Dynamic properties of solitons in the Frenkel-Kontorova Model. Application to incommensurate CDW conductors

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An impact of kink-type solitons on infrared lattice vibrations is studied for incommensurate Frenkel-Kontorova model. It is shown that the vibration of particles involved into the kink formation is very similar to that in a gap mode around the force constant defect. IR phonon mode intensity is found to possess a universal dependence on the system parameters and the kink concentration. It is argued that the giant IR peak observed in a number of incommensurate charge density wave conductors can be explained in terms of dynamic charge transfer stimulated by kinks.

Keywords: solitons, infrared spectrum, charge density waves

I. INTRODUCTION

A system of interacting particles in sinusoidal external potential (Frenkel-Kontorova (FK) model) 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 Ref. 3 and references therein), adatoms diffusion on a metal surface, 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. The dynamics of the FK model has also been extensively studied, but mostly in relation to dynamics of incommensurate superstructures rather than to the single kink. Whereas it is not completely clear yet at what system parameters the single-kink effects can be still important.

Incommensurate charge density wave (CDW) conductors are the physical systems for which the single-kink effects can be very important. Vibration and transport properties of these systems attract great interest due to numerous peculiarities. The most striking among them are: i) the giant peak of unknown origin in the low frequency infrared (IR) spectrum of a number of inorganic CDW conductors such as $K_{0.3}MoO_3$, $(TaSe_4)_2I$ and $TaS_3$; ii) nonlinear conductivity and noise generation when conducting dc current by these materials.

The aim of the present study is to investigate an impact of both single kink and kink lattice onto 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. I believe that after comparison of the numerical results with the experimental data and proper justification of the model it can serve as a bases for understanding of the microscopic nature of the aforementioned peculiar features of CDWs.

The investigations were performed in two approaches: i) molecular dynamic (MD) simulation was used for the system to reach an equilibrium state according to the method proposed in Ref. 17, after what all the particles were subjected to a small uniform step-like displacement and subsequent vibrations were analyzed via Fourier-transformation; ii) eigenvector problem (EVP) was solved in the harmonic approximation to study the vibration spectrum of the system. The kinks in this case were taken into account through expansion of the potential energy around particle equilibrium positions obtained from MD simulation.

II. VIBRATION SPECTRUM IN THE PRESENCE OF KINKS

Let us consider a chain of particles of mass $m$ and charge $e$ with nearest neighbor interaction in the sinusoidal external potential $V(x) = -V \frac{a^2}{\pi^2} \cos(2\pi \cdot \frac{x}{a})$ where $a$ is the potential period. In case of harmonic interparticle interaction the motion equation for $n$-th particle is

$$m \cdot \frac{d^2U_n}{dt^2} + \gamma \cdot \frac{dU_n}{dt} + K_2 \cdot (2U_n - U_{n-1} - U_{n+1}) + \frac{V \cdot a}{2\pi} \cdot \sin \left(2\pi \cdot \frac{U_n}{a}\right) = e \cdot E(t),$$

(1)
where $\gamma$ is phenomenological damping and $E(t)$ is external electric field. Let the time dependent position $U_n$ of the particle can be represented as $U_n(t) = n \cdot a + U_n^0 + \delta_n(t)$, 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 $\delta_n(t) = \delta_n(\omega) \cdot \exp(\ii \omega \cdot t)$ and $E(t) = E_0 \cdot \exp(\ii \omega \cdot t)$ the Eq. (1) can be splitted into two equations

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

$$\delta_n(\omega) \cdot \left[V \cdot \cos \left(2\pi \cdot U_n^0\right) - \omega^2 + \ii \omega \cdot \gamma\right] + \frac{K_2}{m} \cdot (2\delta_n(\omega) - \delta_{n-1}(\omega) - \delta_{n+1}(\omega)) = \frac{\epsilon}{m} \cdot E_0.$$  

Disregarding the trivial case $U_n^0 = 0$ when number of particles $N_{part}$ is equal to the number of potential minima $N_{pot}$, 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). Eq. (3) describes the particle vibration around the new equilibrium position. In the continues limit Eq. (2) reduces to the sine-Gordon equation [18] with the single-kink solution [19]:

$$U_n^0(i) = 2a \cdot \pi^{-1} \cdot \arctg \left\{ \exp \left[ \pm \frac{2(n-i-\frac{1}{2})}{R_k} \right] \right\}; \quad R_k = 2a \sqrt{\frac{K_2}{\pi}}$$

can be considered as the kink radius, $i$ is the kink position.

Substituting this solution into Eq. (3) one can obtain the complex susceptibility $\chi(\omega) = \frac{1}{E_0} \cdot \sum \delta_n(\omega)$, where the peaks in $\text{Im} (\chi(\omega))$ correspond to resonances $\omega_r$ and $\text{Re} (\delta_n(\omega_r))$ corresponds to suitably normalized eigenvector of the mode at $\omega_r$.

Fig.1 shows the $\omega(k)$ plot without (a) and with (b-c) kinks in the model system. One can see the smearing of the resonances in the presence of single kink (Fig.1a) while this smearing is gone in the system with the kink lattice (Fig.1c). Instead, the phonon band folding due to the kink lattice and the additional low frequency vibration arise. The latter is a so-called phason, which is related to translational motion of kink(s) (domain wall(s)). In case of negligible Peierls-Nabarro potential barrier the phason frequency tends to zero. The phason is IR active and looks like a steep increase at $\omega \rightarrow 0$ in the optical conductivity spectrum $\sigma(\omega) = \omega \cdot \text{Im} (\chi(\omega))$ (see Fig.2). The high frequency peaks in Fig.2 correspond to phonons, the strongest one being related to in-phase vibration of the particles situated near bottom of potential wells.

### III. SIMILARITY BETWEEN KINK AND THE FORCE CONSTANT DEFECT

The smearing of the vibrational states in the presence of single kink shown in Fig.1b suggests that the kink is acting like a point defect. Moreover, the particles involved into the kink formation are almost completely eliminated from the high frequency phonon-like normal modes while these particles obviously possess a higher vibration amplitude (local vibration density) at low frequencies (see Fig.3). This is quantitatively illustrated in Fig.4 where the eigenvectors of phason mode and that of IR phonon mode are shown. Accordingly, one could try to describe vibration properties of kinks in terms of localized vibrations around force constant defect. That means the original incommensurate ($N_{part} \neq N_{pot}$) FK model is replaced by commensurate one (or the ordinary harmonic chain of particles with harmonic incite and interpaticle potentials) and some particle cites possess a defect force constant. The strength of the defect has been determined from equation [20]

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

what means the zero-frequency gap mode formation in the vicinity of the defect cite. As it is shown in Fig.4 the eigenvector of the gap mode is very close to that of the phason while the eigenvectors of the phonon-like mode nearly coincide in both cases. The corresponding spectrum of the 1D crystal with the force constant defect is also shown in Fig.2. Note, that the localization length of the gap mode $S_{gap}$ (the halfwidth of the peak shown by dashed line in Fig.4) is equal to $R_k / \sqrt{2}$ in a wide range of $R_k$ values (see insert in Fig.4).

Thus, one may consider the system with kinks as a defect, or impurity crystal taking for the description of its vibration properties all the results already known. For instance, it is well understood that $S_{gap}$ is determined basically by splitting of the gap mode from the bottom of the optical band $\omega_0 = \sqrt{V}$ and by the optical bandwidth $2\sqrt{K_2}$. One may argue therefore that the similarity between phason and the gap mode eigenvectors and the phason eigenvector itself does not depend on the potential anharmonicity provided that its influence on the above mentioned parameters is small enough. It is thought therefore that the obtained 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 \( n_k \) (\( n_k = \frac{N_k}{N_{part}} \) is the kink concentration and \( N_k = |N_{part} - N_{pot}| \) is the number of kinks) for low kink concentration. This indeed does take place in certain range of \( R_k \) values.

IV. WHEN THE KINK EFFECTS ARE IMPORTANT

Although the N-kink solution of Eq. (2) is also available \([21]\) 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 \( N_k \gg 1 \) the kink lattice can be perfectly described as a sum of the single-kink solutions with \( R_k \simeq 2a\sqrt{K_2} \). Namely, for \( N_k = 8 \) and \( K_2 = 4 \ast V \) \( (R_{theor} = 4.0a) \) the value of \( R_k^{exp} \simeq 3.94a \) 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 \( I(\omega) = \text{Im} \left[ \sum \delta_n(\omega) \right] \) has been both calculated from \([3] \) substituting \( U_0 = \sum U_n(i) \) with \( R_k = R_k^{exp} \) and obtained from MD simulation via fluctuation dissipative approach for various values of \( \eta = R_k \cdot n_k \). 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 eigenvectors of the IR vibrations are presented in Fig.5. The eigenvectors for \( \eta = 0.25 \) can be represented as a superposition of the single-kink eigenvectors while for \( \eta = 0.5 \) they are looking quite different: even those particles which still occupy the potential wells and are not involved into the kinks formation, are strongly involved into the characteristic IR vibration (compare (a) and (b) in Fig.5). 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 \( a \), respectively) if the kink concentration is not too high. Otherwise the difference manifests itself in a small shift of the zero-frequency peak in Fig.2 from its position.

I concentrate here on a question concerned with the intensity of the phonon peaks in Fig.2 as a function of the parameter \( \eta \). The EVP approach (Eq. \([3] \) with various values of \( \frac{\delta_n}{E_0} \) and \( n_k \)) was used for this study. The results are presented in Fig.6. The integrated intensity \( I_2 = \int I(\omega) \, d\omega \) of the phonon peaks reveals a universal dependence on the parameter \( \eta \) \([22]\). It was also found that the eigenvector of the strongest IR vibration obey some sort of scaling invariance: the vectors obtained at different \( n_k \) but for one and the same \( \eta \) can be transformed to each other by proper scaling of \( a \). Note, that the parameter \( \eta \) means a volume fraction (in 1-D case) occupied by the kinks and the observed decrease in \( I_2 \) at low \( \eta \) values can be interpreted as washing out of the high frequency density of states by gap modes associated with kinks. At higher \( \eta \), when the kinks form real lattice and eventually sinusoidal superstructure due to interaction with each other, the decrease in \( I_2 \propto \eta \) slows down because the real kink radius can not exceed at least one half of the kink lattice period. Indeed, the linear decrease in \( I_2 \) shown in Fig.6 ends at a cut-off value of \( \eta \simeq 0.4 \) \((a = 1)\) which implies the above mentioned restriction on the kink radius is \( R_k \leq 0.4 \ast k_s^{-1} \), \((k_s = n_k)\) where \( k_s \) is the kink lattice (or superstructure) wave vector measured in units of \( \frac{n}{a} \). Thus, one can display a range of parameters \( k_s \cdot \sqrt{\frac{K_2}{\omega_0}} \leq 0.2 \) in which the single-kink effects are important, i.e. the system can not be explicitly treated in terms of some sinusoidal superstructure related to the kink lattice. Since the IR eigenvectors has been argued to be not very sensitive to anharmonicity one might expect this criterion holds for more realistic potentials too.

V. CDW COLLECTIVE DYNAMICS

The low frequency excitation spectrum of the CDW ground state have been widely investigated both theoretically and experimentally (see, for example, reviews \([22,23]\) and references therein). It is well established that incommensurate CDW ground state is characterized by two specific collective excitations: IR active phase mode and Raman active amplitude mode. \([2] \) The frequency of the former, \( \omega_p \), in the incommensurate CDW conductors is of the order of \( 1cm^{-1} \) while the amplitude mode frequency \( \omega_a \) is about one-two orders of magnitude higher. These vibrations have been observed experimentally in such model CDW conductors as \( K_0.3MoO_3, (TaSe_4)_2I \) and \( TaS_3 \) \([16,17,27,22]\). Besides the phase and the amplitude modes an additional vibration obeying giant IR activity has been observed in all the above mentioned compounds \([13,16]\). The frequency of this additional feature in \( (TaSe_4)_2I \) is about \( 38cm^{-1} \) in between the phase \((\sim 1cm^{-1} \) \([33]\) and the amplitude \((\sim 90cm^{-1} \) \([29]\) mode frequencies. Several explanations have been proposed to account for the additional giant IR peak, but microscopic origin of this vibration is still not clear (see, for instance, the discussions in Refs.1 and 15). In phenomenological model \([34]\) the additional giant IR peak was
thought to result from a bound collective-mode resonance localized around impurity, but again without emphasis of microscopic origin of the model parameters.

Below it is shown that the giant IR resonance occurs in the incommensurate CDW system even in the absence of any impurities provided that the dynamical charge transfer between adjacent CDW periods is taken into account and the CDW possesses some kink lattice structure rather than sinusoidal structure.

Since the lattice deformation coupled to the CDW is much smaller than the crystal lattice constant it is reasonable to describe the CDW system within the FK model. The CDW periods in this case are associated with particles of mass \( m \) and charge \( e \) which are placed into sinusoidal external (crystal lattice) potential \( V (\mathbf{x}) = -V_{0} \frac{\mathbf{\hat{a}}^2}{a} \cdot \cos \left( 2\pi \cdot \frac{\mathbf{\hat{x}}}{a} \right) \). The interparticle distance in the commensurate phase is accepted to be equal to 2\( a \) what means the CDW is formed due to dimerization. In case of \( 2N_{\text{part}} \neq N_{\text{pot}} \) one again obtains incommensurate structure (kink lattice) and the time dependent position \( U_{n} \) of the particle can be represented as \( U_{n} (t) = 2 \cdot n \cdot a + U_{n}^{0} + \delta_{a}(t) \).

### A. Dynamic charge transfer

As it has been demonstrated by Itkis and Brill [33], spatial redistribution of the charge condensed in CDW takes place under action of static electric field. Obviously a characteristic time for the charge redistribution or, in the other words, for the charge transfer from one CDW period to another is determined by the amplitude mode frequency \( \sim 90 \text{cm}^{-1} \) [29]. Therefore, in the case of the giant peak frequency the adiabatic condition is fulfilled.

To take into account the charge transfer contribution to the IR intensity of any mode let us suppose that the particle charge in our model is determined as

\[
\tilde{e}_{n} (t) = e \cdot (1 + \beta \cdot (\delta_{n+1} (t) - \delta_{n-1} (t))) ,
\]

what means that the charge is transferred from the region of local compression of the CDW to a region of local dilatation. The factor \( \beta \) determines the fraction of the particle charge transferred during vibration. The dipole moment \( P (t) \) is determined as a sum of the part related to the particles displacement \( P_{0} (t) \) and the part, related to the charge transfer between adjacent unit cells \( P_{ct} (t) \)

\[
P (t) = P_{0} (t) + P_{ct} (t) = \sum_{n} e \cdot [\delta_{n} (t) + \beta \cdot (U_{n}^{0} - U_{n-1}^{0}) \cdot (\delta_{n+1} (t) - \delta_{n-1} (t) - \delta_{n} (t) + \delta_{n-2} (t))].
\]

In commensurate phase \( U_{n}^{0} - U_{n-1}^{0} = a \) for all \( n \) and the charge transfer dipole moment \( P_{ct} (t) \) vanishes according to [2]. In incommensurate phase the \( P_{ct} (t) \) value can be rather high. It will be shown that the charge transfer effect is essentially determined by kink-related disturbance of the periodicity in the particle arrangement. Using the criterion of importance of single-kink effects obtained in the preceding section one can examine if the kinks are important for description of the charge density wave conductor \((TaSe_{4})_{2}I\). The superstructure wave vector in this system is \( K_{s} \simeq 0.085 \) [34], \( \sqrt{V/m} \) can be associated with the giant IR peak frequency \( \omega \sim 0.005 \text{ eV} \) [37] and \( \sqrt{K_{s}} \) can be estimated from the phason dispersion \( \sqrt{K_{s}} \simeq 0.001 \text{ eV} \) [38]. Thus, one obtains \( K_{s} \cdot \frac{\sqrt{K_{s}}}{\omega} \ll 1 \) what implies that the kink effects can be important in this compound.

Fig.7a shows the fragment of MD simulation of arrangement of 128 particles over 264 potential wells, i.e., the CDW with superstructure. The 51-th particle (shown by arrow in the figure) is pinned. The conductivity spectra \( I (\omega) = \omega \cdot \text{Im} \left[ \sum_{E_{0}} \delta_{e} (\omega) / E_{0} \right] \) obtained from MD simulation are shown in Fig.8 for both pinned and depinned system. The features of the interest are the phase mode (PM) and the peak of CT mode (charge transfer mode), marked by PM- and CT-arrows in Fig.8, respectively. The latter peak is genetically related to the vibration with the wave vector equal to that of the superstructure. The corresponding eigenvectors are shown in Fig.7b. Taking into account that the CDW internal deformation can be adiabatically accompanied by charge redistribution one obtains that the CT peak acquires the giant IR intensity. The conductivity spectra in which the charge transfer effect has been taken into account according to Eqs [2] and [2] are shown in Fig.8 by symbols (depinned chain) and thin solid line (pinned chain). The phase mode intensity is almost independent on the charge transfer effect while the CT mode intensity increases several orders in magnitude.

Fig.9 shows that the CT mode intensity \( \left( \text{Im} \left[ \sum_{E_{0}} \delta_{e} (\omega) / E_{0} \right] \right) \) with charge transfer contribution decreases with the increase of the parameter \( 4a \sqrt{K_{s}} \) and possesses a universal dependence regardless the superstructure wave vector.
Physically this feature can be understood in the following way. The charge transfer dipole moment consists of a sum of elementary dipole moments resulting from the charge transfer over the inter-kink distance. The longer is the latter the higher is the elementary dipole moment, but the smaller is the number of these dipole moments. Thus, the total charge transfer dipole moment does not depend on the kink concentration (probably unless $4a\sqrt{\frac{K_2}{V}} < a/n_k$). On the other hand, this dipole moment strongly depends on the kink-mediated distortion of the chain. The latter decreases with the increase of the kink radius resulting in the observed decrease in CT mode intensity in Fig.9.

It was experimentally proved that the giant IR peak intensity in $(TaSe_4)_2I$ increases with the increase of the sample temperature [33]. This unusual feature can be naturally explained in terms of the charge transfer effect discussed above. Indeed, as it is clear from Fig.9 the integrated intensity of the CT mode as a function of the system parameters can be approximated as (see dashed line in Fig.9)

$$I \simeq C_0 \cdot e^{2 \cdot \left[ \sqrt{\frac{K_2}{V}} \right]^{-2.25}}$$

where $C_0$ is constant. The interparticle force constant, obviously, depends on the particle charge $K_2 = e^2 K'_2$ since the particles are associated with the charges condensed in CDW. The (7) can be then rewritten as

$$I \simeq C_0 \cdot e^{-0.25 \cdot \left[ \sqrt{\frac{K_2}{V}} \right]^{-2.25}}$$

Thus, despite the decrease of the particle charge (the CDW amplitude) the CT mode integrated intensity increases upon approaching $T_p \simeq 261K$ from below! Due to short range order the particle charge (CDW amplitude) remains finite even at very high temperatures and accounts for the high CT mode intensity well above $T_p$.

Note one more peculiarity of the CT peak. It does not depend on the number of particles in the coherent CDW domain or, in the other words, on the effective mass of CDW condensate. The latter can explain why the corresponding frequency has nearly the same value in such different compounds as $K_{0.3}MoO_3$ and $(TaSe_4)_2I$ [32,33].

VI. SUMMARY

The kink-like solitons in the incommensurate Frenkel-Kontorova model are investigated regarding to their impact on the vibration spectrum. It is found that the IR phonon intensity possesses universal dependence on the product of the kink radius and the kink concentration suggesting some sort of scaling invariance for the corresponding eigenvector. The model accounting for the giant IR peak in the incommensurate inorganic CDW conductors is proposed. It is shown the giant IR peak is related to the fundamental vibration with the wave vector equal to that of the superstructure and the giant IR intensity is caused by dynamical charge transfer accompanying the CDW internal motion.

VII. ACKNOWLEDGMENTS

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Fig. 1. Dispersion of vibration band obtained via EVP solution (system of linear equations (3)) for the FK model containing 64 particles arranged over: (a) 64 potential wells (no kinks); (b) 63 potential wells (one kink); (c) 56 potential wells (four kinks). The dark regions correspond to the higher vibration amplitude of particles excited by external field \( E = E_0 \cos(k \cdot n) \cdot \cos(\omega t) \).

Fig. 2. Conductivity spectra of the FK model with one kink. (1) is the calculated spectrum; (3) is that obtained by MD simulation (32 particles with cyclic boundary conditions) for \( K_2 = 4 \cdot V, \sqrt{V} = 72 \, \text{arb.un.} \); (2) is the spectrum corresponding to the force constant defect \( \Delta V = -4.1231 \cdot V \) (see text), in the position of the particle no.16.

Fig. 3. MD study of local density of states distribution over the particles in the commensurate (a) and containing one kink (b) FK model. The particles were initially subjected to random displacements and the temporal evolution of the spatial harmonics was analysed via Fourier-transformation. The dark regions correspond to the maxima in the Fourier spectrum.

Fig. 4. The kink and the phonon (the strongest peak in Fig.1) eigenvectors obtained as described in the caption to Fig.1. By symbols in the insert is shown the dependence of the gap mode radius upon kink radius \( R_k = 2 \sqrt{K_2} \).

Fig. 5. (a) The particle arrangement in the FK model of 128 particles (shown by symbols) in 120 potential wells (solid line). (b) The eigenvectors of the kink-(1,3) and phonon-like (2,4) modes. \( K_2 = 4 \cdot V \) (solid symbols) and \( K_2 = 16 \cdot V \) (open symbols), \( \sqrt{V} = 72 \, \text{arb.un.} \).

Fig. 6. Integrated intensity of the phonon-like modes upon \( \eta = R_k \cdot n_k \) calculated using (4) for FK model of 128 particles arranged over: (1) 112 potential wells \( (n_k = 1/8); \) (2) 120 potential wells \( (n_k = 1/16) \); and (3) 124 potential wells \( (n_k = 1/32) \).

Fig. 7. (a) Fragment of particle arrangement obtained via MD simulation in the FK model containing 128 particles arranged over 272 potential wells \( (n_k = 1/16, \text{see text}) \) for \( K_2 = 16 \cdot V \). The particle No.51 is pinned by an extra local potential. (b) Eigenvectors of phason mode without pinning (dotted line) and with pinning (thick solid line), and those of CT-mode (see Fig.2) shown by thin solid line for both pinned and depinned chain.

Fig. 8. IR conductivity spectra of the FK model (see caption to Fig.7), calculated using Eqs. (3)-(5) for \( 4 \sqrt{K_2} = 8 \) \( (a = 1) \). Thin solid line is for \( \beta = 0 \) and thickness solid line is for \( \beta = 30 \) in case of pinned chain. Dashed line is for \( \beta = 0 \) and symbols are for \( \beta = 30 \) in case of depinned chain. PM are the phase modes and CT are the modes which intensity may contain the charge transfer contribution. For \( \beta = 30 \) the 0.03 \( \cdot e \) of the particle charge is transferred during the CT mode vibration while for \( \beta = 0 \) it is 0.

Fig. 9. Dependence of the CT mode integrated intensity on the potential parameters of the FK model containing 128 particles arranged over 264 minima \( (n_k = 1/32) \): (1) is for \( \beta = 30 \) and (4) is for \( \beta = 0 \); over 272 minima \( (n_k = 1/16) \): (2) is for \( \beta = 30 \) and (5) is for \( \beta = 0 \). (3) is the dependence \( y = 0.45/x^{2.25} \). Arrow shows the parameters for the spectra presented in Fig.8.
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