

S. A. Brazovskii. *Theory of conducting polymers.*

Most quasi-one-dimensional conductors are narrow-band dielectrics, at least at low temperatures. In charge-transfer complexes and in the polymer trans-polyacetylene, trans-(CH)_x, the formation of a dielectric gap at the Fermi surface is due to the deformation of the lattice with wave vector $2k_F$ (the Peierls effect).¹ This deformation (dimerization in the case of trans-(CH)_x is a spontaneous symmetry breaking, so that the ground state of the system is degenerate) is continuous for charge-transfer complexes having incommensurable superstructures, and twofold for trans-(CH)_x. This degeneracy, and also the specifically strong interaction of the electron excitations near the boundaries of the spectrum $\pm \Delta$ with the phonons, leads to fundamental differences between the properties of the Peierls dielectric and those of ordinary dielectrics and semiconductors. The most complete experimental picture was obtained as a result of recent investigations of polyacetylene.²

For trans-(CH)_x, it has been established that as a result of optical pumping and alloying there are highly autolocalized states with electron levels in the region of the center of the forbidden band. In a pure material

(according to the data of electron paramagnetic resonance and nuclear magnetic resonance), there are spin carriers which retain high mobility up to 4.2°K but give no contribution to the conductivity. On the contrary, the current carriers in the alloyed material [(CH)A_y]_x have no spin moment—there is no Curie paramagnetism in the region of jump conductivity $\gamma < 0.005$ or Pauli paramagnetism in the metallic region $0.005 < \gamma < 0.05$.

These data can be explained in terms of the picture of soliton carriers of spin and charge. Analytic and computer calculations of the stationary states^{3,4} and computer simulation of the dynamics of autolocalization³ in the Peierls model for polyacetylene have led to the following results:

The main elementary excitations are solitons connecting domains with opposite dimerization. In the soliton region, there is a change in the local density of wave functions of the occupied electron states with energy $E < -\Delta$, as a result of which a soliton acquires a charge $e^* = -e$ for zero spin $s = \frac{1}{2}$. The quantum numbers of the soliton vary according to the occupation number $\nu = 0, 1, 2$ of the electrons of the local level $E = 0$ in the soli-

ton potential. We obtain spinless charge carriers for $\nu=0, 2$; $e^*=-e, +e$; $s=0$ and uncharged spin carriers for $\nu=1$, $e^*=0$, $s=\frac{1}{2}$. The topological character of the soliton explains the exceptional anisotropy ($\sim 10^6$) of the spin diffusion. The soliton energy is $E_s=(2/\pi)\Delta < \Delta$. The autolocalization of electron-hole ($e-h$) and $e-e$ and $h-h$ pairs is barrier-free for a time $\sim \omega_{ph}^{-1} \sim 10^{-13}$ sec and is accomplished by the formation of diverging pairs of solitons.

For other polymers [cis-(CH) $_x$, polyphenylene, polydiacetylene, etc.], the structure of the polymer skeleton is such that there is no degeneracy of the ground state. Then the effect of autolocalization is preserved, but dispersion of the domain walls becomes impossible, since between them there appears a state with greater energy density.⁴ The nondispersion of the $e-h$ pairs explains the difference between the optical properties of cis- and trans-(CH) $_x$. At the same time, the theory predicts the existence of bound $e-e$ and $h-h$ pairs (bipolarons). This

may explain the absence of paramagnetism in conducting alloyed polypyrrole.⁵

In incommensurable systems such as charge-transfer complexes, there can exist only uncharged spin solitons $s=\frac{1}{2}$, $e^*=0$, while the excitation of charge density becomes nonactivated (Fröhlich conductivity).

¹L. N. Bulaevskii, Usp. Fiz. Nauk **115**, 263 (1975) [Sov. Phys. Usp. **18**, 131 (1975)].

²A. J. Heeger and A. G. MacDiarmid, in: Physics in One Dimension, Springer-Verlag, Berlin-Heidelberg-New York (1981).

³J. R. Schrieffer and S. Kivelson, in: Physics in One Dimension, Springer-Verlag, Berlin-Heidelberg-New York (1981).

⁴S. A. Brazovskii and N. N. Kirova, in: Trudy mezhdunarodnoi konferentsii po nizkorazmernym sinteticheskim materialam (Proc. Intern. Conf. on Small-Dimension Synthetic Materials), Vol. 17 (1981), p. 171.

⁵M. Peo, S. Roth, and J. Hocker, *Ibid.*, p. 133.