CHARGE TRAPPING BY SOLITONS—A POSSIBLE TRANSPORT MECHANISM IN MACROMOLECULAR SYSTEMS

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Macromolecules and their aggregates possess polar modes which, when excited, cause deformations, which provoke in turn elastic restoring forces. Even the simplest of such models (involving polarization and elastic modes along a chain) admit localized excitations (solitons) endowed with a characteristic degree of stability; and these provide a mechanism for charge trapping which may be of importance in the understanding of the elusively high efficiency of charge transfer over macroscopic distances evidently involved in various biomolecular processes.

Introduction. The role of localized excitations propagating along macromolecules (or their aggregates) has been emphasized by several authors in the context of energy transport and transduction processes and the kinetics of conformational transformations occurring in biology. Thus for instance, Davydov (1976, 1977, 1979, 1981) has implicated stable localized excitations (solitons) of α-helical protein molecules in their function (such as, for instance, the contractile activity of the actin–myosin complex in muscle fibres) and this approach has been extensively developed in a series of important papers by Scott (1981, 1982a, 1982b). Although the validity of the method used by Davydov to obtain the non-linear Schrödinger equation and to arrive at quantum soliton has been recently put to question (Brown et al., 1986a,b), the importance of localized structures in biological function of macromolecules remains undiminished. In fact an alternative theoretical model for the
understanding of muscle action in terms of solitons has been proposed by Yomosa (1985). Englander et al. (1980), as also Yomosa (1983, 1984), have posited the possibility of solitonic modes being involved in the movement of open segments (below the melting point) in the DNA-molecule. Jensen, Jaric and Bennemann (1983) have in a similar manner considered right–left (B–Z) conformational changes in DNA, while Balanovski and Beaconsfield (1982), as well as the present authors (Khan et al., 1985), addressed themselves to the question of $A \rightarrow B$ transitions in DNA. Sobell et al. (1983) have speculated on the role of soliton–anti-soliton breather bound states in pre-melting dynamics of DNA. Krumhansl and his group (Krumhansl et al., 1985) have been systematically and vigorously pursuing conformation motions in double-helical DNA. Furthermore, Skinner and Wolynes (1980) have studied the interaction of solitons with the surroundings leading to translational Brownian motion.

Since most of the studies involve drastic approximations to admit analytical treatment, it is encouraging to note that numerical computer experiments of Scott et al. (1979) as well as by Krumhansl (1983) have borne out the essential validity of some of the underlying ideas.

As far as the experimental support for the existence of solitons in molecules is concerned, the ground is rather tenuous and uncertain, and interpretations are being severely debated. Nevertheless, it is being claimed by Careri et al. (1983, 1984) in Italy that the observation of a band in the IR spectrum of acetoanilide, red-shifted from the main amide-I maximum, with an intensity increasing at low temperatures, may find its interpretation in terms of absorption by the solitonic mode. Furthermore, low frequency laser Raman spectra measured by Webb (1980) on metabolically active cells, is cited by some authors as evidence for internal vibrations of Davydov-like solitons, while Layne et al. (1985) call these data into question.

The purpose of the present study is to consider the trapping of charged particles (electrons or ions) by solitons, providing thereby a possible mechanism for efficient and directed charge-transfer over macroscopic distances (along a biomolecule or a channel formed from an aggregate) a process of considerable functional importance. To pose the problem within the confines of a tractable framework we adopt a model proposed by Fröhlich (1973) and developed by Bhaumik et al. (1977) who have also obtained (1982) solitonic solutions for the system. The trapping of charged particles by the soliton is formulated in a manner analogous to that invoked by Zmudzinas (1978) in the context of solid state physics.

\textbf{The Model.} Fröhlich (1973) has conjectured that macromolecules often possess polar modes which, when excited, tend to deform the system, calling into play and counteracted by elastic restoring forces. Several experimental