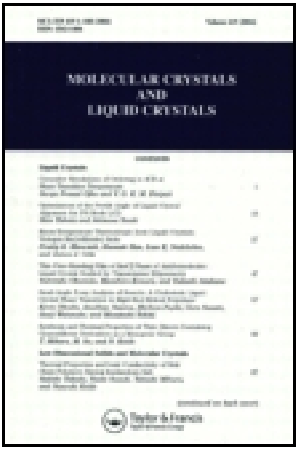

Molecular Crystals and Liquid Crystals
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/gmcl16

The Peierls Instability in Pinning Potentials from Counterions

Lars Kai Hansen [a] & Kim Carneiro [a]
[a] Physics Laboratory I, University of Copenhagen Universitetsparken, 5, DK-2100, Copenhagen ø, Denmark
Version of record first published: 17 Oct 2011.

To cite this article: Lars Kai Hansen & Kim Carneiro (1985): The Peierls Instability in Pinning Potentials from Counterions, Molecular Crystals and Liquid Crystals, 119:1, 471-474

To link to this article: http://dx.doi.org/10.1080/00268948508075200

Mol. Cryst. Liq. Cryst. 1985, Vol. 119, pp. 471-474
0026-8941/85/1194-0471/$10.00/0

THE PEIERLS INSTABILITY IN PINNING POTENTIALS FROM COUNTERIONS

LARS KAI HANSEN and KIM CARNEIRO
Physics Laboratory I, University of Copenhagen
Universitetsparken 5, DK-2100 Copenhagen Ø, Denmark

Abstract In the presence of a pinning potential both the nature of the Peierls transition and the dynamics of the Charge Density Wave are affected. We argue that the periodic potential stabilizes phase solitons, while amplitude solitons can be polarons or bipolarons. For these excitations we give both the extension along the chain as well as the energies of formation. We only discuss the case of a periodic pinning potential as arising from a counterion lattice; neglecting randomness from impurities.

INTRODUCTION

In one-dimensional molecular crystals, ordering of the counterions will give rise to a periodic electrostatic potential on the conducting chains. In several cases[1,2] it is expected that the period will be the same as the period of the Charge Density Wave (CDW) formed under the Peierls transition (some examples are given in Fig.1). This potential is known as a pinning potential, and several authors have considered the dynamics of the CDW in this case.[3-6]

Recently we pointed out that the pinning potential can have a strong effect on the Peierls transition itself.[7] In this paper we extend these results emphasizing the established connection between the nature of the transition and the CDW dynamics. Further we characterize the possible solitary wave excitations, comprising phase solitons as well as polaron and bipolaron amplitude solitons.

The possibility of phase solitons in general periodic potentials (from commensurability) were considered by Rice et al.[8] and by Artemenko and Volkov.[9] Thomas[10] used these results to explain the decrease of the (conductivity) activation energy in $K_2[Pt(CN)_4]\cdot Br_{0.30}\cdot 3.2H_2O$ at low temperatures.

MEAN FIELD THEORY AND CDW DYNAMICS

We consider the one-dimensional electron-phonon system exposed to a periodic potential V_Q of wavenumber $2k_F$:

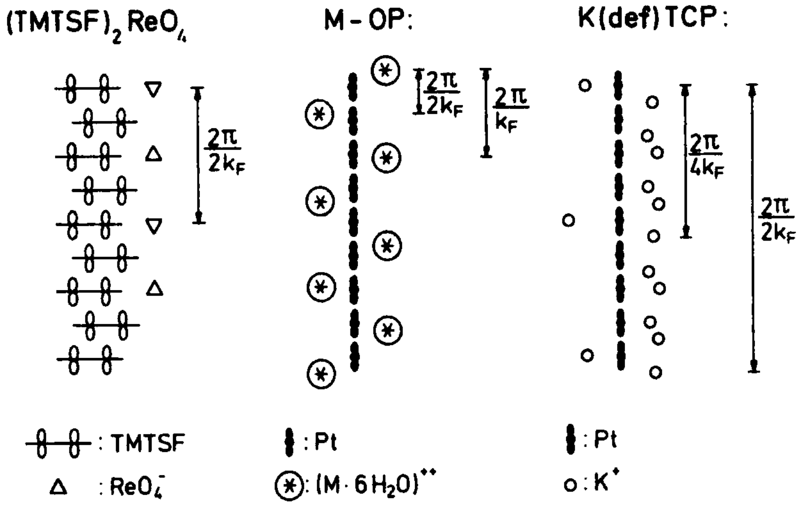

FIGURE 1 Examples of $2k_F$-potentials formed by ordered counterions in molecular conductors. In $(TMTSF)_2ReO_4$ the tetrahedral, monovalent ReO_4-anions order in one column per conducting chain. In class A of $M_{0.84}[Pt(C_2O_4)_2]\cdot 6H_2O$, (M-OP's), the divalent $(M\text{-}6H_2O)$-cations order in two equivalent columns. In $K_{1.75}[Pt(CN)_4]\cdot 1.5H_2O$, K(def)TCP, monovalent K-cations are in two inequivalent columns!

$$H = \sum_{k,\sigma} \varepsilon_k C^+_{k\sigma} C_{k\sigma} + \sum_q \hbar\omega^o_q \, b^+_q b_q \tag{1}$$
$$+ \sum_{k\sigma} \sum_q \frac{ig}{\sqrt{N}} C^+_{k+q\sigma} C_{k\sigma}(b_q + b^+_{-q}) + \sum_{k\sigma} \sum_{Q=\pm 2k_F} V_Q C^+_{k+Q} C_k$$

$C^+_{k\sigma}$, b^+_q are creation operators for electrons of energy ε_k and spin σ, and phonons of frequency ω^o_q respectively. g is the electron-phonon coupling constant while N is the number of host lattice sites, we consider N to be incommensurate with N_e , the number of electrons on a chain.

In mean field theory we find[7] that the presence of V_Q fixes the phase of the gap parameter Δ (and thereby the CDW position), and that $|\Delta(T)|$ obeys the modified gap equation

$$1/\lambda \, \frac{|\Delta| - |V_Q|}{|\Delta|} = \int_0^{\varepsilon_F} d\varepsilon \, \frac{\tanh(E/2kT)}{E} \quad , \; E = \sqrt{\varepsilon_k^2 + |\Delta|^2} \tag{2}$$

where λ is the dimensionless electron-phonon coupling constant.

In the presence of V_Q the CDW phase mode acquires a finite frequency in the long wavelength limit (corresponding to the finite potential against a uniform translation). In the adiabatic limit ($\hbar\omega^o_{2k_F} \ll \Delta_0$) we find at zero temperature:

$$\omega_\phi = \sqrt{v_Q} \cdot \omega^0_{2k_F} \quad , \quad v_Q = V_Q/\Delta_o \tag{3}$$

The threshold electric field E_0, necessary to depin the CDW of the pinning potential, is given by[6,9]

$$E_0 = \frac{2\Delta_0^2 m}{e\hbar k_F \lambda} v_Q \tag{4}$$

m being the electronic band mass.

In conclusion eqs.(2-4) establish a connection between the CDW dynamics and the nature of the Peierls transition in the presence of a pinning potential.

SOLITON EXCITATIONS

Phase solitons

It is readily veryfied that the external potential acts as a M=1 commensurability potential, and by neglecting the electric field associated with the redistribution of charge,[8,9] a static sine-Gordon equation for the phase χ of the gap parameter can be established

$$-L_\phi^2 \frac{\partial^2\chi}{\partial x^2} + \sin\chi = 0 \quad , \quad L_\phi^2 = \frac{\lambda}{2v_Q}\xi^2 \tag{5}$$

where $\xi = v_F/\Delta_0$ is the zero temperature coherence length. Taking the electric field into consideration, the length of the soliton L_ϕ diverges at T = 0.[9] The divergence is suppressed by the presence of impurities or other defects that gives rise to a finite density of states in the Peierls gap. In the dirty limit, ξ is replaced by the mean free path of the normal metal.[9]

Amplitude Solitons

In the general incommensurate case (absence of V_Q) a number of amplitude solitons are possible:[11] neutral kinks and polarons. In the presence of V_Q the continuously degenerate ground state becomes non-degenerate and we obtain a structure that resembles cis-polyacetylene.[11,12] Neutral kinks are excluded while the bipolaron (kink-antikink pair) becomes possible together with minor modifications of the polaron. The characteristics of polarons and bipolarons are summarized in Figure 2a) together with the extension vs. the parameter v_Q/λ. In Fig.2b we show the formation energy associated with the defect and the distance from the gap center of the bound state energies as a function of v_Q/λ, taking a simple analogy with cis-polyacetylene.[11,12]

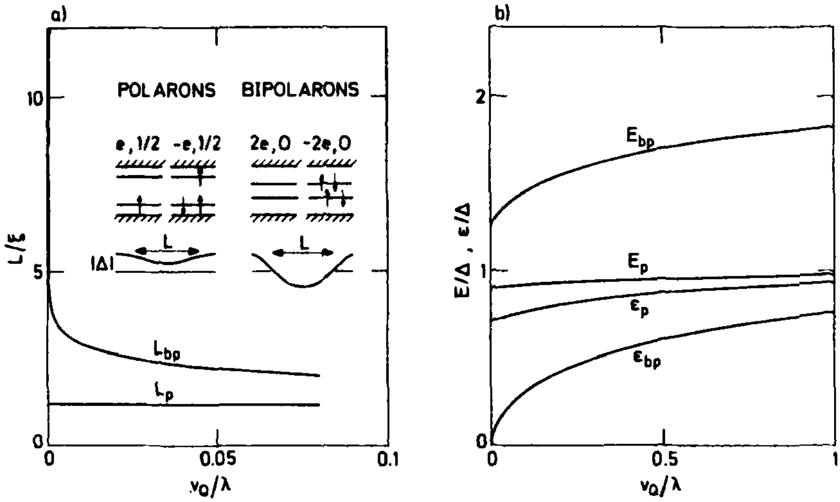

FIGURE 2 Characteristics of amplitude solitons in an incommensurate system exposed to a pinning potential $V_Q = v_Q \cdot \Delta_Q$, taking a simple analogy with cis-polyacetylene.[11,12] a) The length of the soliton vs. strength of the potential. In the inset is shown the charge/spin relation together with the occupancy of the associated bound states. b) The energy of formation, E, and the bound state energy, ε, measured from mid gap.

REFERENCES

1. K. Carneiro, L.K. Hansen, A. Braude, K. Mortensen, C.S. Jacobsen, D. Turner and A.E. Underhill, in these proceedings and references therein.
2. C.S. Jacobsen, H.J. Pedersen, K. Mortensen, G. Rindorf, N. Thorup, J.B. Torrance and K. Bechgaard. J.Physics C 15,2651 (1982).
3. P.A. Lee, T.M. Rice and P.W. Anderson, Solid State Commun.14 703 (1974).
4. M.J. Rice, Phys.Rev.Lett. 37, 36 (1976).
5. T.M. Rice, P.A. Lee and M.C. Cross, Phys.Rev.B 20, 1345 (1979).
6. G. Grüner, A. Zawadowski and P.M. Chaikin, Phys.Rev.Lett. 46, 511 (1981)
7. L.K. Hansen and K. Carneiro, Solid State Commun. 49, 531 (1984).
8. M.J. Rice, A.R. Bishop, J.A. Krumhansl and S.E. Trullinger, Phys.Rev.Lett. 36, 432 (1976).
9. S.N. Artemenko and A. Volkov, Sov.Phys. JETP 54, 992 (1981).
10. J.F. Thomas, Solid State Commun. 42, 567 (1982).
11. S.A. Brazovskii, Sov.Phys. JETP 51, 342 (1980).
12. A.R. Bishop and D.K. Campbell in A.R. Bishop, D.K. Campbell and B. Nicolaenko (eds.): Non-Linear Problems: Present and Future, North-Holland, Amsterdam, p.195. (1982)