DYNAMICS OF THE 1D SYSTEM WITH A COMPLEX ORDER PARAMETER

E. Tutiš[1] and S.Barišić[2]
[1] Institute of Physics of the University, POB 304,
Zagreb, Croatia, Yugoslavia
[2] Department of Physics, Faculty of Sciences, POB 162,
Zagreb, Croatia, Yugoslavia

Abstract

The dynamics of the one dimensional CDW system with a complex order parameter is investigated using the combined Monte Carlo - molecular dynamics simulations. The results for the the dynamic structure factor are presented. The dynamics of thermally activated phase slips in the system with inertial dynamic is examined in the intermediate temperature region, where the one dimensional fluctuation regime is still appropriate.

Introduction

The dynamics of the phonons with wave vectors close to to the wave vector of the Peierls transition was much investigated in the past using the method of inelastic neutron diffraction[1],[2]. However the theoretical understanding of this subject is still not complete and even the dynamics of strictly one dimensional system is not fully understood. This is the problem that we address in the present contribution. The Peierls chain is described here by the effective Lagrangian

$$L=\int dx\ [m|\partial_t\psi|^2 - c|\partial_x\psi|^2 - a|\psi|^2 - (b/4)|\psi|^4], \qquad (1)$$

The coefficients of this Lagrangian, in usual notation, are given by

$$a = a'(T/T_{MF}-1), \qquad a' = \lambda m\omega_0^2, \qquad (2)$$
$$b = (7\zeta(3)/8\pi)v_F(a'/T)^2, \qquad c = 2a'v_F^2/(2\pi T)^2.$$

where the electron-phonon coupling is assumed to be weak, $\lambda<<1$. The complex field ψ describes the lattice deformation with wave vectors near $\pm 2k_F$ (hereafter the wave vector will be measured with respect to $2k_F$). It should be noted that the Lagrangian (1), derived as a Landau expansion[3] near the mean field transition temperature, T_{MF}, gives also a qualitatively good description of the dynamics of the system for $T<<T_{MF}$ if coefficients b and c are fixed to their values at T_{MF}. This can be checked by comparing Lagrangian (1) with the Lagrangian obtained from the low temperature ($T<<T_{MF}$) approach [4]. With appropriate change of the coefficients (2) Eq.(1) can also account for the lattice dynamics of the 1d system with Coulomb correlated charge density wave [5]. It should be noted that damping mechanisms from external sources (nonadiabatic effects from electrons, impurities etc.) are not included in our description of the lattice dynamics. It turns out that damping which arrises from anharmonicities is dominant at high temperatures $T\sim T_{MF}$. At lower temperatatures the low frequency properties (phasons) may be affected by the damping effects that we neglected. However we do not expect them to affect those properties (phase slips) that are connected with amplitude fluctations at higher frequencies. In fact, the amplitude mode was experimentally identified [2] as a well defined phonon branch.

Dynamic structure factor

We have studied the dynamics of the classical system described by the Lagrangian (1) using the combined Monte Carlo - molecular dynamic (MC/MD) numerical simulation. Let us first describe the results for the

(received December 31, 1989)

dynamic structure factor $S(k,\omega)$ defined as the Fourier transform of $\langle\psi_1(x,t)\psi_1(0,0)\rangle=\langle\psi_2(x,t)\psi_2(0,0)\rangle$. Since the usual phonon picture applies for high temperature $T>>T_{MF}$ where the renormalization of the phonon dynamics by electrons is not important we will restrict ourselves only about temperatures which are close to and bellow T_{MF}.

It is convenient to write $S(k,\omega)$ in terms of reduced variables. Introducing the dimensionless function s we write $S(k,\omega)$ as $S(k,\omega) = [(mc)^{1/2}/b]\, s(\vartheta,k/K,\omega/\Omega)$. Here ϑ is the only dimensionless parameter of the system $\vartheta=(bT/|a|c)(c/|a|)^{1/2}$ which for the Peierls system of Eq.(2) is the fuction of T/T_{MF}, $\vartheta \approx (3/2)(T/T_{MF})\cdot(1-T/T_{MF})^{-3/2}$. Ω and K are some combinations of parameters with a dimension of frequency and the wave vector. The choice

$$\Omega = (|a|/m)^{1/2} + m^{-1/2}(bT/c^{1/2})^{1/3}, \qquad (3)$$
$$K = (|a|/c)^{1/2} + c^{-1/2}\,(bT/c^{1/2})^{1/3}$$

proves convenient both for $T/T_{MF}<<1$ and $T\approx T_{MF}$.

The result for $S(k,\omega)$ obtained by MC/MD in the region near T_{MF} shows a dispersive mode behaviour with a finite frequency at k=0. This is different from the conventional picture in which the Kohn-Peierls phonon softens to $\omega=0$ at T_{MF} due to the vanishing harmonic a-term in the Lagrangian (1). Thus, the effect of fluctuations and the quartic b-term is to shift the frequency to the finite value and to retain there the underdamped phonon picture present for $T>>T_{MF}$. The frequency of the phonon with k=0 is $\omega_O=0.71\Omega=0.62\lambda^{1/2}\omega_O$. It should be noted that the ratio of this frequency and the frequency $\omega_A(T=0)$ of the amplitude mode at T=0, $\omega_A=\lambda^{1/2}\omega_O$ [6],[4] is a pure number, 0.62. This may be compared with the experiments provided that the interchain coupling is not too pronunced at T_{MF}. In the blue bronze [2] T_{MF} was estimated to 320K but the two dimensional correlations also start in that temperature region (Peierls transition occurs near 180K). The measured ratio ω_O/ω_A is however 0.71, not very far from our result. The damping (half width of the peak in $S(k,\omega)$ at half maximum) of the k=0 phonon is obtained equal to $0.1\omega_O$. This is also within the order of magnitude (factor 2 difference) of the observed damping[2]. For other Peierls materials the neutron measurements at T_{MF} are not available because T_{MF} is not within the experimental range (eg. the crystal changes chemically before T_{MF} is reached). However extrapolations, as for example in KCP where T_{MF} was estimated[1] to be approximately 400K, show that the system is actually described by the dispersive mode at T_{MF}.

When the temperature is lowered below T_{MF} we can follow the transformation of the Peierls phonon towards the phase and the amplitude mode. Fig.1. illustrates $S(0,\omega)$ down to $T/T_{MF}=0.443$. The k=0 mode becomes overdamped below $0.4T_{MF}$ and the separation into the phase and the amplitude mode starts below $0.3T_{MF}$. The phase mode dominates in $S(k,\omega)$ while both modes contribute equally in the sum rule for the velocity-velocity correlation function $V(k,\omega)= \omega^2 S(k,\omega)$ (entering the sum rule for the oscillator strengths). Temperature dependence of $V(k,\omega)$ is illustrated in Fig.2.. Let us mention again that it was conventionally believed that the ampliton-phason separation starts close below T_{MF}.

Finally, let us note that the obtained temperature dependence of $S(k,\omega)$ has the implication [5] on the electronic pseudogap. The change in the pseudogap from the "shallow" form, produced by the low frequency $2k_F$ phonon, to the "sharp" form, characteristic for the system with well defined CDW amplitude, occurs in the temperature range which is well below T_{MF}.

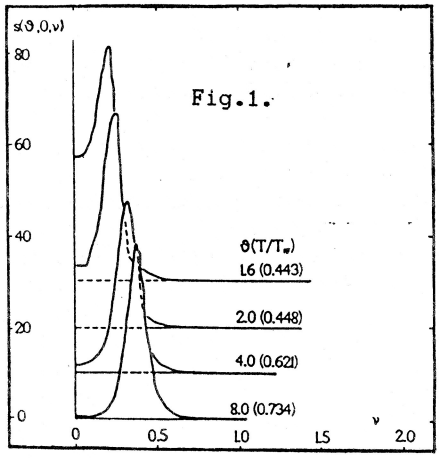

Fig.1.

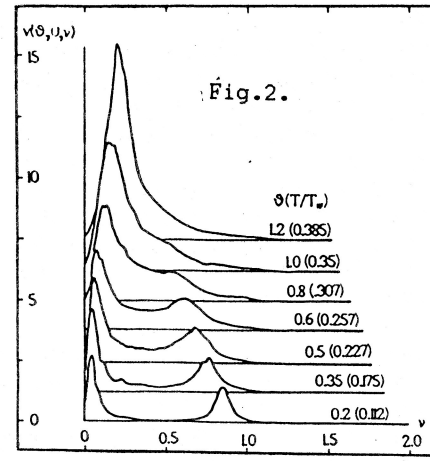

Fig.2.

Thermally activated phase slips

Now we turn to the processes that are characteristic for the low temperature dynamics of the order parameter and are partly responsible for the crossover from the low temperature phason-ampliton dynamics to the high temperature phonon dynamics. Qualitatively speaking this crossover takes place in the temperature region where the fluctuation of the amplitude is of the order of the average amplitude itself. Numerical simulation showed that this happens above $0.3T_{MF}$. However, the local fluctuations in which the amplitude vanishes occur even at lower temperatures, i.e. before than the thermal fluctuation destroy the amplitude of the order parameter on the whole chain. The local destruction of the amplitude may be accompanied by the sudden slip in the phase of the order parameter by 2π. These phase slip processes are essentialy of the same topological type as the processes induced near the electrical contacts when an external electric field is applied to the system. Their important characteristics is that they put the electron into or out of the CDW condensate depending on the sign of the phase jump. Formally, they are similar to phase slip fluctuations in thin whisker superconductors. However the dynamics of phase slips is different in superconductors because the order parameter obeys the time dependent Ginzburg-Landau equation. Instead of the relaxational dynamics in superconductors the inertial dynamics described by the Lagrangian (1) comes in our problem. Nevertheless, the potential energy functionals are of the same form and therefore the expression for the potential energy barrier involved in phase slips are analogous. For the Peierls chain this barrier is given by $V_{PS}=2.54\cdot T_{MF}(1-T/T_{MF})^{3/2}$. The different type of the dynamics involved shows in different prefactor ν in the expression for the average time τ_{PS} between successive phase slips. For the section of the chain with the length L it is given by[7] $1/\tau_{PS}(L)=(L/d_{PS})\cdot\nu\cdot\exp(-V_{PS}/T)$. d_{PS} measures the region in which significant change of the amplitude occurs in the phase slip (essentially the amplitude coherence length).

In our simulations at low temperatures we made an extensive examination of thermally induced phase slips. The assumption of their random occurrence (Poisson distribution with characteristic time τ_{PS}) was checked together with the dominant temperature dependence that comes from $\exp(-V_{PS}/T)$. The next step is to determine ν. In contrast to the time dependent Ginzburg-Landau equation two time scales are present in our problem - one of them is the inverse ampliton frequency, $1/\omega_A$, and the other is the inverse of the phason peak linewidth, $1/\Gamma$. The absence of the significant temperature dependence of ν in the temperature range covered by our simulations and the comparison of the numerical values

for ν with those for ω_A and Γ (ω_A is an order of magnitude larger than Γ at the lowest temperature reached) suggest that essentially $\nu=\omega_A$. Thus, the fluctuations of the amplitude are responsible for crossing of the potential energy barrier.

It should be mentioned here that phase slips can hardly be seen in $S(k,\omega)$. The reason is that other mechanisms which lead to finite widths of ampliton and phason peaks are much more pronounced. The dominant low temperature dependence of the linewidth is linear in T, due to the purely kinematical reasons. The finite lifetime effects that come from anharmonicities in the amplitude - phase Lagrangian [4] are also masked by this linear term.

The effect of phase slips may be seen if the impurities [8] are present in the system because they shift the phase oscillations to finite frequencies while the contribution of the phase slip noise remains near $\omega=0$. Also, it should be recalled that in the system with impurities the free movement of the charge density wave is hindered by the pinning. However it may be argued [8] that the thermally activated phase slips lead, at least when pure one dimensional systems are concerned, to a finite contribution of the charge density wave to the DC conductivity. The point is that the charge density wave deformed by the static electric field may relax through thermally induced phase slips which are accompanied by the conversion of the CDW current to the normal current. These normal electrons may pass over the impurity and enter the CDW condensate again.

The solution of the full problem of 1d electron in the random potential produced by impurities [10], the possibility to interact with the lattice fluctuations and enter the Peierls condensate trough phase slips seems rather complicated and is not yet fully investigated. However under the assumption that the phase slip rate regulates the contribution of CDW to the electronic conductivity and that impurities may be considered as transparent for electrons which jump from one section of the chain to another, a rather simple reasoning gives [9]

$$J_{CDW} \sim E \cdot \pi(n_c e/2k_F \cdot c \cdot d_{PS})^2(\omega_A/T)\exp(-V_{PS}/T)$$

where n_c is the effective density of electrons in the condensate and the linear concentration c of impurities is assumed to satisfy the condition $c\xi_A<<1$.

References:

[1] Comes R. and Shirane G. in "Highly conducting one-dimensional solids" (J.T. Diversee, R.P. Evrard and V.E. van Doren eds.) Plenum, New York, 1979 and references therein.

[2] Pouget J.P. et al., Mol.Cryst.Liq.Cryst **121** (1985) 111; Phys. Scr. **T25** (1989) 58.

[3] Allender D., Bray J.W, Bardeen, J., Phys.Rev **B9** (1974) 119

[4] Brazovskii S.A. and Dzyaloshinskii I.E., Zh.Exp.Theor.Fiz. **71** (1976) 2338

[5] Tutiš E. and Barišić S., Europhys.Lett. **8** (1989) 155; Tutiš E., Barišić S. to be published

[6] Lee P.A. Rice T.M. and Anderson P.W., Solid State Commun. **14** (1974) 703

[7] Langer J.S., Ambegoakar V., Phys.Rev. **164** (1967) 498; McCumber D.E.,Halperin B.I. Phys.Rev **B1** (170) 1054

[8] Koehler T.R., Lee P.A. Phys. Rev. **B16** (1977) 5263

[9] Tutiš E., Thesis, University of Zagreb,Yugoslavia, 1989

[10] for review of the 1d system with impurities see eg. Abrikosov A.A., Phys.Scr. **T27** (1988) 148