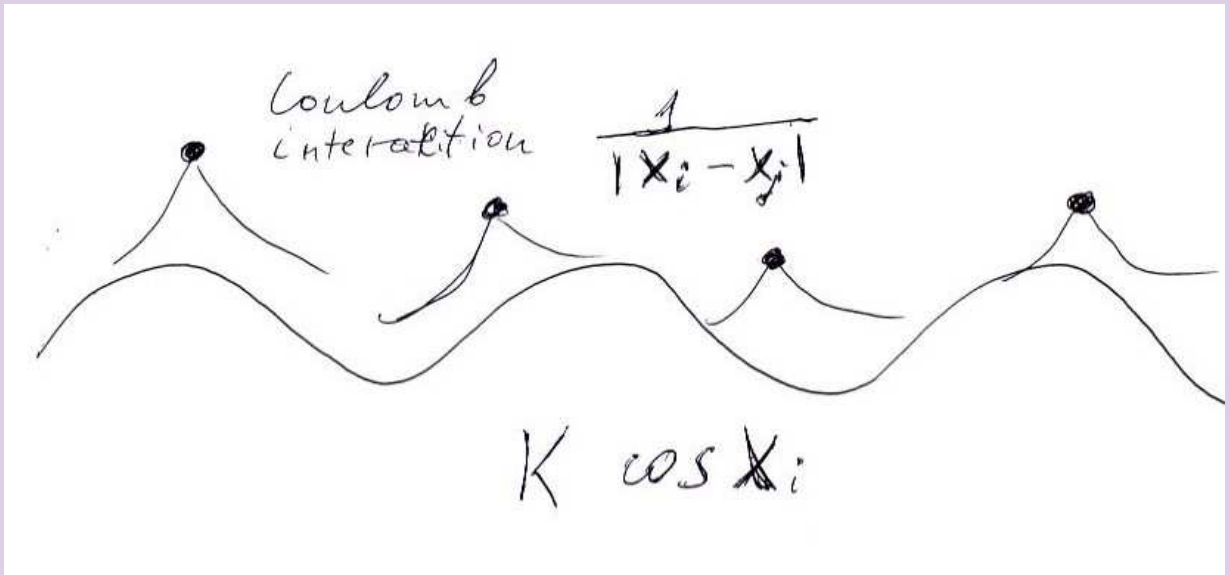
Formfactor of charge density

$F(k) = < |\sum_j \exp(ikx_j(\tau))|^2 >$

(a) The classical incommensurate phase at $K = 0.03$, $\hbar = 0$, arrows mark the peaks at integer multiples of golden mean density ν_g. (b) The pinned phase case at $K = 0.2$ for $\hbar = 0$ (bottom black curve), $\hbar = 0.1$ (red curve shifted 10 units upward), $\hbar = 2$ (green curve shifted 20 units upward, for clarity $F(k)$ is multiplied by factor 5); temperature is $T = \hbar/400 \ll K$. The quantum phase transition takes place at $\hbar_c \approx 1$.

$\rightarrow$ **SLIDING at $\nu_{c1} < \nu$, PINNING at $\nu < \nu_{c1}$**

Thermoelectricity of Wigner crystal in a periodic potential



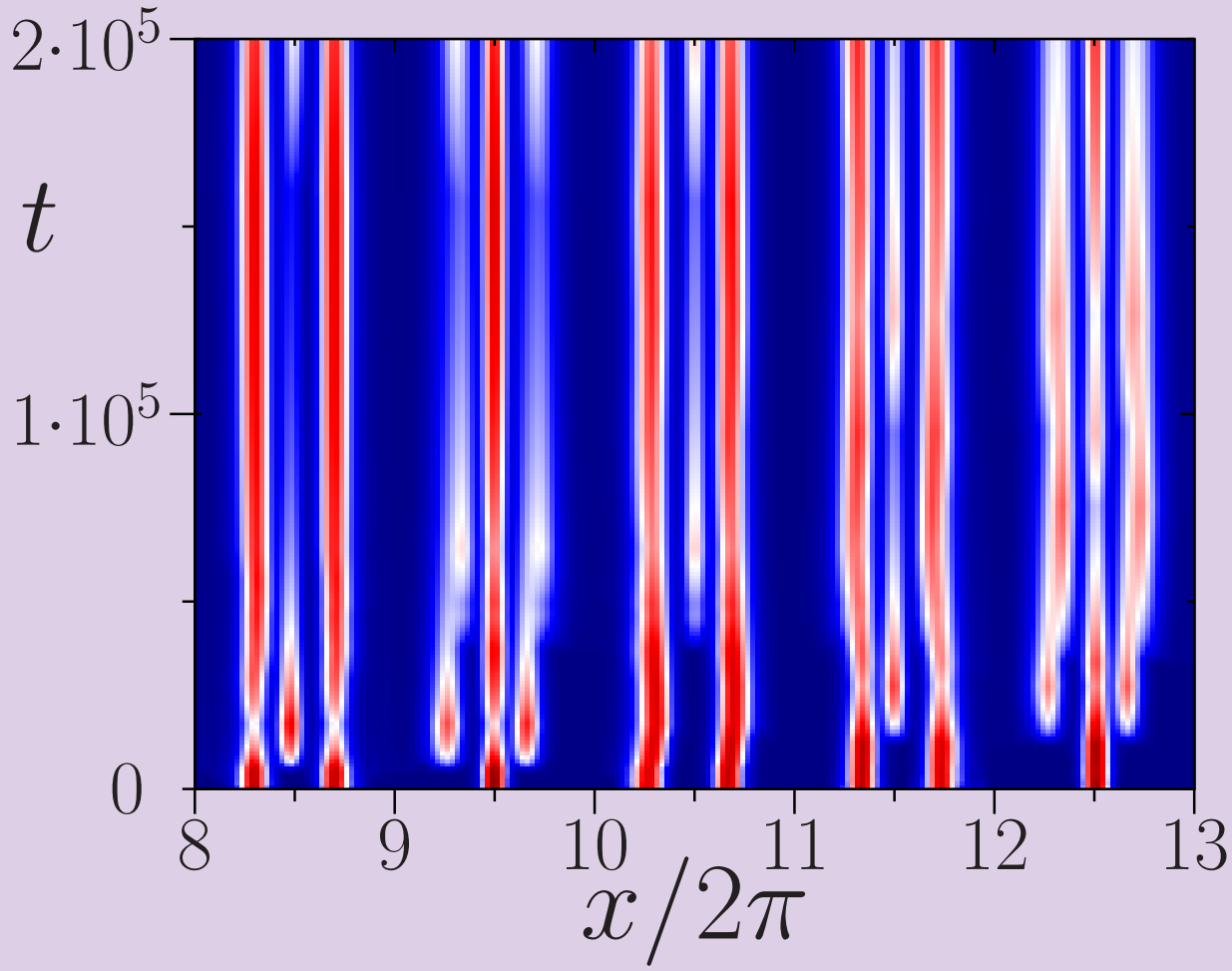
Hamiltonian $H = \sum_i \left(\frac{p_i^2}{2} + K \cos x_i + \frac{1}{2} \sum_{j \neq i} \frac{1}{|x_i - x_j|} \right)$

Dynamic equations $\dot{p}_i = -\partial H / \partial x_i + E_{dc} - \eta p_i + g\xi_i(t)$, $\dot{x}_i = p_i$

Here the Langevin force is given by $g = \sqrt{2\eta T}$, $\langle \xi_i(t) \xi_j(t') \rangle = \delta_{ij} \delta(t - t')$;
$n_e = \nu / 2\pi$, $\nu = \nu_g = 1.618...$ Fibonacci rational approximates.

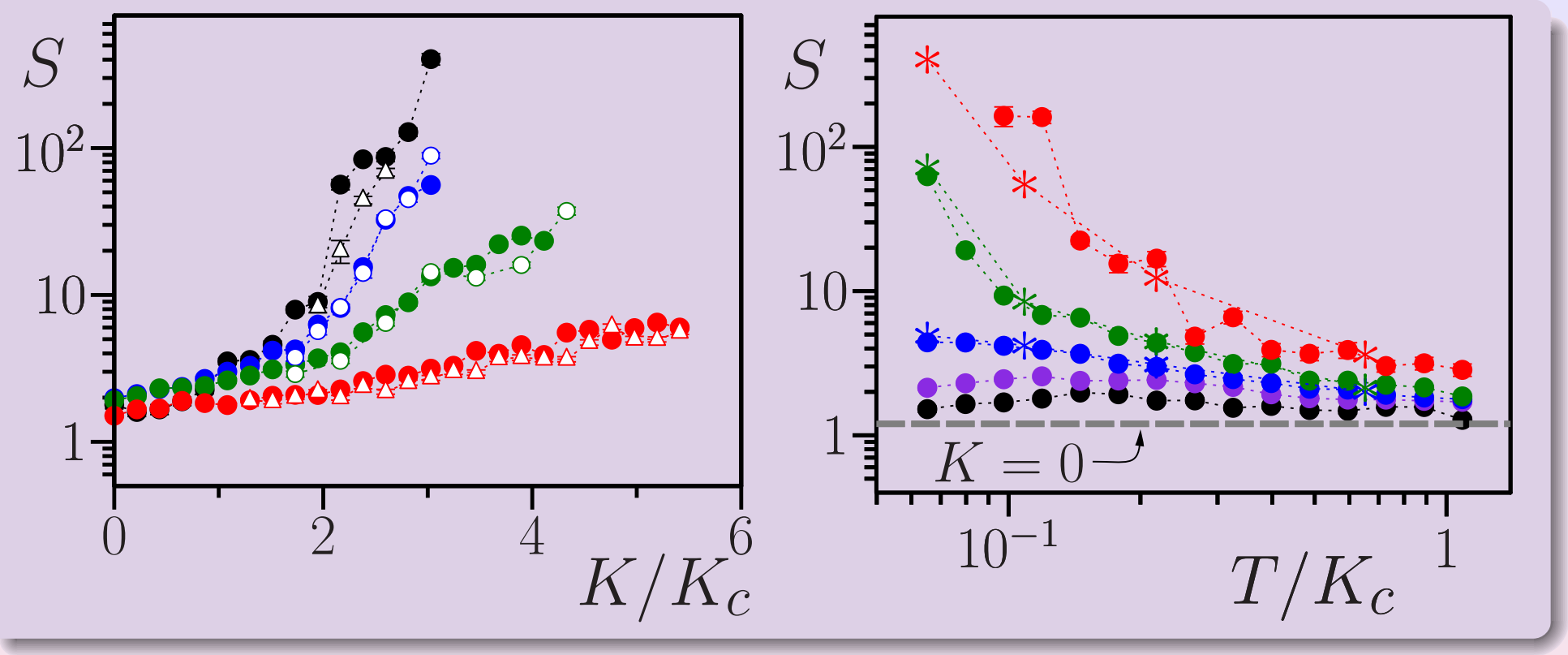
Aubry transition at $K = K_c = 0.0462$ => KAM theory + chaos
I.Garcia-Mata, O.Zhirov, DLS EPJD **41**, 325 (2007)

Time evolution of Wigner crystal



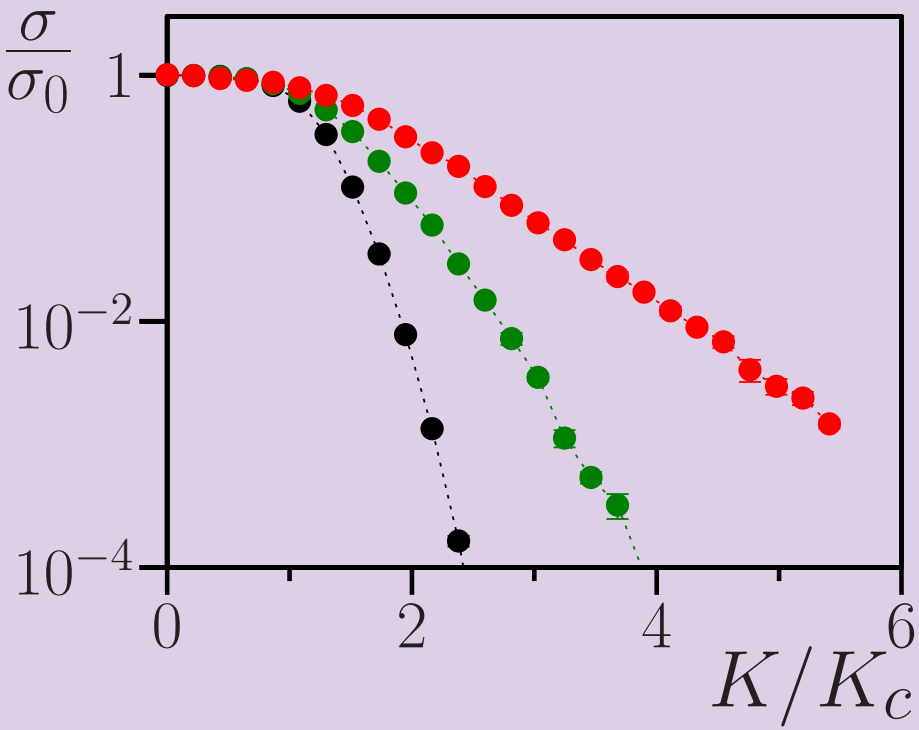
Electron density variation in space and time from one Langevin trajectory at $K/K_c = 2.6$, $T/K_c = 0.11$, $\eta = 0.02$, $N = 34$, $M = L/2\pi = 21$; density changes from zero (dark blue) to maximal density (dark red); only a fragment of x space is shown.

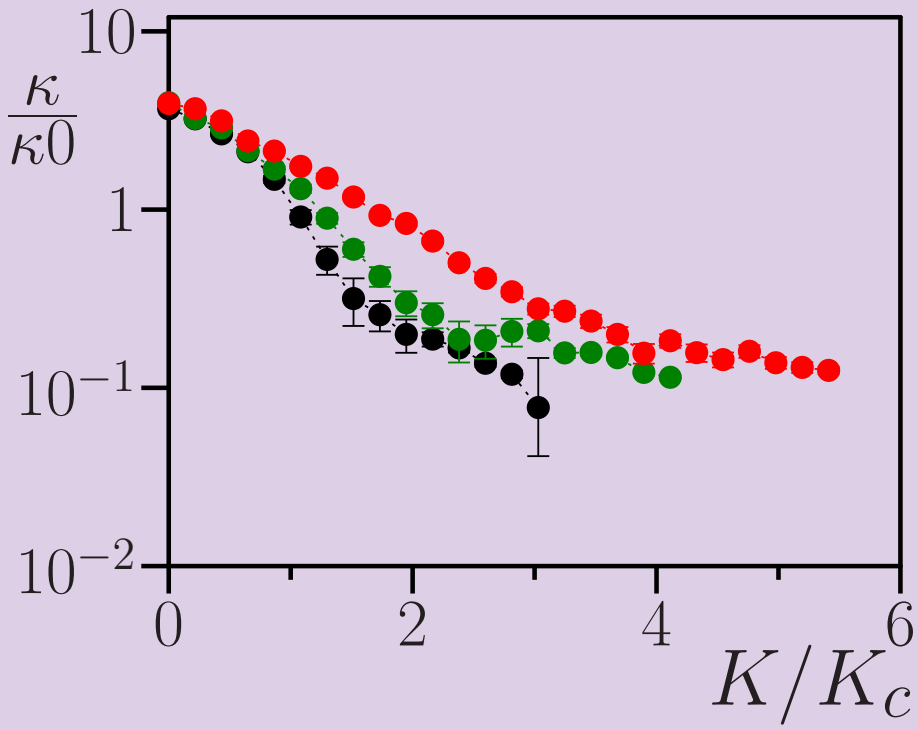
Seebeck coefficient



Left panel: Dependence of the Seebeck coefficient S on rescaled potential amplitude K/K_c at temperatures $T/K_c = 0.065, 0.11, 0.22$ and 0.65 shown by black, blue, green and red colors, respectively from top to bottom. The full and open symbols correspond respectively to chains with $N = 34$, $M = 21$ and $N = 55$, $M = 34$. *Right panel*: Dependence of S on T/K_c at different $K/K_c = 0, 0.75, 1.5, 2.2, 3$ shown respectively by black, violet, blue, green and red points; $N = 34$, $M = 21$; the dashed gray line shows the case $K = 0$ for noninteracting particles. The stars show corresponding results from left plane at same N, M. Dotted curves are drown to adapt an eye. Here and in other Figs. the statistical error bars are shown when they are larger than the symbol size. Here $\eta = 0.02$.

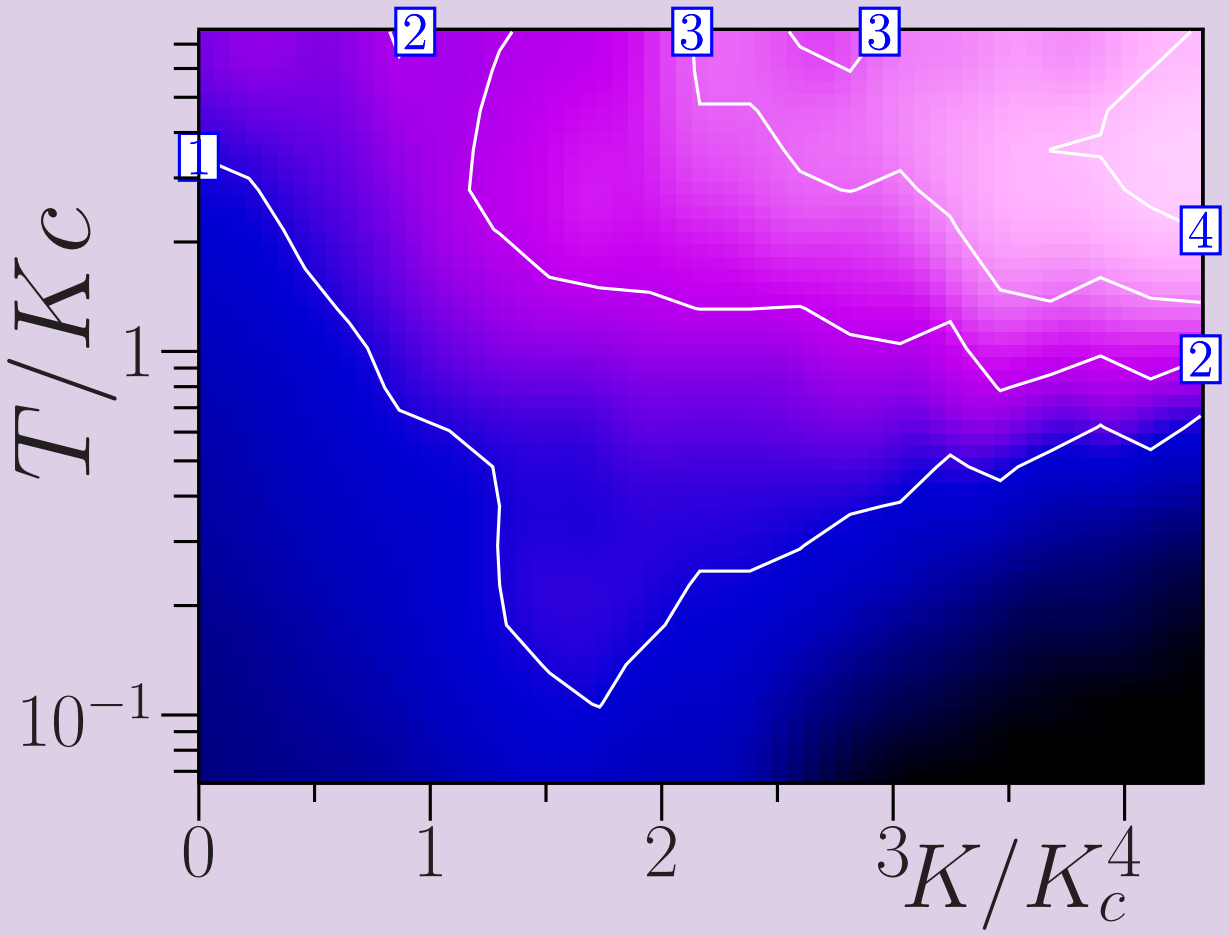
Conductivity and thermal conductivity





Left panel: Rescaled electron conductivity σ/σ_0 as a function of K/K_c shown at rescaled temperatures $T/K_c = 0.065, 0.22, 0.65$ by black, green and red points respectively. *Right panel*: Rescaled thermal conductivity κ/κ_0 as a function of K/K_c shown at same temperatures and colors as in left panel. Here we have $N = 34$, $M = 21$, $\eta = 0.02$, $\sigma_0 = \nu_g/(2\pi\eta)$, $\kappa_0 = \sigma_0 K_c$.

ZT dependence on parameters



Dependence of ZT on K/K_c and T/K_c shown by color changing from $ZT = 0$ (black) to maximal $ZT = 4.5$ (light rose); contour curves show values $ZT = 1, 2, 3, 4$. Here $\eta = 0.02$, $N = 34$, $M = 21$.

Physical picture in oil ...

* In physical units we can estimate the critical potential amplitude as $U_c = K_c e^2/(\epsilon d)$, where ϵ is a dielectric constant, Δx is a lattice period and $d = \nu \Delta x/2\pi$ is a rescaled lattice constant Ref.5. For values typical for a charge density wave regime we have $\epsilon \sim 10$, $\nu \sim 1$, $\Delta x \sim 1nm$ and $U_c \sim 40mV \sim 500K$ so that the Aubry pinned phase should be visible at room temperature. The obtained U_c value is rather high that justifies the fact that we investigated thermoelectricity in the frame of classical mechanics of interacting electrons.

* - Experimental observation of Aubry transition with cold ions in a periodic optical lattice by Vuletic group (MIT) Nat. Mat. **11**, 717 (2016)

* - A lot of numerical computations for different materials (e.g. Kozinsky et al. (Bosch-Harvard) Jour. Appl. Phys. **119** 205102 (2016))

BUT ELECTRON-ELECTRON INTERACTIONS
ARE NOT TREATED CORRECTLY
=> NEW CHALLENGE FOR MATERIAL-COMPUTER SCIENCE

* - Interacting electrons in presence of disorder ?

Mountain snow heights view March 2015