Wigner crystal in snaked nanochannels

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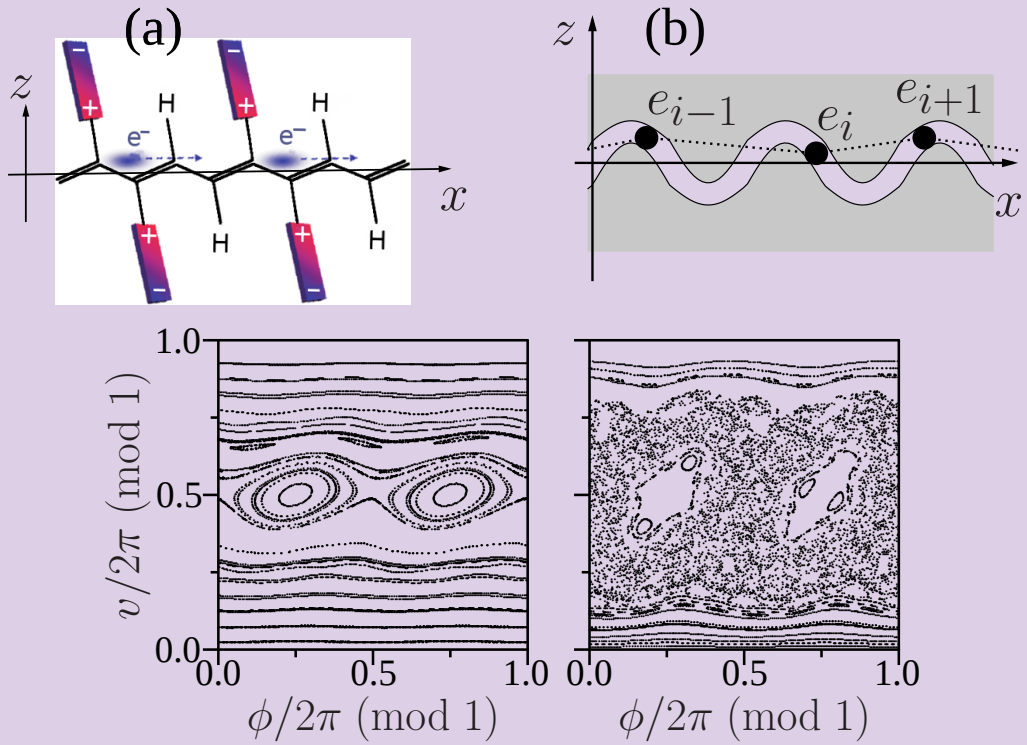


O.V.Zhirov, DS arXiv:1102.1277 (2011) [EPJB **82**, 63 (2011)]

Frenkel-Kontorova model (1938)

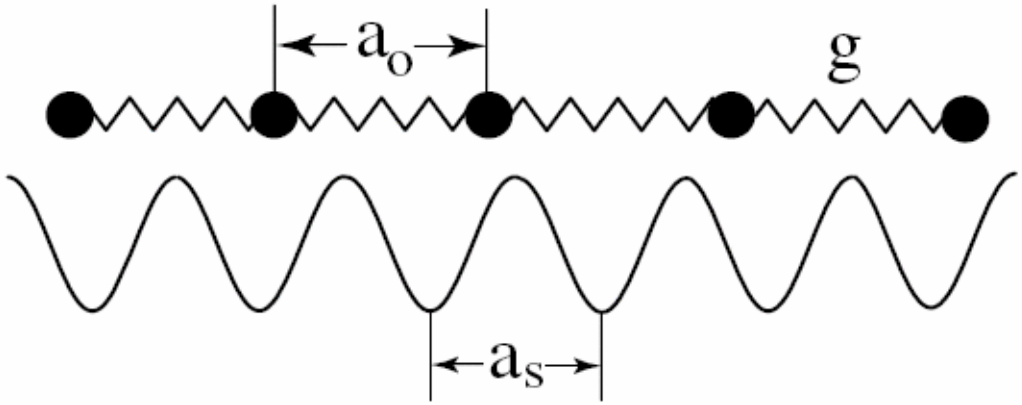


Fig. 1.1. Schematic presentation of the Frenkel-Kontorova model: A chain of particles interacting via harmonic springs with elastic coupling g is subjected to the action of an external periodic potential with period a_s.

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

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

see details in O.M.Braun abd Yu.S.Kivshar, *The Frenkel-Kontorova model: concepts, methods, adn applications*, Spriner, Berlin (2004)

Wigner snake sliding

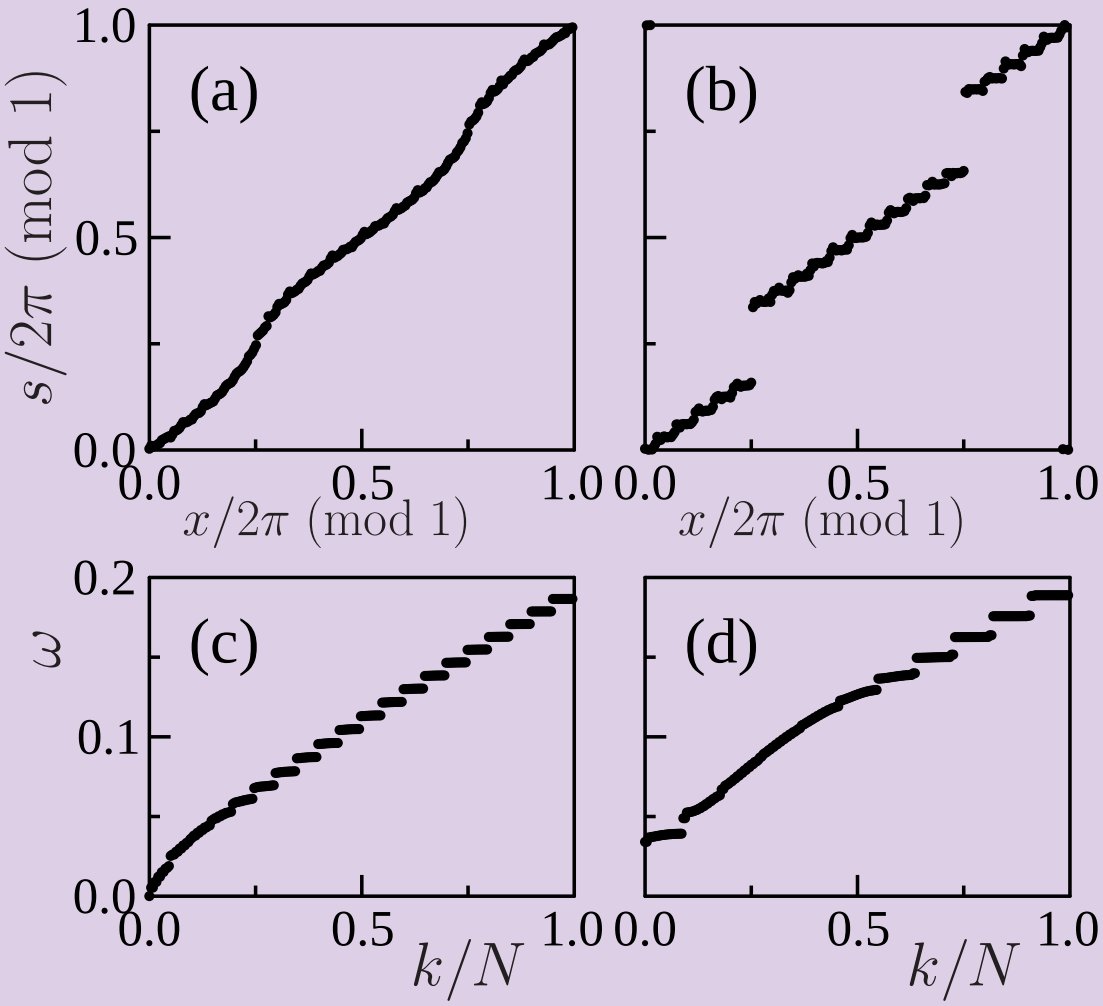
We take a finite number of electrons N for L periods of a channel of finite length. In numerical simulations we put the channel on a cylindrical surface in 3D with electron coordinates being $x_i = L\sin(s_i/L)$, $y_i = L\cos(s_i/L)$, $z = a\sin(s_i)$ where s_i is coordinate along channel for electron i. Thus the channel, filled by N electrons, wiggles in the $z-$direction making L periodic oscillations along cylinder of radius L with periodic boundary conditions. The Coulomb energy of the system is

$$E = \sum_{j>i} 1/R(s_i, s_j) \tag{1}$$

where $R(s_i, s_j)$ is the distance between two electrons. We find from geometry $R^2(s_i, s_j) = 4L^2\sin^2[(s_i - s_j)/2L] + a^2(\sin s_i - \sin s_j)^2$. Here we choose dimensionless units for charge e and length, so that the channel period length is $\ell = 2\pi$ and dimensionless amplitude of channel oscillations is a. The equilibrium static configurations are defined by the condition $\partial E/\partial s_i = 0$ with a minimal ground state energy configuration determined numerically.

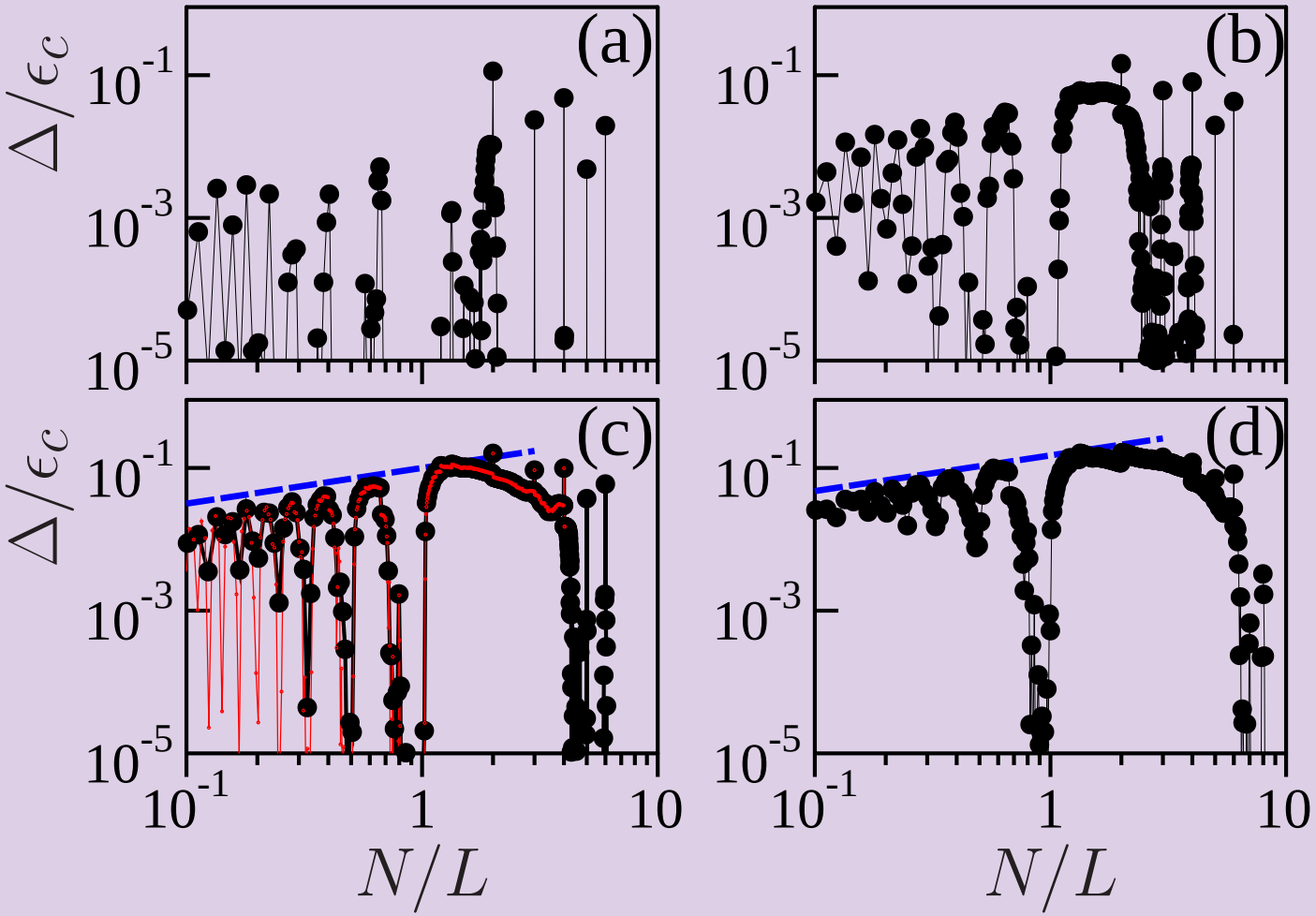
The total energy E is invariant for a homogeneous shift of all electrons by δs when the distance between nearby electrons is $s_{i+1} - s_i = 2\pi m$ that corresponds to electron density $\nu = N/L$ with resonant values $\nu_m = 1/m$.

Wigner snake sliding



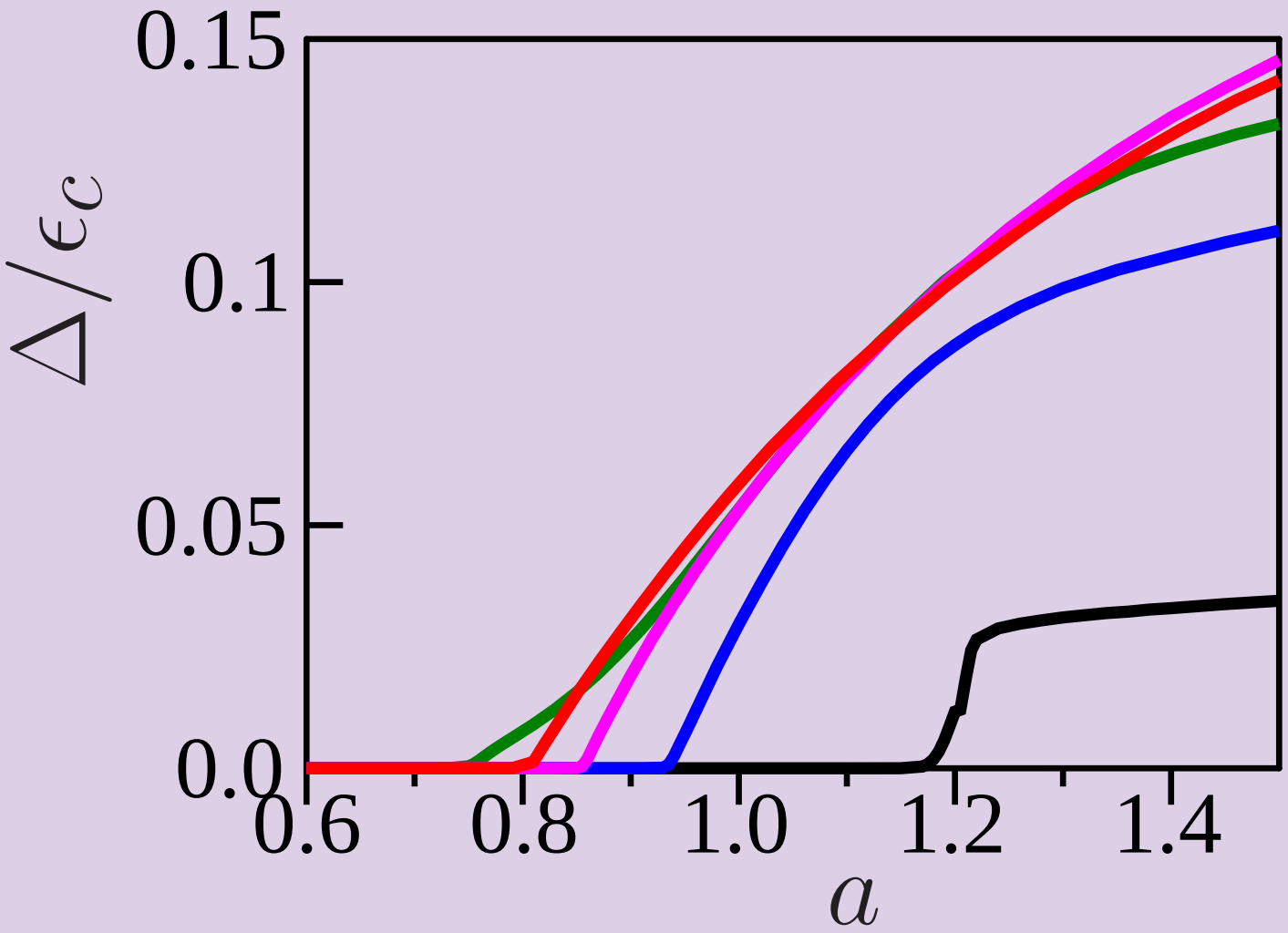
Hull function $s = h(x)$ (a,b) and phonon spectrum $\omega(k/N)$ (c,d) for incommensurate electron densities $\nu = N/L = 239/233$ (a,c) and $\nu = N/L = 244/233$ (b,d). Here $a = 1.2$ and x gives the positions s_i of electrons at $a = 0$.

Phonon gap: density dependence



Dependence of the dimensionless phonon gap Δ/ϵ_c on the electron density $\nu = N/L$ for $a = 0.7(a), 1(b), 1.2(c), 1.5(d)$. Here $L = 89$ (black), 233 (red). The straight line shows empirical dependence $\Delta/\epsilon_c \propto (N/L)^{1/2}$ for (c, d), where $\epsilon_c = 2\pi e^2 \nu/\ell = \nu$ is the Coulomb energy.

Phonon gap: deformation dependence



Dependence of rescaled phonon gap Δ/ϵ_c on channel deformation amplitude a at various values of electron density ν with the number of electrons $N = 241$ (black), 269(blue), 337 (magenta), 377 (red), 307 (green) at $L = 233$.

Dynamical map description

An approximate dynamical map determines recursively the electron positions along the channel. The recursion is given by equilibrium conditions $\partial E/\partial s_i = 0$. Assuming that $a \ll 1$ we can expand R in a that, after keeping only nearest electron interactions, gives recursive relations between s_{i-1}, s_i, s_{i+1}. They can be presented in a form of dynamical map

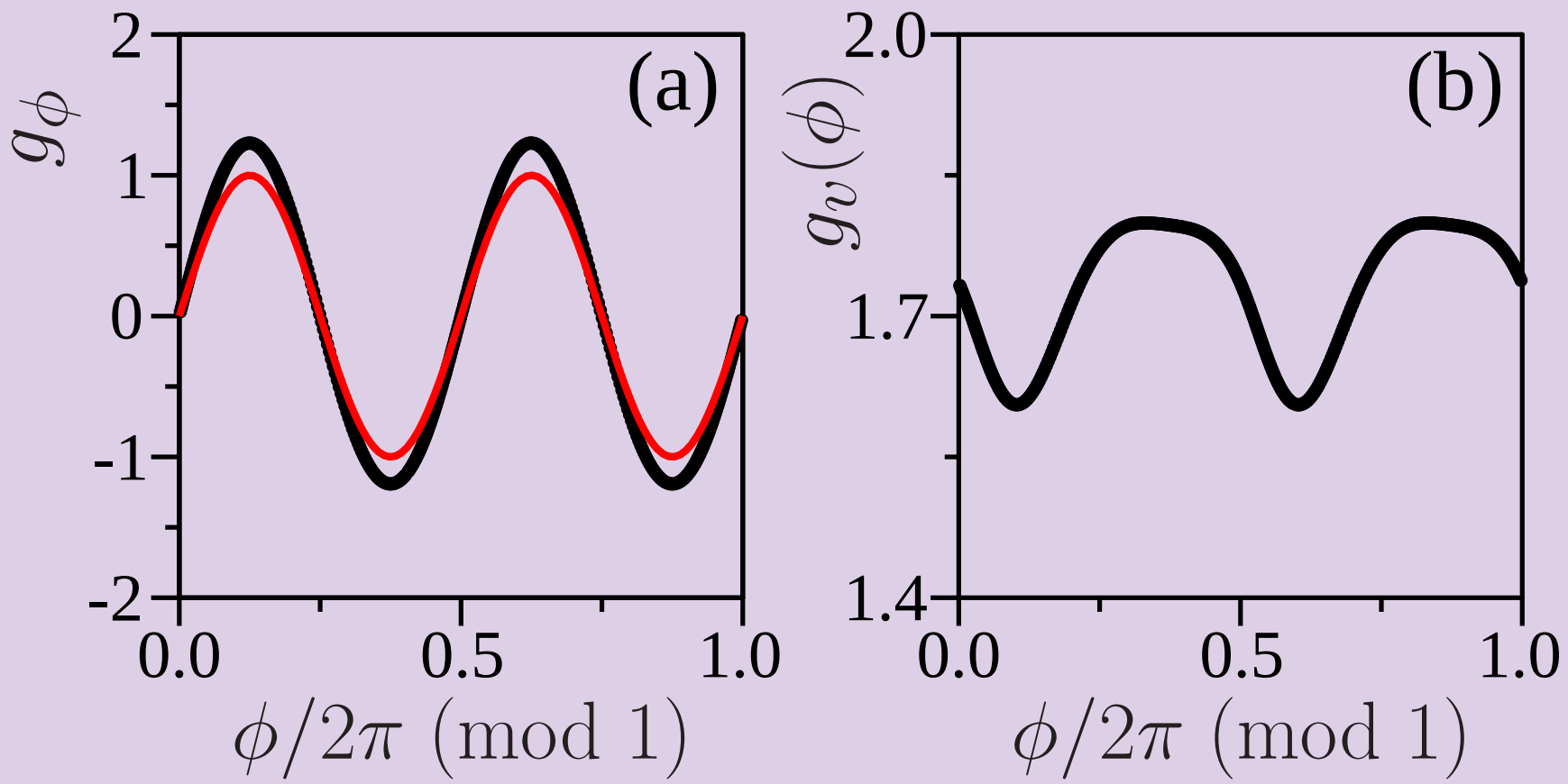
$$\begin{aligned} \bar{v} &= v + 2a^2(1-\cos\bar{v})\sin 2\phi\,, \\ \bar{\phi} &= \phi + \bar{v} + a^2 \sin\bar{v}\cos 2\phi\,, \end{aligned} \tag{2}$$

where $v = s_i - s_{i-1}$, $\phi = s_i$ are conjugated action-phase variables, bar marks their values after iteration. The map is implicit but symplectic. To check its validity we use the values s_i obtained for the groundstate configuration and extract from them the kick function $g_\phi = \sin 2\phi$ from the values $\bar{v} - v = 2a^2 g_v(v) g_\phi(\phi)$ with $g_v(v) = 1 - \cos v$. Such a check shows that the map indeed gives a good description of actual electron positions s_i up to moderate values of a.

Kolmogorov-Arnold-Moser (KAM) invariant curves $\rightarrow$ sliding phase

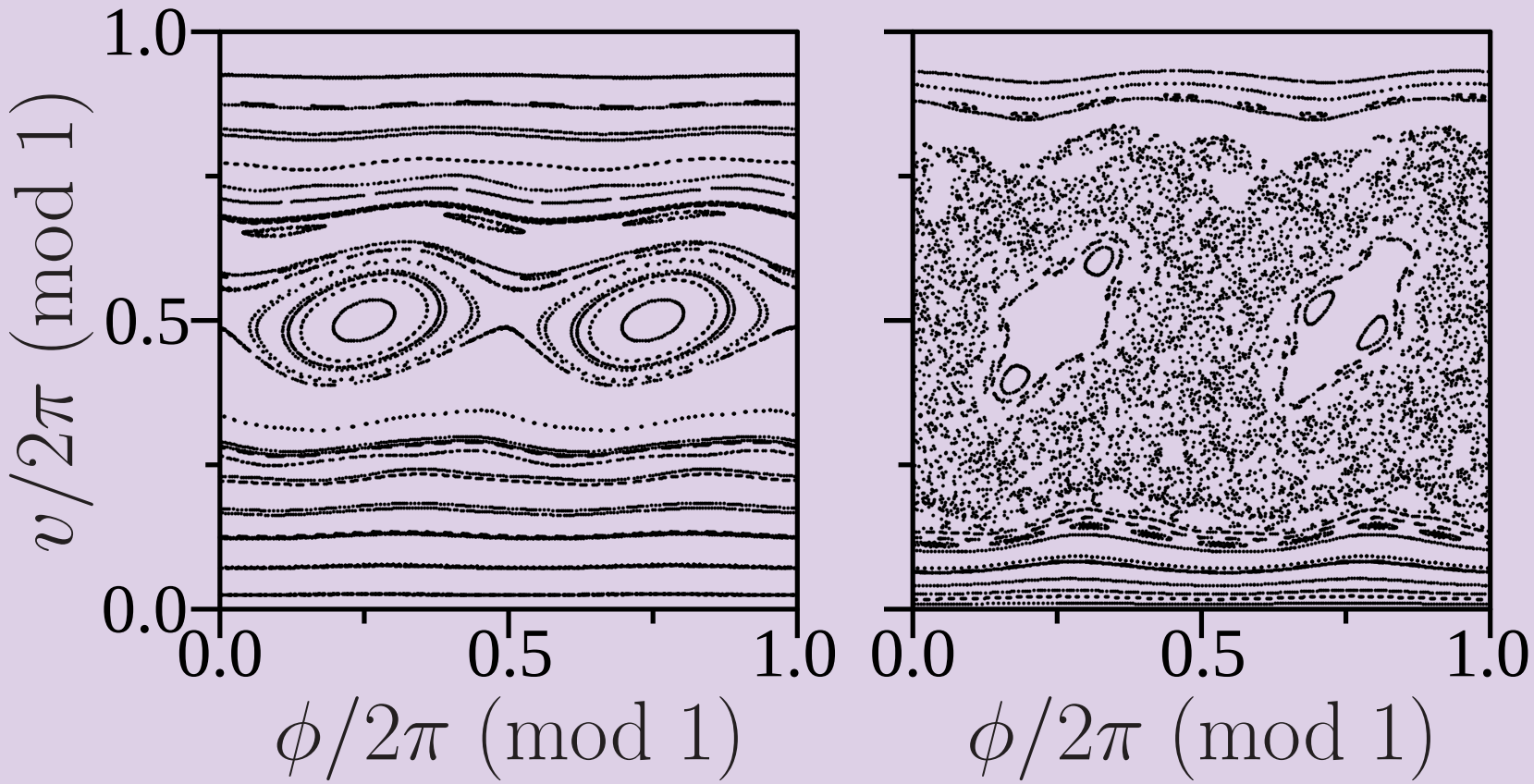
Aubry (cantori) phase $\rightarrow$ pinned phase

Dynamical map desciption



Map kick functions $g_\phi(\phi)$ (a) and $g_v(v)$ (b) obtained from the groundstate electron positions s_i in nanochannel (points), full red curve in (a) shows the theoretical dependence from the map. Here N=377, L=233, $a = 0.5$.

Poincaré section and Aubry transition



Poincare section for the dynamical map at $a = 0.25$ (left panel), 0.5 (right panel).

Dynamics is approximately described by the Chirikov standard map with the chaos parameter $K \approx 4a^2(1 - \cos v)$; the KAM curves are destroyed at $K > 1$. At small charge density ν the parameter K is small $K \approx 2a^2\nu^2 \ll 1$ that corresponds to the KAM regime and a conducting phase of Wigner crystal.

$\rightarrow$ **SLIDING at $\nu < \nu_{c2}$, PINNING at $\nu > \nu_{c2}$**

Wigner crystal in a periodic potential

The dimensionless Hamiltonian has the form:

$$H = \sum_{i=1}^{N} \left(\frac{P_i^2}{2} - K \cos x_i \right) + \sum_{i>j} \frac{1}{|x_i - x_j|} \tag{3}$$

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 (3) 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:

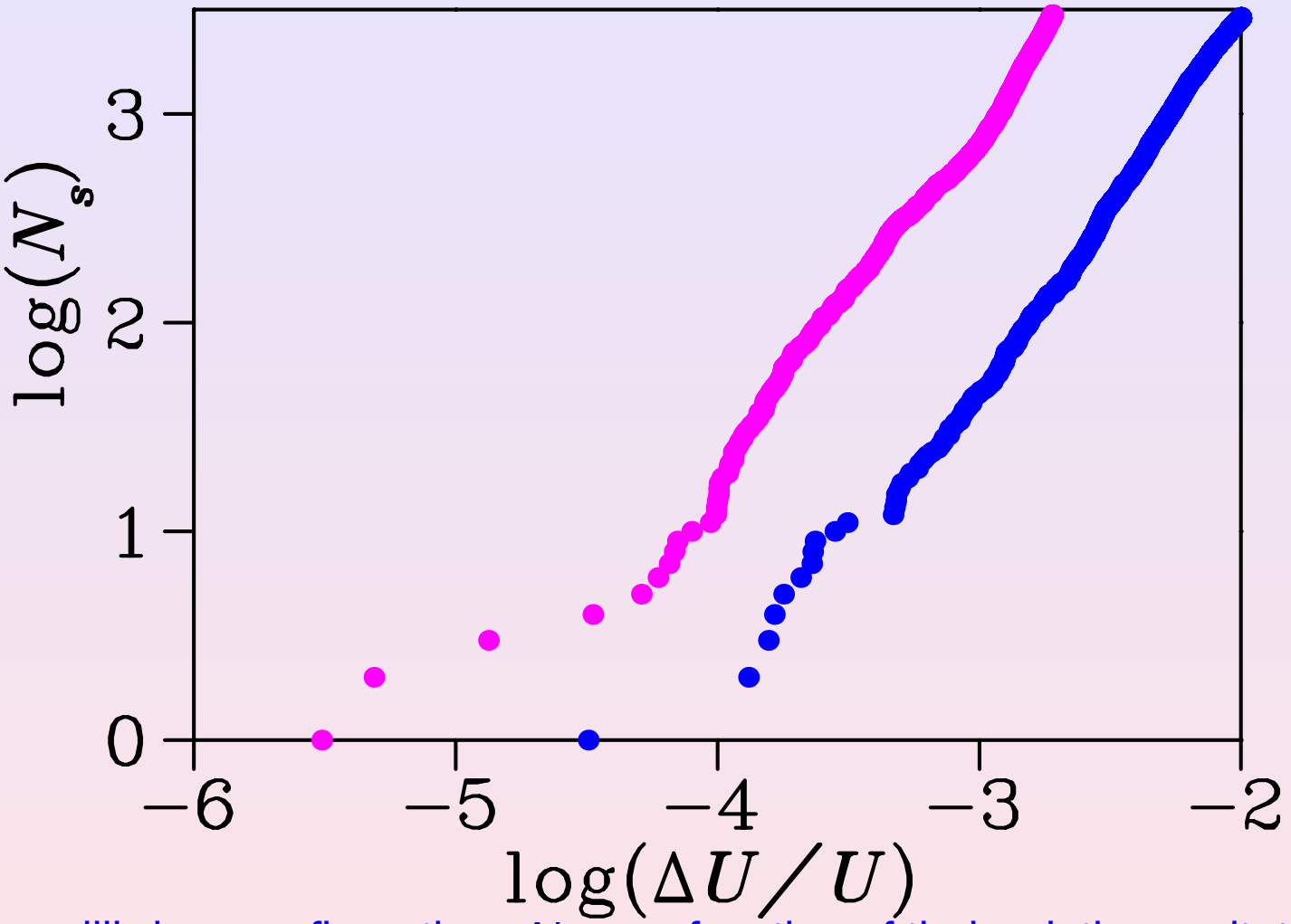
$$p_{i+1} = p_i + Kg(x_i)\ , \quad x_{i+1} = x_i + 1/\sqrt{p_{i+1}}\ , \tag{4}$$

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 $\nu = (\sqrt{5} - 1)/2$.

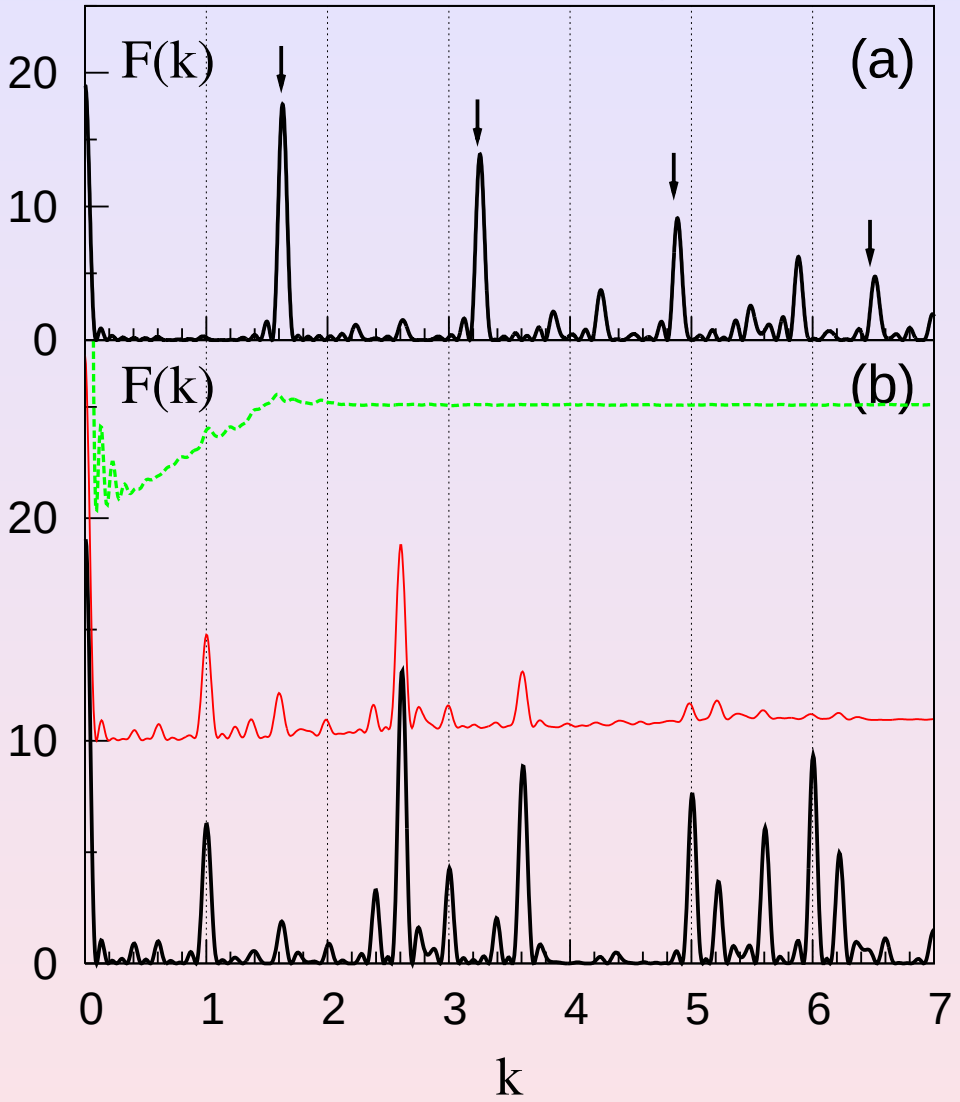
I.Garcia-Mata, O.V.Zhirov, D.S. EPJB **41**, 325 (2007)

Wigner crystal in a periodic potential



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 $\hbar_c \approx 1$.

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

Discussion:

Kolmogorov-Arnold-Moser concept of superconductivity in organic conductors

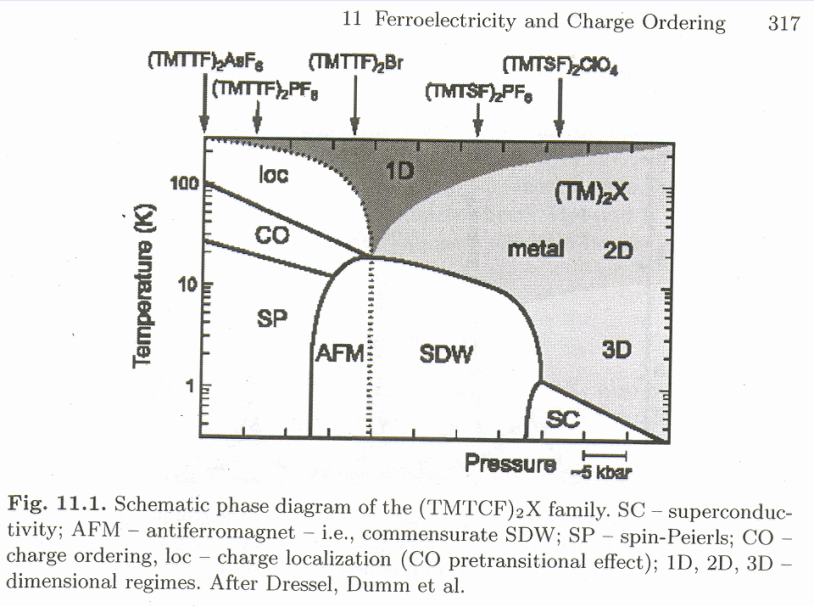
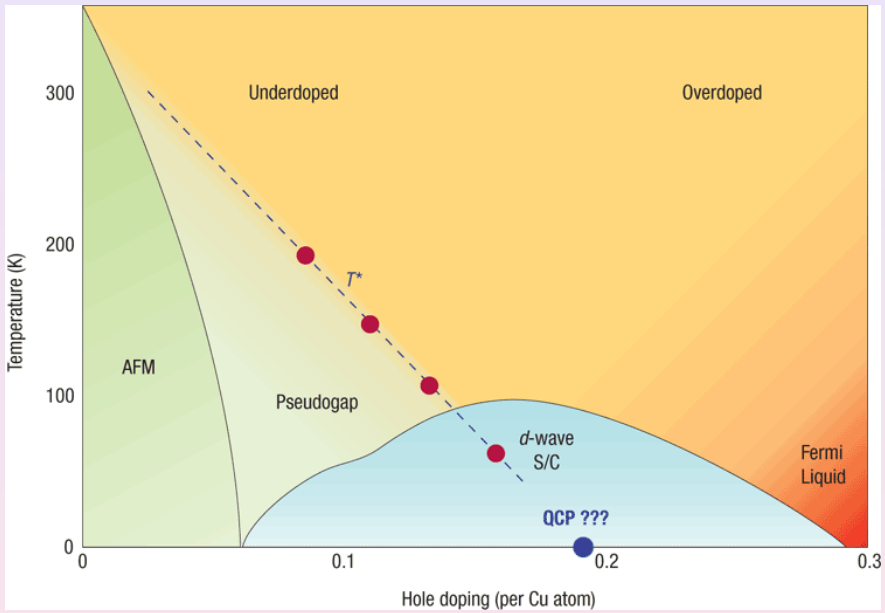


Fig. 11.1. Schematic phase diagram of the $(TMTCF)_2X$ family. SC – superconductivity; AFM – antiferromagnet – i.e., commensurate SDW; SP – spin-Peierls; CO – charge ordering, loc – charge localization (CO pretransitional effect); 1D, 2D, 3D – dimensional regimes. After Dressel, Dumm et al.



KAM CONCEPT: KAM curves and free sliding correspond to a superconducting phase induced by Coulomb repulsion in molecular wires, this phase appears at filling factors

$\nu_{c1} < \nu < \nu_{c2}$.

References:

1. F.Borgonovi, I.Guarneri, D.L.Shepelyansky, "Quantum Effects in the Frenkel-Kontorova Model", Phys. Rev. Lett. v.63, p.2010 (1989)

2. O.V.Zhirov, G.Casati and D.L.Shepelyansky, “Fractal Spin Glass Properties of Low Energy Configurations in the Frenkel-Kontorova chain ”, Phys. Rev. E v.65 p.026220 (2002)

3. O.V.Zhirov, G.Casati and D.L.Shepelyansky, “Quantum phase transition in the Frenkel-Kontorova chain: from pinned instanton glass to sliding phonon gas”, Phys. Rev. E v.67 p.056209 (2003)

4. I.Garcia-Mata, O.V.Zhirov and D.L.Shepelyansky, "Frenkel-Kontorova model with cold trapped ions", Eur. Phys. J. D v.41, p.325 (2007)

5. O.V.Zhirov and D.L.Shepelyansky, "Wigner crystal in snaked nanochannels", Eur. Phys. J. B v.82, pp.63 (2011)