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Published in:
 Synthetic Metals

DOI:
[10.1016/S0379-6779\(98\)00827-3](https://doi.org/10.1016/S0379-6779(98)00827-3)

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Document Version
 Publisher's PDF, also known as Version of record

Publication date:
 1999

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Figge, M. T., Mostovoy, M. V., & Knöster, J. (1999). Disorder-induced neutral solitons in degenerate ground state polymers. *Synthetic Metals*, 101(1-3), 388 - 389. [https://doi.org/10.1016/S0379-6779\(98\)00827-3](https://doi.org/10.1016/S0379-6779(98)00827-3)

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Disorder-induced neutral solitons in degenerate ground state polymers

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Abstract

We study the effects of weak off-diagonal disorder on π -conjugated polymers with a doubly degenerate ground-state. We find that disorder induces a finite density of neutral solitons in the lattice dimerization of a polymer chain. Interchain interactions result in a linear potential between the solitons and, if sufficiently strong, bind them into pairs resulting in an exponential suppression of the soliton density. As neutral solitons carry spin $1/2$, they contribute to the polymer's magnetic properties. We calculate the magnetic susceptibility and suggest measurements of the magnetic susceptibility in *trans*-polyacetylene at low temperatures.

Keywords: Polyacetylene and derivatives, Magnetic measurements, Ising models, Order-disorder phase transitions

1. Introduction

Conjugated polymers belong to a large class of quasi-one-dimensional Peierls materials, in which the lattice distorts due to its interaction with itinerant electrons. Much attention has been devoted to *trans*-polyacetylene, which has a doubly degenerate ground state. The degeneracy allows for topological excitations, solitons, which are kinks in the lattice dimerization accompanied by a local distortion of the electron density. Solitons survive the presence of on-site Coulomb repulsion. Although solitons are usually associated with excited states, we show in this contribution that off-diagonal disorder may induce a finite density of kinks in the ground state of *trans*-polyacetylene. We discuss the effects on the magnetic response.

2. Mapping on the Random-Field Ising Model

We describe the polymer chains by a Peierls-Hubbard model, which accounts for both a static electron-lattice interaction and electron-electron interactions. The lattice dimerization at position n of the chain is given by:

$$\Delta(n) = \Delta_{lat}(n) + \eta(n). \quad (1)$$

Here, $\Delta_{lat}(n)$ describes the Peierls distortion and corresponds to the alternating part of the electron hopping amplitude along the chain direction. The second term, $\eta(n)$, represents the disorder and stems from the small fluctuations in this amplitude. While in the absence of disorder the ground state energy does not depend on the sign of the

dimerization $\Delta(n) = \pm\Delta_0$, the weak-disorder correction to the energy,

$$\delta E \propto - \sum_n \Delta_{lat}(n) \eta(n), \quad (2)$$

removes this degeneracy. As we explained in Ref. [1], the energy correction Eq. (2) stabilizes neutral solitons in the lattice dimerization of a chain's minimal-energy lattice configuration.

As a consequence of the form Eq. (2), the statistics of neutral solitons in a weakly disordered Peierls-Hubbard chain can be described by the random-field Ising model (RFIM) [2,3]:

$$E\{\sigma_m\} = \sum_{m=1}^M \left[\frac{\mu}{2}(1 - \sigma_m \sigma_{m+1}) - h_m \sigma_m - B \sigma_m \right]. \quad (3)$$

The Ising variable $\sigma_m = \pm 1$ corresponds to the two possible values of the lattice dimerization $\Delta_{lat} = \pm\Delta_0$ between neighboring kinks. Thus, the first term in Eq. (3) is the energy cost related to the occurrence of kinks, where μ is the kink creation energy. As the RFIM Eq.(3) is an effective model, obtained by integrating out small lattice fluctuations, μ weakly depends on temperature and is renormalized by electron-electron interactions [2]. Comparing Eq. (3) to Eq. (2) reveals that the role of the disorder is taken over by the random "magnetic" field h_m , which we assume to have a Gaussian distribution with zero mean and correlator $\langle h_m h_n \rangle = \epsilon \delta_{m,n}$ with the disorder strength $\epsilon \ll \mu^2$.

Finally, the third term in Eq.(3) describes the interchain interactions, which tend to establish a coherence between the phases of the order parameter on different chains.

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These interactions are taken into account in the chain mean-field approximation, so that the homogeneous “magnetic” field B is proportional to the average order parameter: $B = W\langle\langle\sigma\rangle\rangle$. Here, the double brackets denote both the thermal and the random-field average. The validity of the chain mean-field approximation requires the interchain interaction energy to be sufficiently weak, $W \ll \mu$, which holds in quasi-one-dimensional materials such as conjugated polymers.

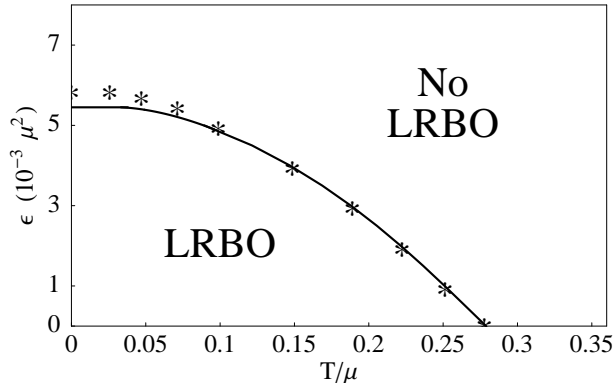


Fig. 1. Phase diagram of the RFIM.

We have analytically solved the model Eq. (3) by noticing that the disorder averaged free energy of its continuum version has the form of a matrix element of the Green function describing the relaxation of a spin 1/2 in a time-dependent magnetic field. The coordinate along the chain plays the role of the (imaginary) time in which the relaxation takes place. The Green function was found by solving the corresponding Fokker-Planck equation [2,3].

For a single chain ($B \propto W = 0$) the ground state density of solitons is then found to be proportional to the disorder strength,

$$n_s = \epsilon / \mu^2. \quad (4)$$

The solitons occur randomly positioned along the chain and destroy the long-range order in the lattice dimerization at any temperature [2-4]. This turns out to be the same for interacting chains ($W \neq 0$), as long as the disorder strength is larger than the critical value $\epsilon_c = 2W\mu/3$. However, for $\epsilon < \epsilon_c$, the long-range bond order (LRBO) in the lattice dimerization is re-established as solitons are bound into pairs by the interchain interactions (soliton confinement). As a consequence, the density of neutral soliton pairs n_p is found to be exponentially suppressed at low temperatures:

$$n_p = 2 \frac{W^2}{\epsilon} \exp\left(-2 \frac{W\mu}{\epsilon}\right). \quad (5)$$

In Fig. 1 we plot the phase diagram for the existence of LRBO in the RFIM Eq. (3) using parameters typical for *trans*-polyacetylene. The result of a numerical calculation (stars) and our analytical result (solid line) are seen to be

in excellent agreement.

3. Magnetic Susceptibility in the Ordered Phase

As neutral solitons carry a spin 1/2, they contribute to the polymer’s magnetic properties. For $\epsilon \ll \epsilon_c$, solitons only occur in isolated pairs. Within the RFIM Eq. (3), we have analytically calculated the pair size distribution $p(R)$, which turns out to be sharply peaked around a typical pair size $R = R^*$. As the antiferromagnetic exchange between the neutral solitons of a pair is a known (exponentially decaying) function $J(R)$ of the pair size [6], knowledge of $p(R)$ allows us to calculate the magnetic susceptibility due to the disorder-induced solitons.

At temperatures T larger than the typical exchange value $J^* = J(R^*)$, we find the magnetic susceptibility to obey the Curie law, $\chi(T) \propto 1/T$. At temperatures $T \ll J(R^*)$, however, most of the spin pairs are in the singlet state, and the magnetic susceptibility (up to logarithmic corrections) reads [5]:

$$\chi(T) \propto \left(\frac{1}{T}\right)^{1-\alpha} \quad (6)$$

with $\alpha \propto W^2/\epsilon$. Thus, the interplay between interchain interactions (W) and disorder (ϵ) determines the low-temperature behaviour of the magnetic susceptibility.

4. Conclusions

Off-diagonal disorder induces neutral solitons in the ground state of *trans*-polyacetylene. These solitons contribute to the magnetic susceptibility. At low temperatures their magnetic response shows deviations from Curie behavior, and the thermal behavior of the susceptibility strongly depends on disorder and interchain interactions [Eq. (6)]. Our theory may explain the observed deviation from Curie behavior in Durham polyacetylene below 30K [7]. To get better insight into the parameter α , experiments should be extended to temperatures of the order of 1K.

Acknowledgments

This work is supported by the Stichting Fundamenteel Onderzoek der Materie (FOM).

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