Frenkel-Kontorova Model with Cold Trapped Ions

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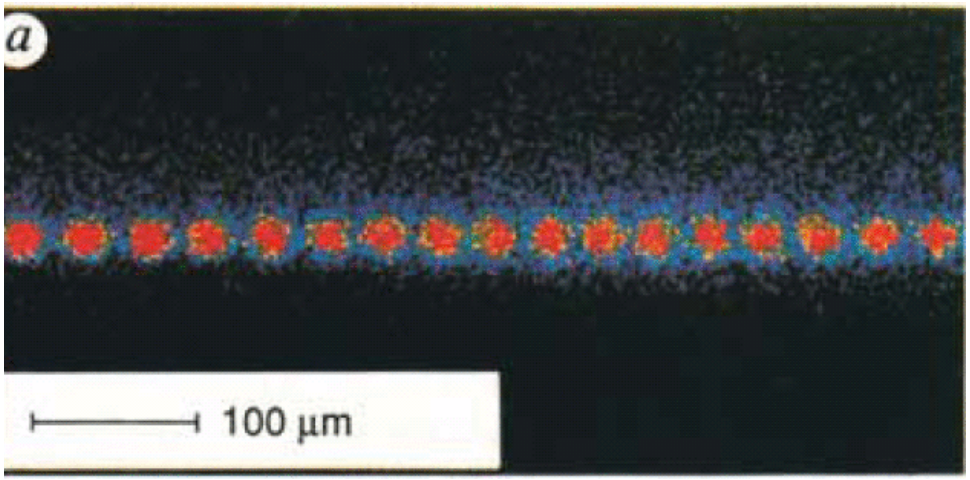
Crystal structure of laser-cooled $^{24}M^{+}$ ions

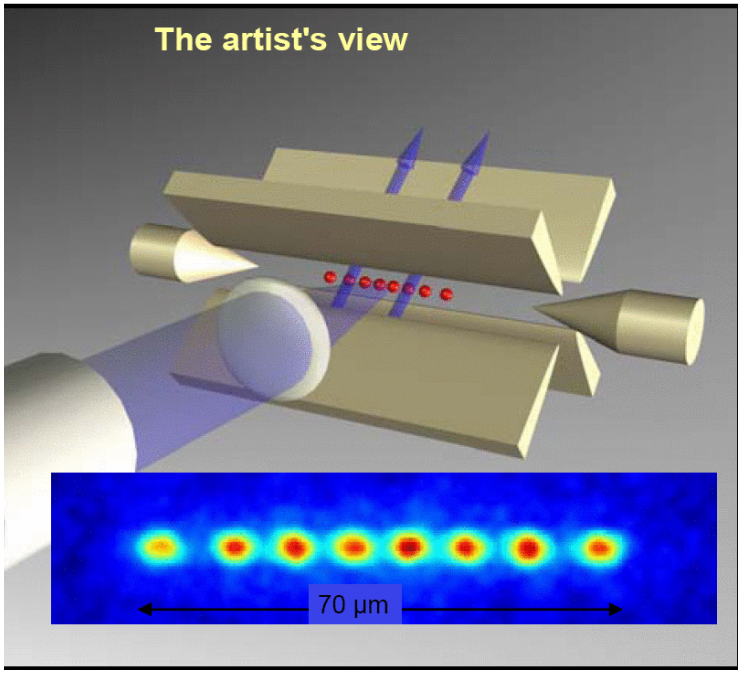
Experiments with cold ions in a quadrupole storage ring
(G.Bikl, S.Kassner and H.Walther, Nature **357**, 310 (1992)):



Observed structures include the one-dimensional Wigner crystal, zig-zag and helical structures in three dimensions with up to thousands of ions.

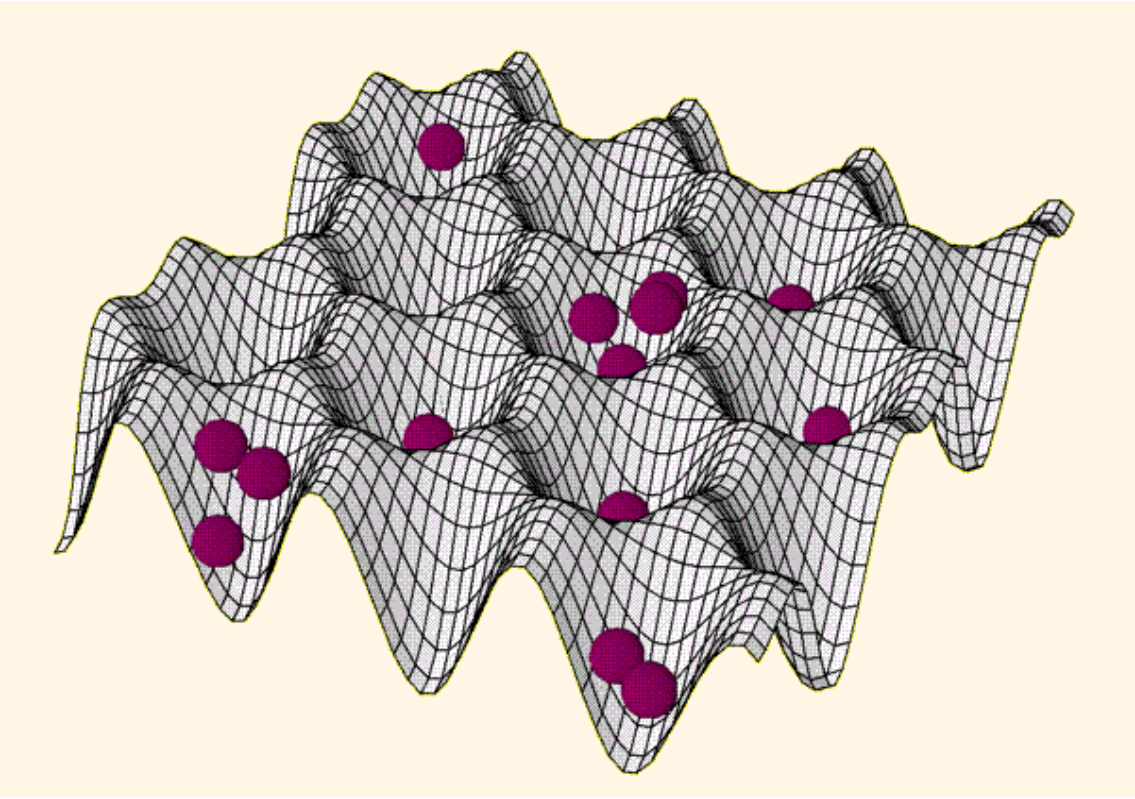
Cold Ions for Quantum Computing

Proposal Cirac-Zoller (1995); Experiments of the Blatt group at Innsbruck (slide from J.Eschner lecture at Varenna school 2005)



Ions in a global oscillator potential, at to 8 qubits has been realized.

Atoms and Ions in Optical Lattice



Thousands of cold atoms can be placed in an optical lattice

Wigner Crystal in a Periodic Potential

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On the Interaction of Electrons in Metals

E. WIGNER, *Princeton University*

(Received October 15, 1934)

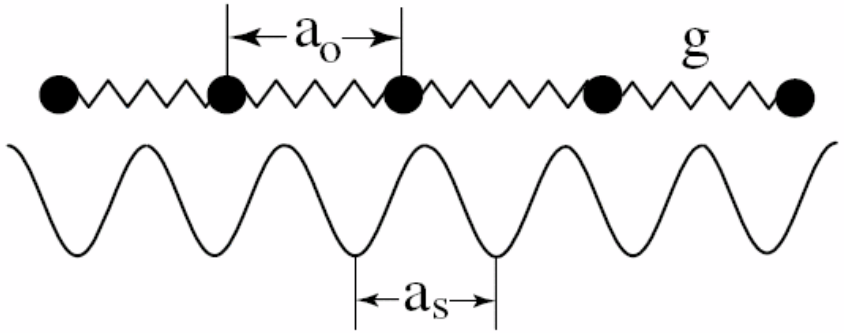
raction between free electrons in an idered. The interaction energy of l spin is known to be that of the exchange integrals, and these terms he wave functions but slightly. The rons with antiparallel spin, contains, nteraction of uniformly distributed er term. This term is due to the fact that the electrons repell each other and try to keep as far apart as possible. The total energy of the system will be decreased through the corresponding modification of the wave function. In the present paper it is attempted to calculate this "correlation energy" by an approximation method which is, essentially, a development of the energy by means of the Rayleigh-Schrödinger perturbation theory in a power series of e^2.

1.

has been made in previous e a more general expression ion of free electrons in metals d by Hartree's method of the [1,2,3] or Fock's equations. The function assumed in Fock's tem of $2n$ electrons, occupying electron at the point u is given by adding to the Coulomb field of the ions the fields of all electrons with parallel and with antiparallel spin. The former distribution may be obtained by inserting u for x_n in (1) and integrating over all coordinates except x_1 and u, while the latter is obtained by a similar operation with the exception that the integration should be carried out over all coordinates except x_1 and u.

From Wikipedia, the free encyclopedia: A Wigner crystal is the solid (crystalline) phase of electrons first predicted by Eugene Wigner in 1934. Such a phase can be realized if the electron density is sufficiently low. In 2-dimension (2D), it can also be realized by applying a sufficiently strong perpendicular magnetic field. ($http://en.wikipedia.org/wiki/Wigner\_crystal$)

The Frenkel-Kontorova Model (1938)



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

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

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

See detailed description in O.M. Braun and Yu.S. Kivshar, *The Frenkel-Kontorova Model: Concepts, Methods, and Applications*, Springer-Verlag, Berlin (2004).

The Frenkel-Kontorova Ion Model

The dimensionless Hamiltonian has the form:

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

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 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 $\hbar \to \hbar/(e\sqrt{md})$. 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. At $K = 0$ the frequencies of small oscillations are ω, $\sqrt{3}\omega$ and independent of charge (D.H.E. Dubin and T.M. O'Neil, Rev. Mod. Phys. **71**, 87 (1999)).

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 developed by Aubry (1979-1983). The harmonic frequency ω 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.

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 $K_c = 0.971635\ldots$.

Numerical Results for the Classical FKI Model

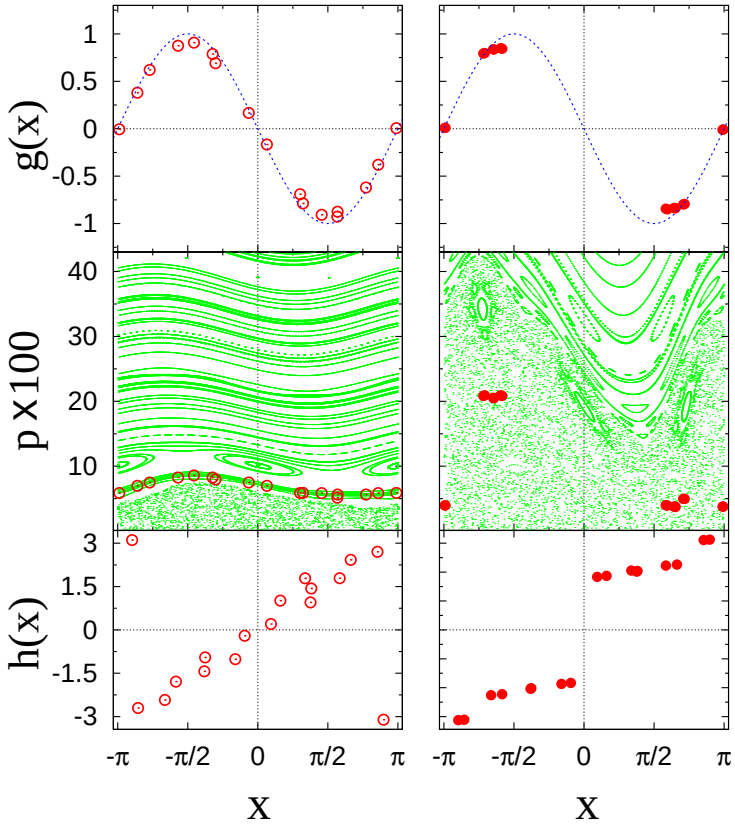


Fig.1 Functions related to the dynamical map (2) obtained from the ground state equilibrium positions x_i of $N = 50$ ions for $\omega = 0.014$ at $K = 0.03$ (open circles, left column) and $K = 0.2$ (full circles, right column). Panels show: the kick $g(x)$ function (top); the phase space (p, x) of the map (2) with $g(x) = -\sin x$ (green/gray points) and actual ion positions (red/black circles) (middle); the hull function $h(x)$ (bottom). The ion positions are shown as $x = x_i (mod 2\pi)$ for the central $1/3$ part of the chain.

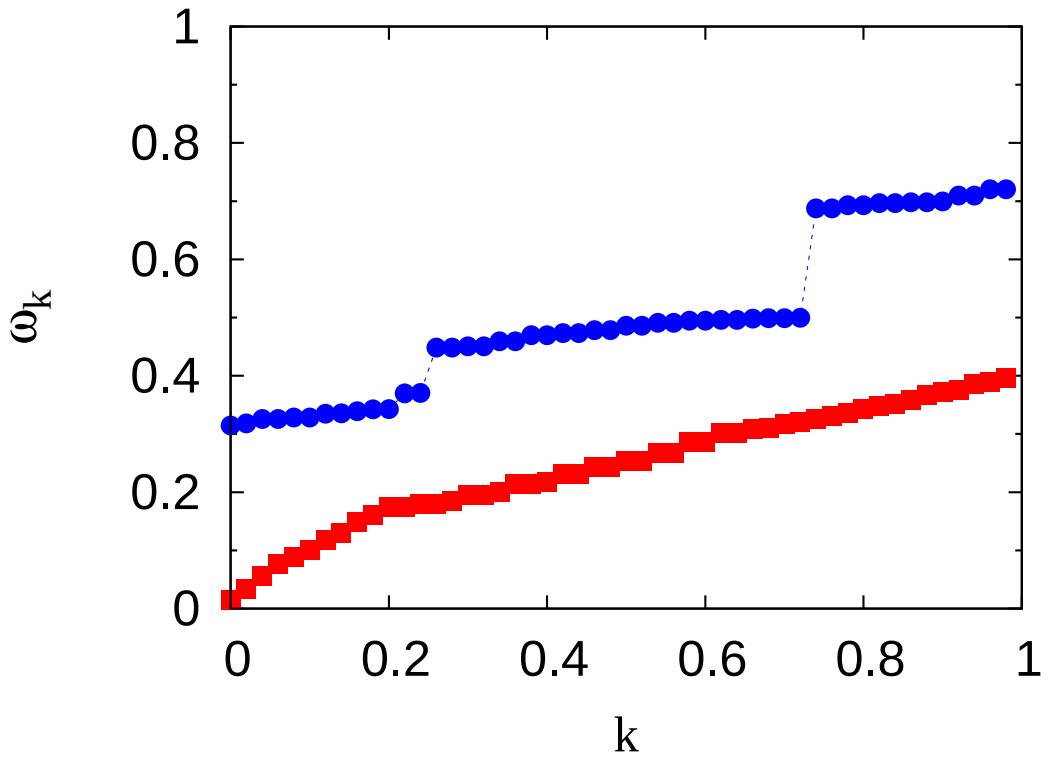


Fig.2 Phonon spectrum $\omega(k)$ as a function of scaled mode number $k = i/N$ $(i = 0, \ldots, N-1)$, for $K = 0.03$ (bottom curve, squares) and $K = 0.2$ (top curve, points) for the case of Fig.1

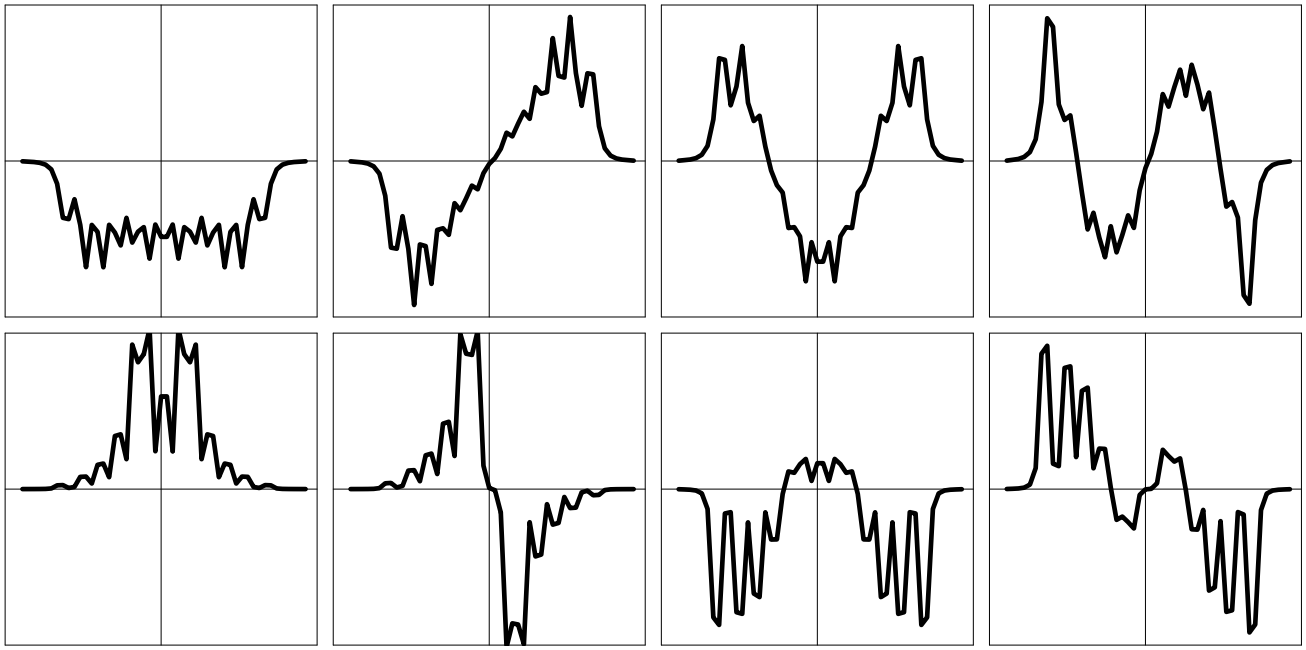


Fig.2bis Phonon eigenmodes in the chain with $N = 50$ ions at the golden mean ion density with $\omega = 0.014$. Panels show the amplitude of eigenmode (in arbitrary linear units) vs. ion positions x_i varied from minimal to maximal value for lowest 4 modes with number 0, 1, 2, 3 (from left to right).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

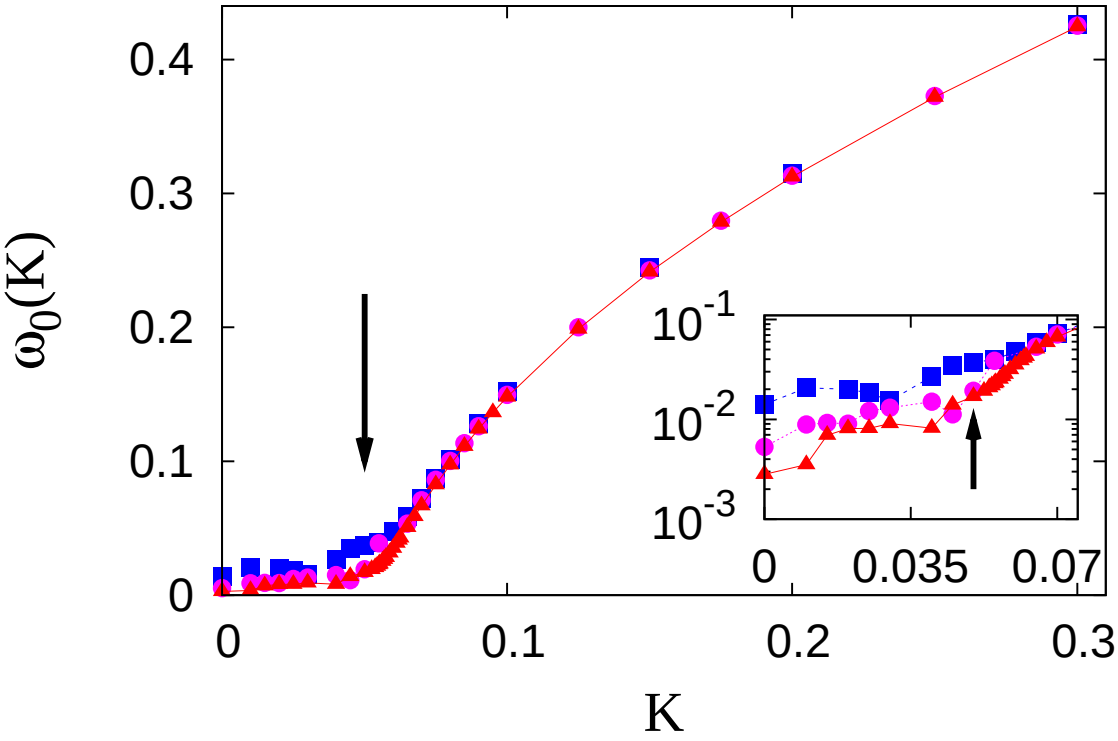


Fig.3 Minimal excitation frequency $\omega_0(K)$ as a function of periodic potential strength K for the golden mean ion density ν_g and number of ions $N = 50$ (squares; $\omega = 0.014$), $N = 150$ (circles; $\omega = 0.00528$), $N = 300$ (triangles, $\omega = 0.00281$). The critical point $K_c \approx 0.05$ is marked by arrow; inset shows data near K_c.

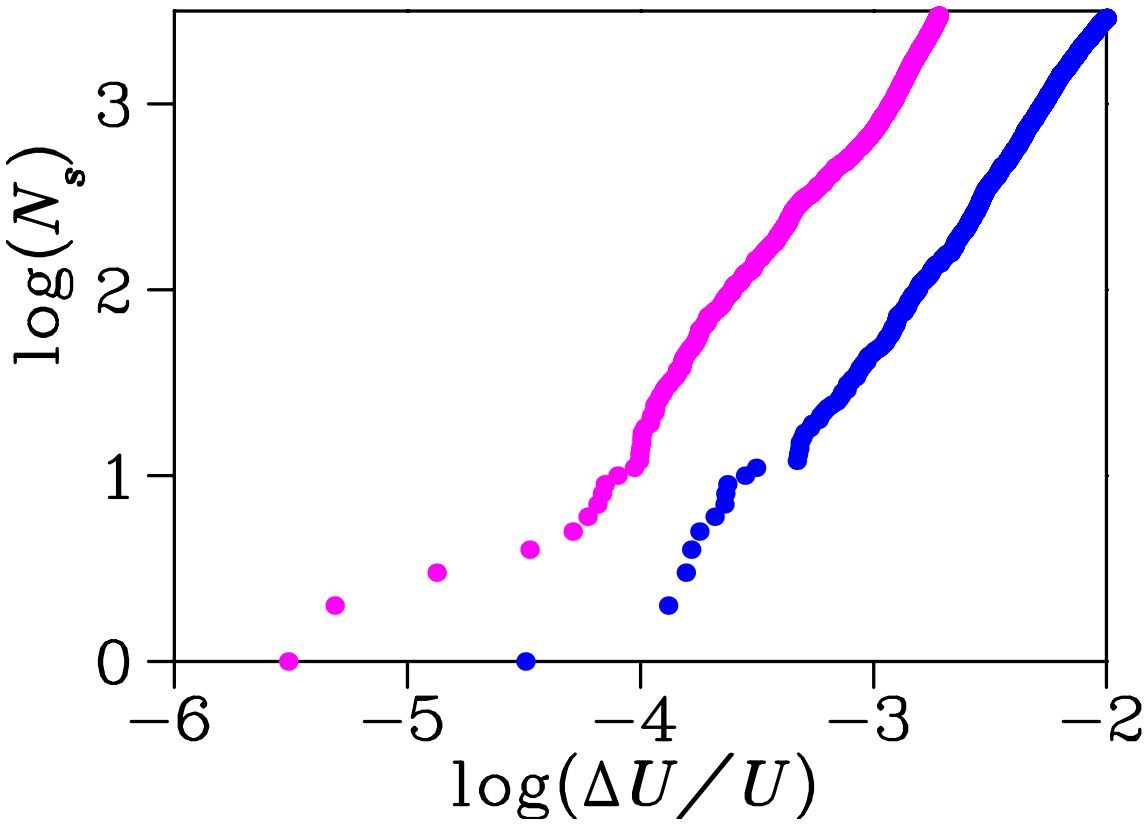


Fig.4 Number of equilibrium configurations N_s as a function of their relative excitation energy $\Delta U/U$ above the ground state for 50 (blue/black) and 150 (magenta/gray) ions at $K = 0.2$ with ω as in Fig.3 (logarithms are decimal).

Numerical Results for the Quantum FKI Model

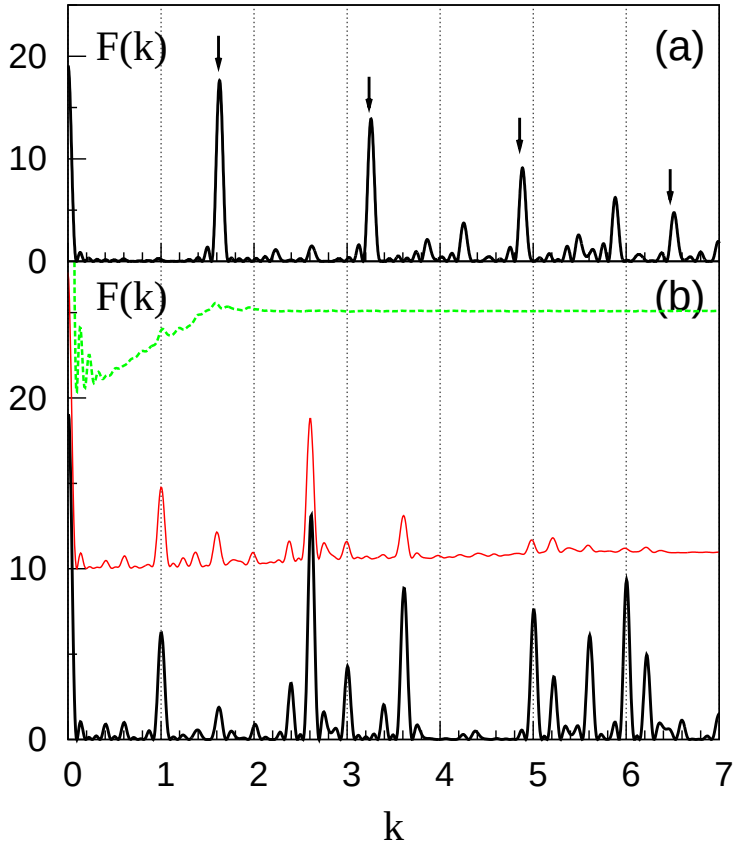


Fig.5 Formfactor of the chain $F(k) = \langle \sum_i \left| \exp(ikx_i(\tau)) \right|^2 \rangle / \delta N$ for $N = 50$ ions and $\omega = 0.014$. **(a)**: The classical incommensurate phase at $K = 0.03$, $\hbar = 0$, arrows mark the peaks at integer multiples of golden mean density ν_g. **(b)** The 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). The temperature of the quantum chain is $T = \hbar/\tau_0$ with $\tau_0 = 400$ so that $T \ll K$ and $T \ll \hbar\omega_0(K)$. The quantum phase transition take place at $\hbar_c \approx 1$.

Physical Parameters for the FKI Model

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 of Blatt experiments the distance between Ca ions is about $\Delta x \approx 5\mu m$ so that the golden mean density ν_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 $V = K_c e^2/d \approx 0.6K$ that in principle can be reached in strong laser fields. For $^{40}Ca^+$ ions with such d the dimensionless Planck constant is $\hbar_{eff} = \hbar/(e\sqrt{md}) \approx 3 \times 10^{-5}$. 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 ω_k for $K > K_c$ (Figs.2,3) may be useful for protection of quantum gate operations in quantum computations.

Higher values of dimensionless $\hbar$ can be reached with electrons forming a Wigner crystal placed in a periodic potential where $\hbar \approx 0.1$ for $d \approx 5nm$. Such a situation may appear in 1D electron wires, molecular structures or nanotubes where a devil's staircase behavior has been discussed recently. 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.