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ABOUT PROPERTIES OF IR ACTIVE LATTICE VIBRATIONS IN THE VICINITY OF KINKS IN THE FRENKEL-KONTOROVA MODEL

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We present an analysis of an impact of kinks in the Frenkel-Kontorova model on infrared lattice vibrations. Our results show that the vibration of particles involved into the kink formation is very similar to that in a gap mode around a force constant defect. We found that the IR phonon mode intensity possess a universal dependence on certain combination of system parameters and the kinks concentration. On the bases of these results a criterion, which allows to separate the regime of weakly interacting kinks in the system from the regime of kink lattice is proposed.

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A system of interacting particles in sinusoidal external potential (Frenkel–Kontorova (FK) model [1]) is widely used for description of a broad variety of physical phenomena, such as statics and dynamics of incommensurate phases (see, e.g. [2]), transport properties in quasi-one dimensional conductors (see [3] and references therein), adatoms diffusion on a metal surface [4], etc. Peculiar features of the FK model usually explored are related to the kink-like solitons. Properties of the kinks have been described in a number of publications [5–10]. The dynamics of the FK model has also been extensively studied, but mostly in relation to the kink lattice rather than to the single kink [11–14]. Whereas it is not completely clear yet at what system parameters the single-kink effects can be still important.

The aim of the present study is to investigate an impact of both single kink and kink lattice onto infrared (IR) active phonon spectrum and to specify the range of the model parameters in which its properties can be treated in terms of nearly independent kinks rather than in terms of superstructure, associated with the kink lattice.

The investigations have been performed in two approaches: i) molecular dynamic (MD) simulation has been used for the system to reach an equilibrium state according to the method proposed in [15], after what all the particles have been subjected to a small uniform step-like displacement and subsequent vibrations has been analyzed via Fourier-transformation; ii) eigen vector problem (EVP) has been solved in the harmonic approximation to study the vibrational spectrum of the system. The kinks in this case have been taken into account through expansion of the potential energy around particle equilibrium positions determined from MD simulation.

Let us consider a chain of particles of mass m and charge e with nearest neighbor interaction in the sinusoidal external potential $V(x) = -(V \cdot a^2/4\pi^2)\cos(2\pi x/a)$ where a is the period of the potential. In case of harmonic interparticle potential

the motion equation for n-th particle is

$$m\frac{\partial^2 U_n}{\partial t^2}+\gamma\frac{\partial U_n}{\partial t}+K_2(2U_n-U_{n-1}-U_{n+1})+\frac{Va}{2\pi}\sin\left(2\pi\frac{U_n}{a}\right)=eE(t), \qquad (1)$$

where γ is phenomenological damping and $E(t)$ is external electric field. Let the time dependent position U_n of the particle can be represented as $U_n = na+U_n^0+\delta_n(t)$,where U_n^0 is quasistatic variable describing a shift of the equilibrium position of the particle with respect to the corresponding potential minimum, $\delta_n(t)$ describes a vibration of the particle around the new equilibrium position U_n^0. Then suggesting $\delta_n(t) = \delta_n(\omega)\exp(i\omega t)$ and $E(t) = E_0\exp(i\omega t)$ the Eq. (1) can be splitted into two equations

$$K_2(2U_n^0-U_{n-1}^0-U_{n+1}^0)+\frac{V}{2\pi}\sin\left(2\pi U_n^0\right) = 0, \qquad (2)$$

$$\delta_n(\omega)\left[V\cos\left(2\pi U_n^0\right)-\omega^2+i\omega\gamma\right]+K_2(2\delta_n(\omega)-\delta_{n-1}(\omega)-\delta_{n+1}(\omega)) = E_0, \qquad (3)$$

here and below we accepted $m = 1$, $e = 1$ and $a = 1$. Disregarding the trivial case $U_n^0 = 0$ Eq. (2) describes quasistatic kink-like deformation of the chain (due to neglection of the dynamical term we restrict our consideration by standing kinks only), while Eq. (3) describes the particle vibration around the new equilibrium position. In the continuous limit Eq. (2) reduces to the sine-Gordon equation [16] with the single-kink solution [17] $U_n^0(i) = 2\pi^{-1}\mathrm{arctg}\{\exp[\pm 2(n-i)a/R_k]\}$, $R_k = 2\sqrt{K_2/V}$ can be considered as the kink radius measured in a units, i is the kink position. Substituting this solution into Eq. ($\chi(\omega) = E_0^{-1}\sum\delta_n(\omega)$, where peaks in $\mathrm{Im}(\chi(\omega))$ correspond to resonances ω_r and $\mathrm{Re}(\delta_n(\omega_r))$ corresponds to properly normalized eigen vector of the mode at ω_r.

It is well established that the presence of kinks (or domain walls) in case of negligible Peierls–Nabarro potential barrier results in zero-frequency peak (phason mode) in the optical conductivity spectrum $\sigma(\omega) = \omega\,\mathrm{Im}(\chi(\omega))$ (see Fig.1) corresponding to translational motion of kinks. The high frequency peaks in Fig.1 correspond to the phonons, the strongest one being related to the inphase vibrations of particles inside potential wells. The particles involved into the kink formation obviously possess a higher vibration amplitude at low frequencies, while, as it is shown in the Fig.2, they are almost completely eliminated from the phonon-like normal mode (the strongest one in the Fig.1). By dashed lines in Fig.2 there are shown the eigen vectors also for the case of the external force constant defect $\Delta V(i)$ in the particle site i and the rest particles being situated inside the potential wells. The corresponding spectrum is also shown in Fig.1. The strength of the defect has been determined from equation [18]

$$1+\frac{\Delta V}{N}\sum\frac{1}{V+4K_2\cdot\sin^2\left(\frac{k}{2}\right)} = 0, \qquad (4)$$

which means the zero-frequency gap mode formation in the vicinity of the ivery close to that of the kink while the eigen vectors of the phonon-like mode nearly coincide in both cases. Also the localization length of the gap mode S_{gap} (the halfwidth of the peak shown by dashed line in Fig.2) is equal to $R_k/\sqrt{2}$ in a wide range of R_k values (see insert in Fig.2). On this basis one may consider the system with kinks as a defect, or impurity crystal taking for the description of its vibrational properties all the results already known. For instance, it is well

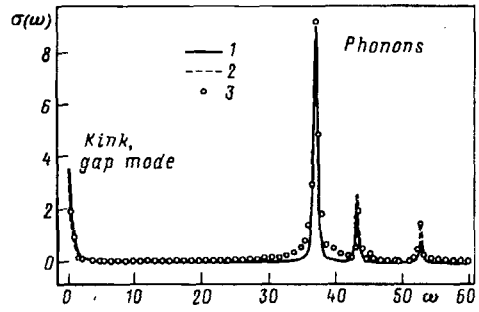

Fig.1. Conductivity spectra of the Frenkel–Kontorova model containing 32 particles arranged over 31 potential wells: *1* is the spectrum calculated by (3) and (o) is that obtained by MD simulation for $K_2 = 4V$, $\sqrt{V} = 36$ arb.un.; *2* is the spectrum corresponding to the force constant defect $\Delta V = -4.1231V$ (see text), in the position of the kink middle particle no.16

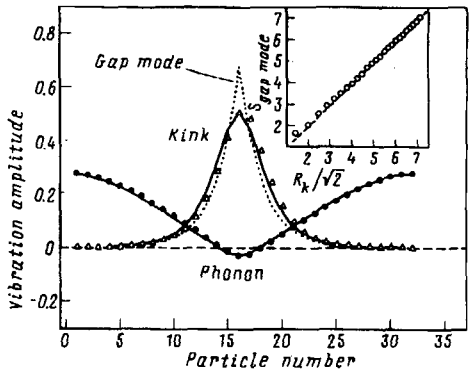

Fig.2. The kink and the phonon (the strongest peak in Fig.1) eigen vectors obtained in the ways corresponding to those in Fig.1. By symbols in the insert the dependence of the gap mode radius upon kink radius $R_k = 2\sqrt{\frac{K_2}{V}}$ is shown

understood that S_{gap} is determined basically by separation of the gap mode from the optical band $\sqrt{V}$ and by the bandwidth $2\sqrt{K_2}$. One may argue therefore that the similarity between kink and the gap mode eigen vectors and the kink eigen vector itself does not depend on the potential anharmonicity provided that its influence on the above mentioned parameters is small enough. Thus, we expect that our results will be applicable for a more realistic interparticle potential too. From the analogy between the kinks and the defects it follows also that the IR phonon mode intensity will show a linear decrease versus n_k for low kink concentration. It really takes place in certain range of R_k values.

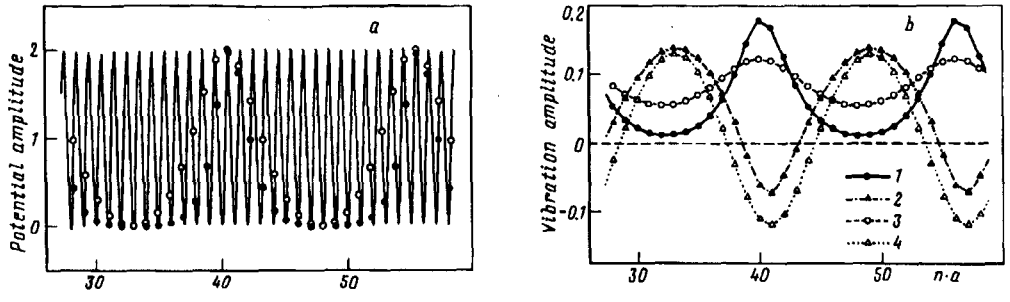

Fig.3. *a*) The particle arrangement in the FK model of 128 particles (shown by symbols) in 120 potential wells (solid line). *b*) The eigen vectors of the kink-(*1*, *3*) and phonon-like (*2*, *4*) modes. $K_2 = 4V$ (solid symbols) and $K_2 = 16V$ (open symbols), $\sqrt{V} = 36$ arb.un

Although the N-kink solution of Eq. (2) is also available [19] it is more convenient to approximate it with the sum of single-kink solutions. Our MD study of the ground state of a system consisting of 128 particles arranged in 128-N_k

potential wells with cyclic boundary conditions showed that even for $N_k \gg 1$ (N_k is a number of kinks) the kinks lattice can be perfectly described as a sum of the single-kink solutions with $R_k \simeq 2\sqrt{K_2/V}$. Namely, for $N_k = 8$ and $K_2 = 4V$ ($R_k^{theor} = 4.0$) the value of $R_k^{exp} \simeq 3.94$ has been obtained. Similar results have been obtained also for the case when the number of potential wells exceeds that of the particles. The dipole moment spectrum $I(\omega) = \mathrm{Im}[\sum \delta_n(\omega)/E_0]$ has been both calculated from (3) substituting $U_n^0 = \sum U_n^0(i)$ with $R_k = R_k^{exp}$ and obtained from MD simulation via fluctuation dissipative approach for various values of $\eta = R_k n_k$ ($n_k = N_k/128$ is the kink concentration). Both approaches agree rather well even at very low frequencies although the harmonic approximation obviously fails at $\omega = 0$. Two examples of the particles arrangement and corresponding eigen vectors of the IR vibrations are presented in Fig.3. The eigen vectors for $\eta = 0.25$ are looking quite similar to those for the single kink or gap mode while for $\eta = 0.5$ even the particles which still occupy the potential wells and not involved into the kinks formation are strongly involved into the characteristic IR vibration (compare the *a* and the *b* panels in Fig.3). It should be pointed out that there is no noticeable difference between the commensurate and incommensurate cases (kink lattice period is equal and is not equal to an integer number of the *a*, respectively) if the kink concentration is not too high. Otherwise the difference manifests itself in a small shift of the zero-frequency peak shown in Fig.1 from its position.

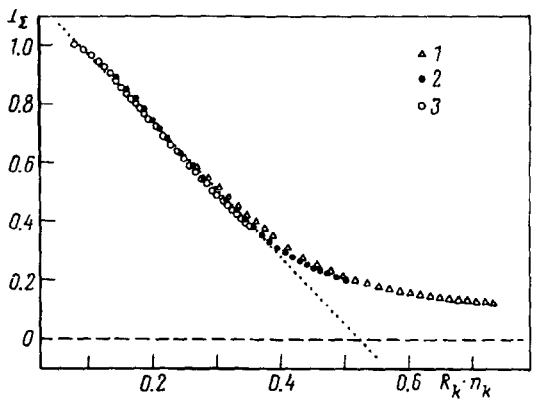

Fig.4. Integrated intensity of the phonon-like modes upon $\eta = R_k n_k$ calculated using (3) for FK model of 128 particles arranged in 112 wells (*1*) ($n_k = 1/8$), 120 wells (*2*) ($n_k = 1/16$), and 124 wells (*3*) ($n_k = 1/32$)

We concentrate here on a question concerned with the intensity of the phonon peaks shown in Fig.1 as a function of the parameter η. For investigation we used the EVP approach using Eq. (3) for various values of K_2/V and n_k. The results are presented in Fig.4. The integrated intensity $I_\Sigma = \int I(\omega)\, d\omega$ of the phonon peaks reveals a universal dependence on the parameter $\eta = R_k n_k$. We found also that the eigen vectors of the strongest IR vibration obtained for different n_k but for one and the same η values, can be transformed to each other by proper scaling of *a*, i.e. they obey some sort of scaling invariance. Note, that the parameter η means a volume fraction (in $1D$ case) occupied by the kinks and the observed decrease in I_Σ at low η values can be interpreted as washing out of the high frequency density of states by gap modes associated with the kinks. At higher η, when the kinks form real lattice and eventually sinusoidal superstructure due to interaction with each other, the decrease in $I_\Sigma \propto \eta$ slows down because the real kink radius can not exceed at least one half of the kink lattice period. Indeed, the linear decrease in I_Σ shown in Fig.4 ends at a cut-off value of $\eta \simeq 0.4$

which implies the above mentioned restriction on the kink radius is $R_k \leq 0.4k_s^{-1}$ ($k_s = n_k$) where k_s is the kink lattice (or superstructure) wave vector measured in units of $\pi/2a$. Thus, we can display a range of parameters $k_s\sqrt{K_2/V} \leq 0.2$ in which it is possible (or even necessary) to describe the properties of the system in terms of independent kinks rather than in terms of some effective superstructure related to the kink lattice. Since the IR eigen vectors has been argued to be not very sensitive to anharmonicity one might expect this criterion holds for more realistic potentials too.

Using the above criterion one can examine if the kinks are important for description of some particular system. For example, in the charge density wave conductor $(TaSe_4)_2I$ the superstructure wave vector $k_s \simeq 0.085$ [20], $\sqrt{V}$ can be associated with the giant IR peak frequency $\omega \sim 0.005\,eV$ [21] and $\sqrt{K_2}$ can be estimated from above as $\sqrt{K_2} < \omega_p \simeq 1\,eV$ [22], where ω_p is the plasma frequency. Thus, one obtains $k_s\sqrt{K_2/V} < 1$ which implies that the kink effects can be important in this compound. A more detailed consideration of vibrational properties of $1D$ conductors on the basis of the obtained results will be given in the forthcoming paper.

In conclusion we showed that i) the vibrational properties of kinks in the Frenkel–Kontorova model are very similar to those of the gap modes in $1D$ crystal with force constant defects; ii) on the basis of the universal dependence of the IR phonon mode intensity on certain combination of the system parameters it is possible to estimate whether single-kink effects are important for a particular physical system.

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