IOP Publishing Physica Scripta
Phys. Scr. **95** (2020) 035218 (6pp) https://doi.org/10.1088/1402-4896/ab509d

Numerical experiments on the dynamics of two-dimension charge-density-waves (CDW's) system in the presence of the weak interchain interaction effect

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Received 4 June 2019, revised 18 October 2019
Accepted for publication 23 October 2019
Published 6 February 2020

Abstract

Layered charge-density-wave (CDW) materials exhibit a lot of interesting aspects for their potential in a variety of device applications. So, a good understanding of their properties may enable the better development of new devices based on them. We address in this paper a study of the dynamic properties of CDW two-dimension electronic crystal in the presence of weak interchain interaction. This study was done through numerical experiments based on the generalized Fukuyama–Lee–Rice (FLR) model. One of the results of this Letter showed that the time-dependent spatially averaged velocity exhibits the steady-state regime characterized by a series of quasi-periodic fluctuations. Moreover, it was found that the increase in the weak interchain interaction effect reduces the NBN amplitude and normalized excess conductivity. All findings accessed here were discussed in the context of the inhomogeneous nature of CDW's dynamics, damping mechanism as well as the attenuation of phase solitons which are nucleated when the CDW's slide.

Keywords: charge density waves, interchain coupling, generalized Fukuyama–Lee–Rice model, nonlinear transport, numerical simulation

(Some figures may appear in colour only in the online journal)

1. Introduction

Quasi-one-dimensional compounds such as $K_{0.3}MoO_3$ TaS_3, NbSe3, etc, have always attracted wide attention in the last years due to their unconventional physic properties. A common feature of these conductors is that the low-dimensional electron gas undergoes phase transition called Peierls towards charge density waves (CDWs) [1]. When the applied electric field is lower than a threshold field (E_T), the CDWs along different chains do not overcome the pinning force due to under-lattice defects [2, 3] and, also, the presence of a linear part in the current–voltage curves is only carried by uncondensed electrons [4]. Beyond the critical field ($E > E_T$), the CDWs begin to slide, leading to nonlinear conduction accompanied by a narrow-band-noise (NBN) [5–7]. Since this phenomenon has first been reported experimentally in 1979 [8], it has been and continues to push researchers to extreme imagination in terms of understanding its source, but until now they resort just on the assumptions for its interpretation.

Many 3D CDW compounds belong to a group of the van der Waals materials characterized by the layered crystalline structures with strong in-plane bonding and weak out-of-plane interactions. These weak interactions enable to obtain a two-dimensional (2D) layers with few-nanometer thickness from the corresponding bulk CDW crystals [9]. Recently, there has been a new rebirth of interest in 2D CDW compounds around the world [10–13] because of their extraordinary properties that are found to be absent in conventional bulk CDW materials [14–18] and which has opened the way into examining their potential in a lot of applications such as radiation-hard electronics [19], communications [20], etc Furthermore, attempts to detect sliding effect in these systems knew success, despite the fail-over the past [21]. For instance, the nonlinear current–voltage characteristic was found for layered $DyTe_3$ compound [22].

Like in bulk CDW materials, an important local parameter governing the low dimensional electronic properties in 2D CDW compounds is the transverse coupling between conductors through several mechanisms [23–29]. Despite the much attention to this parameter in the physics of quasi-one-dimensional compounds [29–33], few investigations were conducted to learn more about its effect on dynamic properties in 2D CDW system. Our former numerical study has shown that the increase of weak interaction effect between CDWs in the 2D system leads to a suppression of the onset of CDW's sliding. The authors suggested that this type of local effect can be considered as an integral part of the damping force which prevents the CDW's movement in 2D system [34].

Understanding the dynamic properties of the 2D CDW conductor is motivated by the need to integrate this type of material into numerous devices as well as the study of spatio-temporal phenomena appearing at long time scales. However, to our knowledge, the investigation into the NBN in the 2D CDW system under the interchain coupling effect is still lacking in the experimental and theoretical reports and, hence, needs clarification. So, this work aims to fill this void in the existing literature. We will report in this Letter the coupling effect between chains on the dynamic properties of a 2D incommensurate CDW system in the weak pinning limit. This will be carried out in the frame of numerical simulations based on the generalized Fukuyama–Lee–Rice (FLR) model. This paper is ordered as follows: section 2 presents respectively a description of the theoretical model and numerical method as well as the calculation procedure. Section 3 is devoted to present the results derived from numerical experiments accompanied by party of discussions and conclusions of paper are summarized in section 4.

2. Model theoretical and numerical implementation

In order to exhibit our idea as clearly as possible, we assume a model which has a simple structure as the classical CDW compounds characterized by the layered crystalline structures. In this regard, we present the generalized FLR model which treats the position-dependent charge modulation on jth chain (equation (1)) as a deformable elastic medium, taking into account its interaction with only first nearest-neighbour ones

$$\rho_j(x, t) = \rho_c + \rho_0 \cos(Qx + \phi_j(x)) \tag{1}$$

$Q = 2K_F$, K_F is the wave vector at the Fermi energy; $\phi_j(x)$ is the local position of the CDW, ρ_c and ρ_0 are respectively the concentration of uncondensed electrons and the amplitude of

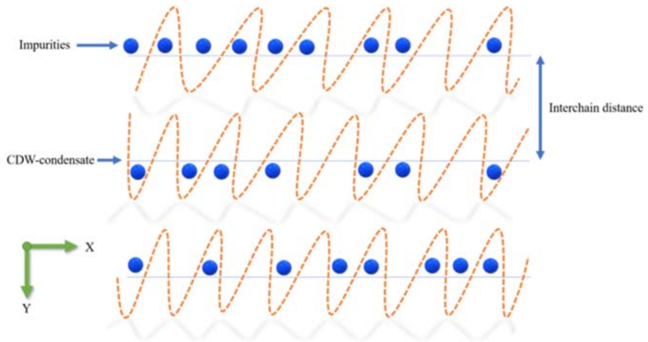

Figure 1. Representative schema of 2D-array of the CDW-carrying linear chains weakly pinned by randomly distributed impurities.

the CDW phase along the jth chain. The phenomenological Hamiltonian of 2D CDW system consisting of weakly coupled linear chains (parallel to the x-axis (see figure 1)), can be written as:

$$H = \sum\nolimits_j (H_{//j} + H_{\perp j}). \tag{2}$$

The first term $H_{//,j}$ of equation (2) is the FLR Hamiltonian for a one dimensional incommensurate CDW, written as (For more detail on this Hamiltonian see [35–37])

$$H_{//,j} = \int \frac{k}{2}\left(\frac{\mathrm{d}\phi_j}{\mathrm{d}x}\right)^2 \mathrm{d}x - \frac{\rho_c E}{\pi}\int \mathrm{d}x \phi_j(x, t) + \sum_i \int \mathrm{d}x \rho_j(x, t) V_i(x - r_i). \tag{3}$$

The second term $H_{\perp,j}$ of equation (2) is the Hamiltonian of interaction between CDWs which was proposed by Nakajima and Okabe, it is to be parameterized as [38]

$$H_{\perp j} = -\frac{1}{2}\sum\nolimits_{j'} \lambda_{jj'} \cos(\phi_j(x) - \phi_{j'}(x)). \tag{4}$$

Here, $\frac{1}{2}$ is introduced, so as not to count any chain twice. j and j' are respectively related to a given chain and its nearest neighbours. $\lambda_{j,j'}$ is the phenomenological parameter of the inter-chain (it is non-zero only for nearest-neighbour ($\lambda_{j,j'} = \lambda$)). Here we consider that $H_{\perp,j}$ represents an additional contribution to the damping force of the system.

The dynamic behavior of CDWs at zero temperature can be specified by the next overdamped equation [35, 39]

$$\gamma\left(\frac{\mathrm{d}\phi(x)}{\mathrm{d}t}\right) = -\frac{\delta H}{\delta\phi(x)} \tag{5}$$

γ is a friction coefficient.

It is worthwhile mentioning that the last equation is strongly nonlinear; it is very complicated to deal with it by means of analytical methods. Therefore, a numerical method is a practical way of diverting this difficulty. In this regard, we must make first some approximations: the damping force is assumed to act only at the impurity's positions r_i [40] and the impurity pining's potential $V_i(x - r_i)$ is chosen as a short-range interaction effect $V_i(x - r_i) = V_0\delta(x - r_i)$ [41]. The index i runs over the impurities whose concentration is c_j. Then, the time and length units are rescaled by kc_j/γ and c_j,

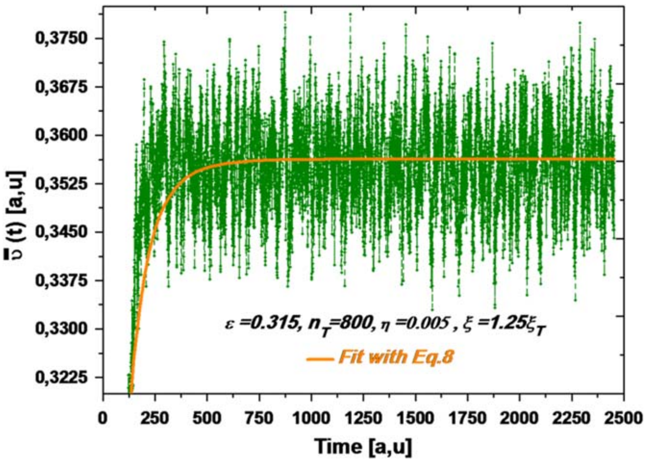

Figure 2. Time-dependent spatially averaged velocity of the 2D CDW system given by equation (7). Solid line is fit according to equation (8).

respectively. In the context of these units the equation describing the dynamics of 2D CDW system can be discretized using a standard finite-difference method on a 2D grid, obtaining [34]

$$\phi_{j,i}(t+1) = \phi_{j,i}(t) + \delta t\Bigg(\Delta\phi_{j,i}(t) + \frac{1}{2}\xi(x_{i+1} - x_{i-1}) + \varepsilon\sin(\theta_i + \phi_{j,i}(t)) + \eta\sum_{j'=j-1}^{j'=j+1}\sin(\phi_j(t) - \phi_{j'}(t))\Bigg) \quad (6)$$

$x_i = c_j r_i$, $\theta_i = Qx_i$. δt is the time step. $\Delta\phi_{j,i}(t)$ is the discrete second derivative. $\xi = \rho_c E/Qkc_j^2$ is a dimensionless electric field along the chain directions. $\varepsilon = \rho_0 V_0/kc_j$ is a dimensionless interaction strength, where V_0 is the pinning potential considered identical for all the impurities. $\eta = \lambda/kc_j$ is a dimensionless interchain coupling constant. The numerical study in this paper is carried out for weakly coupled linear chains in 2D CDW's system containing n_T impurities, using periodic boundary conditions. The initial values of the phase $\phi_i(t=0)$ are randomly chosen in the interval $[0, 2\pi]$. Without losing rigor, a cutoff radius ($R_{\text{cutt-off}}$) is used in the numerical simulation due to the limiting computer capacity; the phase $\phi_{j,i}$ situated on the considered chain j is assumed to interact only with phases of CDW on the first adjacent chain within $R_{\text{cutt-off}}$ equal to $\sqrt{2}\Gamma$, where Γ is the interchain distance.We assume that at zero electric-field in all local velocities are zero and for a given electric field, the CDW system to respond instantaneously between the impurities sites; this neglects the dynamic degree of freedom on short time scales.

3. Results and discussion

The problem of nonlinear collective transport though CDWs in anisotropic conductors has attracted much experimental and theoretical attention due to the spatio-tempoal phenomena. Above the depinning threshold field, the time dependence of the spatially averaged velocity $\overline{\upsilon}(t)$ (equation (7)) of the 2D CDW system exhibited two distinct regimes, a transient period followed by the onset of steady-state response (figure 2) characterized by quasi-periodic fluctuations with wildly varying avalanches sizes. This behavior is of the typical nature of real compounds marked by a random distribution of structural defects along underlying networks. In addition, similar results observed in a variety of nonlinear dynamical systems, such as third-order autonomous memristive chaotic oscillator [42] and the dynamic displacements of shallow shells used in aerospace engineering and civil engineering [43]. Furthermore, the response of 2D CDW system which is described by $\overline{\upsilon}(t)$ obeys a stretched exponential law of the type (equation (8)) [44]

$$\overline{\upsilon}(t) = \frac{1}{N_{\text{imp}}}\sum_i \frac{d\phi_{j,i}(t)}{dt} \quad (7)$$

N_{imp} is the impurity number

$$\overline{\upsilon}(t) = \upsilon_0\left[1 - \exp-\left(\frac{t}{\tau_{\text{on}}}\right)^{\beta}\right] \quad (8)$$

τ_{on} is the relaxation time and β is an exponent, such that $0 < \beta < 1$.

At steady-state, the spatially averaged velocity of 2D CDW system displays irregular spikes. These effects can result from the inhomogeneous nature of CDW's dynamics; the multiple response's coexistence given by CDW domains along or between chains. In the first type of responses, the trajectories and speeds of CDW's domains exhibit invariant function over time (their trajectories in the phase space present unique points but do not have the same values), indicating that they remain constrained in their pin states against the depinning phenomenon of the system. The second type of responses reveal the saddle-node type of bifurcations in the phase space, i.e. trajectories and speeds of CDW's domains are periodic in time, leading to the conclusion that the local dynamic phase transitions have occurred (local tearing transitions from pinned-to-depinned domains). The third type of responses exhibit chaotic behaviors, resulting from the fact that the applied electric field is much higher than that for the tearing of CDW's domains.

The tearing of some CDW domains along or between chains above the threshold field of the system leads to reduce the pinning energy of neighboring domains which result from their interaction. Thus, there is an unstable configuration with the forward motion and local deformation of CDW domains at the same time, which can cause the fluctuation in $\overline{\upsilon}(t)$, characterized by wildly occasionally spikes. This can have a profound implication on CDW transport properties, as a possible source of the NBN that has been observed recently on thin film of CDW compounds [45–48].

For predicting the NBN amplitude in 2D CDW system, the root mean square of $\overline{\upsilon}(t)$ (equation (9)) was adopted. This function has been widely employed to describe the system's kinetic [49, 50]

$$\Delta = [<(\overline{\upsilon}(t) - \upsilon_{\text{CDW}})^2>_t]^{\frac{1}{2}}. \quad (9)$$

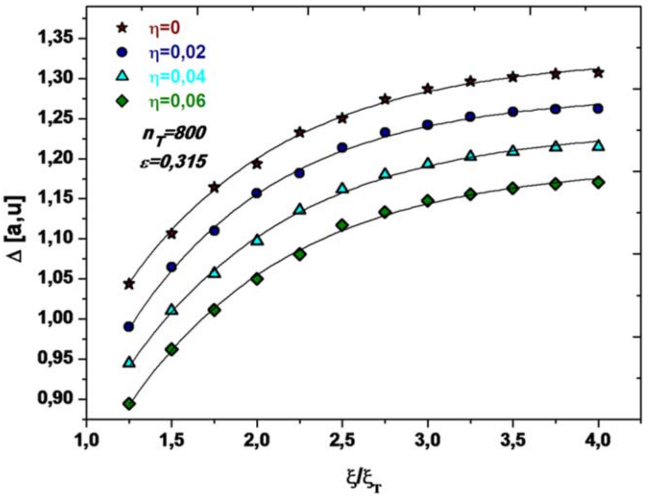

Figure 3. Applied electric field dependence of the root mean square (RMS) of the spatially averaged velocity (Δ) for various η values.

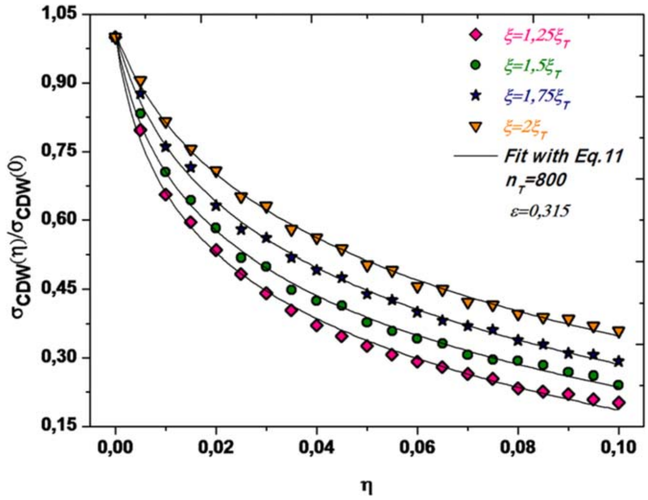

Figure 4. Weak interchain coupling amplitude dependence of normalized excess conductivity ($\sigma_{\mathrm{CDW}}(\eta)/\sigma_{\mathrm{CDW}}(0)$) for various applied electric fields. Solid lines are fit according to equation (11).

Figure 3 displays the field-dependent Δ just above threshold field. It was shown that Δ increases with increasing field, but this dependence becomes very little for high values of field. This finding indicates that the NBN amplitude grows with respect to the applied electric field then reaches a limiting value at larger fields. The behavior of the field-dependent NBN amplitude obtained here is in good agreement with that reported on quasi-1D CDW system of NbSe3 [51].

Since the topologically nontrivial objects like phase dislocations that appear when the CDW's slide [52–55] can move between pinned and unpinned domains of the sample [56] and can make the system more disordered [57, 58], it seems that the field-dependent NBN amplitude obtained in this work can be explained by the fact that when the field is increased, the local pinning barriers vanish gradually (the fraction of CDWs depinning domains increases with the increasing field), but the system is not entirely depinned from the impurities centers, causing greater fluctuations of the phase dislocations between pinned and unpinned domains of CDWs along or between chains. These effects, therefore, can lead to a huge disorder in the system, just as a strong increase in NBN amplitude.

For a given external field, beyond the threshold field, Δ is found to be very sensitive to the interchain coupling effect (figure 3), it decreases when the η increases. This finding indicates that the NBN amplitude is gradually reduced as the weak interchain coupling effect increases. Due to the phase solitons cannot be ignored in the CDWs moving, as experimentally observed [59] and predicted in theoretical researches [60, 61], these topological object's stabilization with the weak interchain coupling [24] can be viewed as a factor in making the CDW's response more homogeneous above the depinning threshold and, therefore, reduce the NBN amplitude (figure 3)

$$\sigma_{\mathrm{CDW}}(\xi) = \frac{\upsilon_{\mathrm{CDW}}(\xi)}{\xi}, \tag{10}$$

where υ_{CDW} is the steady-state time-averaged velocity of the system [34, 39]:

Table 1. Variation of τ as a function of ξ/ξ_T, for $n_T = 800$ and =0.315.

ξ/ξ_T	δ
1.25	0.362
1.5	0.391
1.75	0.448
2	0.502

In contrast to its behavior with the applied electric field, the excess conductivity normalized to the excess conductivity without interchain coupling effect ($\sigma_{\mathrm{CDW}}(\eta)/\sigma_{\mathrm{CDW}}(0)$) decreases when increasing the parameter (figure 4). This finding suggests that the CDW-condensates display a slow dynamic when increasing the interchain coupling effect, demonstrating that this correlation type can be considered as an effective field which represents a resistance that opposes the CDW's motion along the chain axis and, hence, the increase in the damping mechanism of 2D CDW system. Furthermore, it was found that $\sigma_{\mathrm{CDW}}(\eta)/\sigma_{\mathrm{CDW}}(0)$ seems to reach a limiting value for high amplitudes of η figure 4. This is consistent with the unidimensional CDW nature of the system characterized by high anisotropy along the chains [62].

For various values of the applied electric field above threshold field, the variation of normalized excess conductivity according to the parameter η is well fitted by equation (11)

$$\sigma_{\mathrm{CDW}}(\eta)/\sigma_{\mathrm{CDW}}(0) = 1 - \kappa\eta^{\delta}, \tag{11}$$

where κ and δ are respectively, a constant and an exponent, such that $0 < \delta < 1$. δ depend on the force applied to represent the CDWs (external electric field), a fit of the figure 4 curves with equation (11), shows that this exponent increases as a function of the applied electric field (table 1).

As mentioned previously, there is a lot of source of the interchain interactions in the real CDW system, mainly from an interaction between the modes not participating in CDW-condensates such as phonons and free carriers [23]. In this regard, the increase in damping mechanism from the increased influence of interchain interaction effect (figure 4) can, therefore, come from enhanced screening effect of electric fields applied parallel to the x-axis when more electrons and phonons are available to produce coupling sufficiently between the chains.

4. Conclusion

The findings presented in this Letter display that the weak interchain interaction effect affects drastically the dynamic properties of 2D CDW system. It was found that the time-dependent spatially averaged velocity exhibits two distinct regimes; transient period followed by the onset of steady-state response characterized by quasi-periodic fluctuations. Besides, it was established that the increase in the weak interaction effect between CDWs causes greater attenuation of NBN amplitude and diminution of excess conductivity transported by CDWs on parallel linear chains.

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