Frenkel-Kontorova model with cold trapped ions

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We study analytically and numerically the properties of one-dimensional chain of cold ions placed in a periodic potential of optical lattice and global harmonic potential of a trap. In close similarity with the Frenkel-Kontorova model, a transition from sliding to pinned phase takes place with the increase of the optical lattice potential for the density of ions incommensurate with the lattice period. Quantum fluctuations lead to a quantum phase transition and melting of pinned instanton glass phase at large values of dimensional Planck constant. The obtained results are also relevant for a Wigner crystal placed in a periodic potential.

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Nowadays experimental techniques allow to store thousands of cold ions and observe various ordered structures formed by Coulomb repulsion in ion traps. These structures include the one-dimensional (1D) Wigner crystal, zig-zag and helical structures in three dimensions. The Cirac-Zoller proposal of quantum computations with cold trapped ions generated an enormous experimental progress in this field with implementations of quantum algorithms and quantum state preparation with up to 8 qubits. In these experiments ions form a 1D chain placed in a global harmonic potential which frequency determines the eigenfrequencies of chain oscillations being independent of ion charge. Highly accurate experimental control of the chain modes allows to perform quantum gates between internal levels of ions. In addition to ion traps, modern laser techniques allow to create periodic optical lattices and store in them thousands of cold atoms. A single ion dynamics in an optical lattice has been also studied experimentally. The combination of these two techniques makes possible to study experimentally the properties of a 1D chain of few tens of ions placed in an optical lattice and a global harmonic potential at ultra low temperatures.

In this Letter we analyze the physical properties of such a system and show that it is closely related to the Frenkel-Kontorova Model (FKM) which gives a mathematical description of various physical phenomena including crystal dislocations, incommensurate phase transitions, epitaxial monolayers on a crystal surface, magnetic chains and fluxon dynamics in Josephson junctions. As in the classical FKM the ion chain exhibits the Aubry analyticity breaking transition when the amplitude of optical potential becomes larger than a certain critical value. Below the critical point the classical chain can slide (oscillate) in the incommensurate optical lattice while above the transition it becomes pinned by the lattice and a large gap opens in the spectrum of phonon excitations. Above the transition the positions of ions form a devil’s staircase corresponding to a fractal Cantor set which replaces a continuous Kolmogorov-Arnold-Moser (KAM) curve in the phase space below the transition. According to the FKM ground state is unique but in the pinned phase there are exponentially many stable configurations which are exponentially close to the ground state and the system resembles a fractal spin glass. In the quantum FKM the instanton tunneling between quasidegenerate configurations leads to a melting of the pinned instanton glass and the quantum phase transition into sliding phonon phase takes place above a critical value of the effective Planck constant.

The dimensionless Frenkel-Kontorova Hamiltonian has the form:

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

where \( P_i, x_i \) are ion momentum and position, \( K \) the strength of optical lattice potential and all \( N \) ions are placed in a harmonic potential with frequency \( \omega \). To make a transfer from 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 \( e^2/d \) and \( \omega^2 \to m \omega^2 d^3/e^2 \) where \( m \) is ion mass. In the quantum case \( P_i = -i\hbar \partial/\partial x_i \) with dimensionless \( \hbar \) measured in units \( \hbar = \hbar/(e\sqrt{md}) \). In the quantum case we use the approximation of distinguishable ions which is well justified when the distance between ions imposed by the harmonic potential is comparable with the lattice period.

We start the discussion from the classical case. Here
the stable configurations with minimal energy have \( P_i = 0 \) and satisfy the conditions \( \partial H / \partial x_i = 0 \). In approximation of only nearest neighbor interacting ions these conditions lead to the dynamical recursive map for equilibrium ion positions \( x_i \):

\[
p_{i+1} = p_i + K g(x_i), \quad x_{i+1} = x_i + 1/\sqrt{p_{i+1}}, \tag{2}
\]

where the effective momentum conjugated to \( x_i \) is \( p_i = 1/(x_i - x_{i-1})^2 \) and the kick function \( K g(x) = -\omega^2 x - K \sin x \). To check the validity of this description we find the ground state configuration using numerical methods described in [11][12]. The harmonic frequency \( \omega \) is chosen in such a way that in the middle of the chain the ion density \( \nu = 2\pi/(x_1 - x_0) \) at \( K = 0 \) is equal to the golden mean value \( \nu = \nu_g = (\sqrt{5} + 1)/2 \). This corresponds to an incommensurate phase with the golden KAM curve usually studied for the Aubry transition [10][11]. For a fixed \( \nu \approx 1 \) the strength of harmonic potential \( \omega^2 \) drops with \( N \) according to relations found in [3][6]. The numerical values \( x_i \) allow to determine the function \( g(x) \) using relations [2] and show that with good accuracy \( g(x) = -\sin x \) (see Fig 2). We attribute this result to an effective screening of global harmonic potential by long range interactions between ions in the central part of the chain where the ion density is approximately constant. For small values of optical potential \( (K = 0.03) \) the chain is in the sliding phase with a continuous KAM curve in the plane \( (p, x) \) while above the Aubry transition at \( K = 0.2 \) it is in the pinned phase and forms a fractal Cantor set in the phase space (Fig 1). The qualitative change of chain properties is also seen via the hull function \( h(x) \) which gives the ion positions in periodic potential vs. unperturbed positions at \( K = 0 \) both taken \( \mod 2\pi \): for \( K < K_c \) one has a continuous function \( h(x) \approx x \) while for \( K > K_c \) the hull function has a form of devil’s staircase with clustering of ion positions at certain values (Fig 1). More data for a larger number of ions \( N = 150 \) are shown in Appendix (see Fig 1).
The structural changes in the chain below and above the Aubry transition at the critical value $K_c$ are also clearly seen in the spectrum of phonon excitations shown in Fig. 2 (see also Fig. 7 in Appendix for $N = 150$). For $K < K_c$ the spectrum of phonon modes has a sound like form at small wave vectors $k$, going down to a minimal oscillation frequency $\omega_0 \approx \omega$, which is small compared to frequencies of periodic potential. For $K > K_c$ the spectrum of excitations is characterized by a phonon gap when $\omega_0$ becomes independent of number of ions $N$ (Fig. 4). According to the data of Fig. 4 for $\omega_0(K)$ and of Fig. 8 in Appendix for the hull function the critical point is located at $K_c \approx 0.05$. The value $K_c$ can be obtained approximately by a reduction of map 2 to the Chirikov standard map 15. For that the second equation 2 can be linearized near $1/\sqrt{\tau} = 2\pi/\nu_0$ that gives the Chirikov standard map with chaos parameter $K_{eff} = K(2\pi/\nu_0)^3/2$ and the critical value $K_c = 0.034$ corresponding to $K_{eff} = 1$. This value is smaller than the value $K_c \approx 0.05$ obtained from numerical data that can be attributed to a strong dependence of $K_{eff}$ on $\nu_0$.

The obtained results show that the ion chain in a periodic potential has close similarities with the FKM. The map 2 describes quite accurately the central 1/3 part of the chain where the ion density is approximately constant. Outside of this part the ion density starts to grow and deviations from the map start to be visible in $(p, x)$ plain and $h(x)$, even if the $g$-function remains rather close to $g = -\sin x$. A separation on two parts is also seen in the lowest phonon eigenmodes which are localized in the central part of the chain (see Figs. 10 and 11 of Appendix). Also, in similarity with the FKM 12, we find that in the pinned phase at $K > K_c$ the FKIM has properties of a spin glass with enormous number of stable equilibrium configurations $N_s$ in the very close vicinity of the ground state (see Fig. 1).

These quasidegenerate configurations become very important in the quantum chain where quantum tunneling between them leads to nontrivial instanton excitations. To study the quantum case we use the QMC approach 13, 16, 18 with the Euclidean time $\tau$ in the interval [0, $\tau_0$] and system temperature $T = h/\tau_0$. We use large values of $\tau_0$ (e.g. $\tau_0 \geq 400$) so that the temperature $T$ is small compared to periodic potential $K$ and phonon gap $\hbar \omega_0$. To see the structural changes produced by quantum fluctuations it is convenient to compute the formfactor of ion positions defined as $F(k) = \langle \sum_i |\exp(ikx_i(\tau))|^2 \rangle/\delta N$, where summation is taken over the central part of the chain with $\delta N \approx N/3$ ions, $x_i(\tau)$ are ions positions at Euclidian time $\tau$ and brackets mark averaging over $\tau$. In the classical case $x_i$ are the equilibrium positions of ions. For $h = 0$ the formfactor peaks are equidistant in $\nu_0$ that clearly show the incommensurate sliding phase at $K = 0.03 < K_c$ (Fig. 5). For $K = 0.2 > K_c$ the peaks in $F(k)$ are at integer $k$ values showing that ions are pinned by the optical lattice (Fig. 5, bottom). In the quantum case at $K = 0.2 > K_c$ and small values of $h = 0.1$ the density of instantons is small and quantum tunneling does not de-
stroy the pinned phase. However, at large $\hbar = 2$ quantum fluctuations lead to melting of pinned phase, the integer peaks disappear and $F(k)$ becomes continuous (Fig. 3). This means that the ion chain can slide in the optical lattice. The quantum phase transition from pinned instanton glass to sliding phonon gas takes place at zero temperature and certain $\hbar_c \sim 1$. The formfactor $F(k)$ can be experimentally obtained by light scattering on the ion chain and in this way various phases of the system can be detected. For experimental conditions like in [3] the distance between Ca ions is about $\Delta x \approx 5 \mu m$ so that the golden mean density $\nu_g$ corresponds to the lattice constant $d = \nu_g \Delta x/2\pi \approx 1.3 \mu m$. This value can be realized by laser beams crossed at a fixed angle. The transition to pinned phase takes place at the optical lattice potential $V = K_c e^2 / d \approx 0.6 K$ that in principle can be reached in strong laser fields. For $^{40}Ca^+$ ions with such $d$ the dimensionless Planck constant is $\hbar_{eff} = h/(e\sqrt{md}) \approx 3 \times 10^{-5}$. This means that such experiments with cold trapped ions can be performed in a deep semiclassical regime hardly accessible to the QMC numerical simulations. We also note that a strong gap in phonon spectrum $\omega_k$ for $K > K_c$ (Figs. 2, 3) may be useful for protection of quantum gate operations in quantum computations.

Higher values of dimensionless $h$ can be reached with electrons forming a Wigner crystal placed in a periodic potential where $h \approx 0.1$ for $d \approx 5 nm$. Such a situation may appear in 1D electron wires, molecular structures or nanotubes where a devil’s staircase behavior has been discussed recently [19]. In the regime when the number of electrons per period is of the order of $\nu \sim 1$ the effects related to statistics of particles are not so crucial and the quantum melting of the pinned phase should qualitatively follow the scenario described here. Hence, the obtained results describe also a more general problem of a Wigner crystal in a periodic potential.

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**APPENDIX**

Here in Figs. 6-11 we present additional data showing results with larger number of ions.

**Fig. 6:** (Color online) Same as in Fig. 1 but for $N = 150$ ions at $\omega = 0.00528 \ (\omega^2 = 2.794 \times 10^{-5})$ corresponding to the golden mean density of ions in the middle of the chain.

**Fig. 7:** (Color online) Phonon spectrum $\omega(k)$ as a function of scaled mode number $k = i/N \ (i = 0, \ldots, N-1)$, for $K = 0.03$ (bottom curve, squares) and $K = 0.2$ (top curve, points) for the case of Fig. 3 at $N = 150$ (compare with data of Fig. 2 for $N = 50$).

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FIG. 8: (Color online) Evidence of the Aubry transition in the hull function. The hull function $h(x)$ shows the ion positions $x_i(K)$ mod $(2\pi)$ in presence of periodic potential as a function of ion positions $x_i^{(0)} \text{mod}(2\pi)$ without potential ($K = 0$). Here $N = 150$, $\omega = 0.000528$, $\omega^2 = 2.794 \times 10^{-5}$. (a) $K = 0.04$; (b) $K = 0.055$; (c) $K = 0.065$; (d) $K = 0.1$. Only the central 1/3 part of the chain is shown.

FIG. 9: Phonon eigenmodes in the chain with $N = 50$ ions at the golden mean ion density with $\omega = 0.014$, $\omega^2 = 1.986 \times 10^{-4}$. Panels show the amplitude of eigenmode (in arbitrary linear units) vs. ion positions $x_i$ varied from minimal to maximal value for lowest 4 modes with number 0, 1, 2, 3 (from left to right). Top row is for $K = 0.03$ and bottom row is for $K = 0.2$.

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