Physica B 407 (2012) 1909–1911

Contents lists available at SciVerse ScienceDirect

Physica B

journal homepage: www.elsevier.com/locate/physb

Wigner crystal in snaked nanochannels: Outlook

O.V. Zhirov [a], D.L. Shepelyansky [b,*]

[a] Budker Institute of Nuclear Physics, 630090 Novosibirsk, Russia
[b] Laboratoire de Physique Théorique du CNRS (IRSAMC), Université de Toulouse, UPS, F-31062 Toulouse, France

ARTICLE INFO

Available online 28 January 2012

Keywords:
Wigner crystal
Organic conductors
Frenkel–Kontorova model
Aubry transition
Invariant KAM curves

ABSTRACT

We study properties of Wigner crystal in snaked nanochannels and show that they are characterized by a conducting sliding phase at low charge densities and an insulating pinned phase emerging above a certain critical charge density. We trace parallels between this model problem and the Little suggestion for electron transport in organic molecules. We also show that in the presence of periodic potential inside the snaked channel the sliding phase exists only inside a certain window of electron densities that has similarities with a pressure dependence of conductivity in organic conductors. Our studies show emergence of dynamical glassy phase in a purely periodic potential in the absence of any disorder that can explain enormously slow variations of resistivity in organic conductors. Finally we discuss the KAM concept of superfluidity induced by repulsive Coulomb interaction between electrons. We argue that the transition from the sliding KAM phase to the pinned Aubry phase corresponds to the superfluid-insulator transition.

1. Introduction

The Wigner crystal [1] appears when the energy of Coulomb repulsion between charges of same sign becomes dominant comparing to kinetic energy of charge motion. On a one-dimensional (1D) straight line this crystal can move ballistically as a whole at an arbitrary small velocity. Here, we discuss the properties of Wigner crystal sliding in 1d in the presence of a periodic potential and in 1d snaked nanochannel following recent works [2,3]. An example of snaked nanochannel of a sinusoidal form is shown in Fig. 1. The snaked form of a channel is very similar to the Little suggestion [4] on possibilities of superconductivity in organic molecules. As described in Refs. [4,5], it is assumed that organic molecules form some effective wiggled or snaked channel with an effective density of electrons ν which slides along the channel opening a new view on possibilities of superconductivity in such materials.

The question about sliding in such a channel is rather nontrivial being linked with fundamental results of dynamical systems [6,7] which we briefly discuss. In fact in a local approximation of small charge oscillations the forces depend linearly on displacements corresponding to a string of particles, linked locally by linear springs and placed in a periodic potential. The density of particles or charges corresponds effectively to a fixed rotation number in a dynamical symplectic map which describes the recurrent positions of particles in a static configuration with a minimum of energy. For linear springs this map is exactly reduced to the Chirikov standard map [6]. This model in known also as the Frenkel–Kontorova model which detailed description is given in Ref. [8]. At small channel deformation a or small amplitude of periodic potential K the particles can freely slide in the periodic potential that corresponds to the regime of invariant Kolmogorov–Arnold–Moser (KAM) curves which rotation number determines the particle density. In this regime the spectrum of small excitations is characterized by a phonon spectrum with the dispersion relation $\omega = c_s k$ where k is dimensionless wave vector and c_s is dimensionless sound velocity. Above a certain critical strength of deformation the KAM curve at a given ν is destroyed being replaced by an invariant Cantor set known as cantori [9]. In this regime the excitations above the ground state have a gap $\omega^2 = (c_s k)^2 + \Delta^2$ and the chain becomes pinned by the potential. The gap Δ is proportional to the Lyapunov exponent of dynamical orbits on such cantori set [7,9]. The transition between sliding and pinned phases is known as the Aubry transition [8]. In the pinned phase the Aubry theorem guarantees that at fixed ν there is a unique ground state which static equilibrium configuration corresponds to the cantori set with positions of particles forming a devil's staircase. However, from the physical view point this ground state is rather hard to reach since in its vicinity there are exponentially many equilibrium configurations which energy is exponentially close to the energy of the ground state. Numerical studies show that already for 100 particles the energy difference is as small as 10^{-25} in dimensional units [10]. This phase was called the dynamical spin glass (or dynamical instanton glass) since such

* Corresponding author.
E-mail address: dima@irsamc.ups-tlse.fr (D.L. Shepelyansky).

0921-4526/$ - see front matter © 2012 Elsevier B.V. All rights reserved.
doi:10.1016/j.physb.2012.01.061

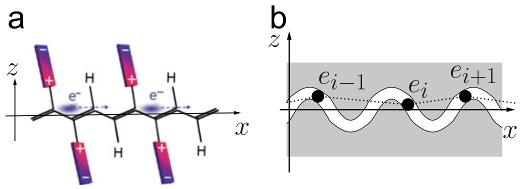

Fig. 1. (a) A schematic image of the Little suggestion for electron transport in organic molecules (after [4,5]). (b) A schematic image of electron Wigner crystal with charges e_i (points) sliding in a snaked sinusoidal nanochannel, dashed lines show force directions between nearby electrons.

properties appear in spin glasses [11] which have random disordered on-site energies and interactions. In contrast to that these properties of the Aubry phase appear in the absence of any disorder being of purely dynamical origin of cantori in a purely periodic potential.

The studies of properties of the quantum Frenkel–Kontorova model has been started in Ref. [12] and further significantly advanced in Ref. [13]. It was shown [13] that quantum fluctuations lead to melting of the pinned phase at sufficiently large values of dimensionless Planck constant $\hbar$. This transition is a zero temperature $T=0$ quantum phase transition. At small $\hbar \ll 1$ an $T=0$ the phonon mode is frozen but quantum tunneling gives transitions between quasi-degenerate equilibrium classical configurations which can be viewed as instantons. At small $\hbar \ll 1$ the density of instantons is small and their interactions are weak. When $\hbar$ increases the instanton density grows and above a certain critical $\hbar_c \sim 1$ the quantum melting of pinned phase takes place at zero temperature leading to zero gap, appearance of quantum phonon mode and quantum chain sliding [13]. The results obtained for the Wigner crystal in a periodic potential [2] in classical and quantum regimes confirm this qualitative picture. At fixed amplitude of periodic potential K the classical Wigner crystal is pinned at small charge densities $\nu < \nu_{c1}$ [2]. Indeed, at $\nu \to 0$ we have a problem of one electron with zero kinetic energy and obviously, an electron is pinned by a periodic potential.

2. Sliding Wigner snake

The situation is different in the case of snaked nanochannel: noninteracting electrons, corresponding to the limit $\nu \ll 1$, move freely inside the wiggled channel and pinning of the Wigner crystal appears only above a certain critical charge density $\nu > \nu_2$. An example of sliding and pinned regimes is shown in Fig. 2. The data clearly show that the sliding phase at $a=0.6$ has a smooth hull function and sound dispersion law for small oscillations of the crystal. In contrast, in the pinned regime at $a=1.2$ the hull function has a form of fractal devil's staircase and gapped spectrum of small oscillations.

More detailed results on dependence of gap Δ on charge density ν and deformation a are described in Ref. [3]. In Ref. [3] it is also shown that for moderate deformations $a<1$ the charge positions in a static configuration are described by a symplectic dynamical map

$$\overline{v} = v + 2a^2(1-\cos \overline{v})\sin 2\phi,$$

$$\overline{\phi} = \phi + \overline{v} + a^2 \sin \overline{v} \cos 2\phi, \qquad (1)$$

where $v = x_i - x_{i-1}$, $\phi = x_i$ are conjugated action-phase variables, bar marks their values after iteration. The map is implicit but symplectic (see e.g. [7]). Examples of Poincaré sections of this map at two values of deformation a are shown in Fig. 3. Phase space region with scattered points corresponds to chaotic dynamics with

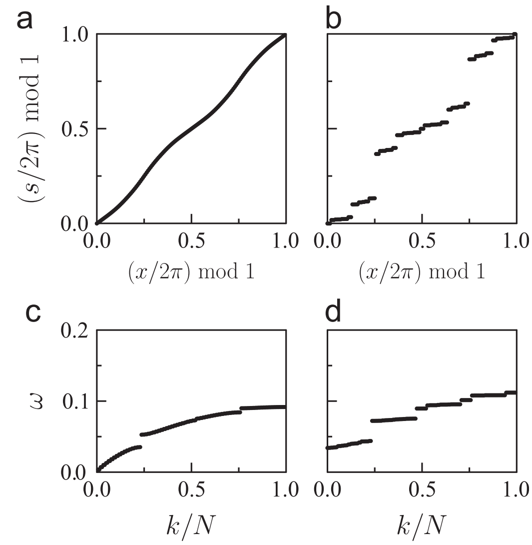

Fig. 2. Hull function $s=h(x)$ (a, b) and phonon spectrum $\omega(k/N)$ (c, d) for incommensurate electron density $\nu = N/L = 144/233$ is shown at $a=0.6$ (a, c) and $a=1.2$ (b, d). Here x gives the positions s_i of electrons at $a=0$. Here a gives the dimensional amplitude of sinusoidal channel described by equation $y = a \sin x$.

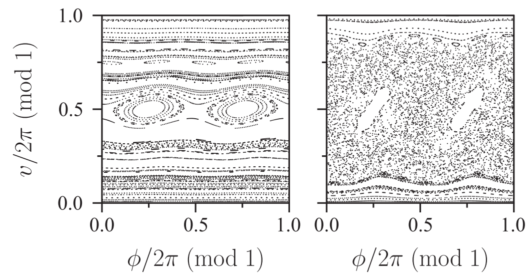

Fig. 3. Poincaré section for the dynamical map (1) at $a=0.2$ (left panel), 0.6 (right panel).

pinned phase, while the smooth invariant KAM curves correspond to the sliding phase.

In many aspects the properties of the Wigner crystal in snaked nanochannels are similar to those of the Frenkel–Kontorov model [10] and the Wigner crystal in a periodic potential [2]: in the pinned phase there are exponentially many static configurations being exponentially close in energy and corresponding to the dynamical glass phase. However, there are also some specific features: for rational values of densities $\nu = \nu_m = 1/m$, where m is an integer, the Wigner snake can slide freely since a displacement does not modify the Coulomb energy of electron interactions.

In analogy with the results presented in Ref. [2], we expect that the quantum Wigner crystal shows a zero temperature quantum phase transition going from a pinned phase at $\hbar < \hbar_c \sim 1$ to a sliding phase at $\hbar > \hbar_c$. However, a direct demonstration of this fact requires further numerical simulations using quantum Monte Carlo methods described in Refs. [2,12,13].

3. Discussion

In the above section we considered the Wigner crystal in a snaked nanochannel without any internal potential. It is natural to assume that a more realistic case of molecular organic conductors, as shown in the Little suggestion in Fig. 1, has not only channel deformation but also a periodic potential inside the channel. Thus the case of organic conductors corresponds to a case of snaked channel with a periodic potential inside it.

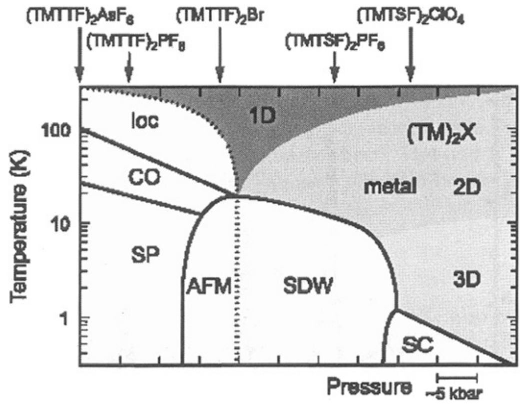

Fig. 4. Schematic phase diagram of the $(TMTCF)_2X$ family taken from Ref. [14] (see details there).

The combination of results of Refs. [2,3] shows that for a given deformation and amplitude of the periodic potential we have the sliding phase in a certain range of charge densities ν

$$\nu_{c1} < \nu < \nu_{c2}. \quad (2)$$

We suppose that the sliding KAM phase may correspond to effective superconducting behavior of electron transport in organic conductors. Indeed, the pressure diagram of organic conductors shown in Fig. 4 from Ref. [14] shows that superconductivity exists only is a finite range of pressure. We assume that pressure gives variation of effective charge density inside the molecular channels in the Little suggestion in Fig. 1. This leads us to the KAM concept of superconductivity of electrons without attractive forces: the Wigner crystal of electrons slides freely inside a snaked molecular crystal channel if the charge density is located inside of KAM phase defined by Eq. (2). Of course, further studies are required for development of this concept. In fact. the sliding KAM phase can be viewed as a superfluid phase of electrons. Indeed, we see that in the KAM phase there is a spectrum of excitations with a finite sound velocity c_s. Thus according to the Landau criterion [15] the sliding of electrons with velocities $v < c_s$ is superfluid. Hence, the transition from the sliding KAM phase to the pinned Aubry phase corresponds to the transition from superfluid to insulator. In this superfluid liquid the charge carries have change "e" and not "2e" as it is the case for BCS pairs. May be effect of interactions between electrons in parallel snaked channels should be taken into account to have 2e-pairs. We note that it is known that repulsive interactions can create superfluid phase in disordered 1d systems, e.g. in the repulsive Hubbard model with disorder [16].

The existence of dynamical spin glass phase with pinned Wigner crystal shows that there should be very slow relaxation processes corresponding to very slow transitions between quasi-degenerate static equilibrium configurations. In fact the experiments with organic conductors show very slow variations of conductivity which take place of a scale of days. Such experimental results have been reported at ECRYS-2011 by Miyagawa [17] and Monceau [18]. Usually it is argued that the glassy phase appears due to impurities. We think that the origin of this phenomenon is not related to disorder and impurities, which presence should be rather small in organic crystals used in experiments [17,18]. In contrast this glassy phase appears as a result of dynamical spin glass phase described in Refs. [2,12,13,3] which exists in purely periodic structures without any impurities and disorder.

Finally, we note that in Ref. [2] it was proposed to study the dynamical spin glass with cold ions in optical lattices which can model the problem of Wigner crystal in a periodic potential. Such experiments with cold ions are now under active discussions [19,20] and their experimental realization is on the way [21].

Acknowledgments

This work is supported in part by ANR PNANO project NANOTERRA.

References

[1] E. Wigner, Phys. Rev. 46 (1934) 1002.
[2] I. Garcia-Mata, O.V. Zhirov, D.L. Shepelyansky, Eur. Phys. J. D 41 (2007) 325.
[3] O.V. Zhirov, D.L. Shepelyansky, Eur. Phys. J. B 82 (2011) 61.
[4] W.A. Little, Phys. Rev. A 134 (1964) 1416;
W.A. Little, Sci. Am. 212 (1965) 21.
[5] D. Jérome, Historical approach to organic superconductivity, in: A. Lebed (Ed.), The Physics of Organic Superconductors and Conductors, Springer-Verlag, Berlin, 2008, p. 3.
[6] B.V. Chirikov, Phys. Rep. 52 (1979) 263.
[7] A.J. Lichtenberg, M.A. Lieberman, Regular and Chaotic Dynamics, Springer, Berlin, 1992.
[8] O.M. Braun, Yu.S. Kivshar, The Frenkel–Kontorova Model: Concepts, Methods, Applications, Springer-Verlag, Berlin, 2004.
[9] S. Aubry, Phys. D 7 (1983) 240.
[10] O.V. Zhirov, G. Casati, D.L. Shepelyansky, Phys. Rev. E 65 (2002) 026220.
[11] M. Mézard, G. Parisi, M.A. Virasoro, Spin Glass Theory and Beyond, World Scientific, Singapore, 1987.
[12] F. Borgonovi, I. Guarneri, D.L. Shepelyansky, Phys. Rev. Lett. 63 (1989) 2010.
[13] O.V. Zhirov, G. Casati, D.L. Shepelyansky, Phys. Rev. E 67 (2003) 056209.
[14] S.A. Brazovskii, Ferroelectricity and charge ordering in quasi-1D organic conductors, in: A. Lebed (Ed.), The Physics of Organic Superconductors and Conductors, Springer-Verlag, Berlin, 2008, p. 313.
[15] L. Landau, Phys. Rev. 60 (4) (1941) 356.
[16] R.T. Scalettar, G.G. Batrouni, G.T. Zimanyi, Phys. Rev. Lett. 66 (1991) 3144.
[17] K. Miyagawa, Y. Muto, M. Kodama, Y. Shimada, K. Kanoda, ^{13}C NMR and resistivity measurements of charge glass state in a charge-frustrated organic conductor, $q-(BEDT-TTF)_2RNZN(SCN)_4$, report at ECRYS-2011, Cargese (see this Phys. B issue).
[18] P. Monceau, Ferroelectricity in organic low-dimensional systems, report at ECRYS-2011, Cargese (see this Phys. B issue).
[19] M. Johanning, A.F. Varon, C. Wunderlich, J. Phys. B: At. Mol. Opt. Phys. 42 (2009) 154009.
[20] A. Benassi, A. Vanossi, E. Tosatti, Nat. Commun. 2 (2011) 236.
[21] T. Pruttivarasin, M. Ramm, I. Talukdar, A. Kreuter, H. Häffner, New J. Phys. 13 (2011) 075012.