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SUBMITTED TO: 26th Annual Meeting of the Society for
General Systems Research
January 5-9, 1982
Washington, D.C.

University of California

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DAVYDOV SOLITONS ON ALPHA-HELIX PROTEIN

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ABSTRACT

Some results are reported from a numerical and theoretical study of solitons on alpha-helix protein. The threshold level of non-linearity for soliton formation is equal to the value obtained for this parameter from SCF calculations. Furthermore the soliton displays a spectrum of internal vibrations that is in agreement with recent laser-Raman measurements.

INTRODUCTION

A soliton (Scott, et al., 1973) is an essentially nonlinear object that maintains dynamic integrity by balancing the effects of nonlinearity against those of dispersion. To date most of the soliton systems discovered by applied mathematicians have been of one space dimension. Thus we are tempted to ask: Where in the physical world does one find one dimensional systems that display both nonlinearity and dispersion? The answer is obvious: Polymers are a natural theater in which to seek real physical (or chemical or biochemical) solitons. Recent developments support this surmise. Simple polymers such as polyacetylene (Su and Schrieffer, 1980) are now being extensively studied both theoretically and experimentally by solid-state physicists to understand the effects of solitons on physical properties. Turning to biological polymers, the prospect becomes even more exciting. The presence of a topological soliton in deoxyribonucleic acid has been inferred to explain deuteration rates by Englander et al. (1980); Pilz et al. (1981) have proposed a general model for biological solitons; and the tails of both chlorophyll and rhodopsin are essentially polyacetylene.

DAVYDOV'S ALPHA-HELIX SOLITON

Perhaps the earliest suggestion for a "polymer soliton" was made by Davydov (1979 a,b) to explain the storage and transport of energy in biological systems. He has concentrated his attention upon the alpha-helix protein and has chosen the relatively isolated amide-I (or C=O "stretch") vibration as the "basket" in which energy is carried. According to a linear analysis, energy transported by this means should spread out from the effects of dispersion and rapidly become disorganized and lost as a source for biological mechanisms. But in the nonlinear analysis of Davydov, propagation of amide-I vibrations is retroactively coupled to longitudinal sound waves of the alpha-helix, and the coupled excitation propagates as a localized and dynamically self-sufficient entity (the soliton). The amide-I vibrations generate longitudinal sound waves which, in turn, provide a potential well that prevents vibrational dispersion; thus the soliton holds itself together.

THE LASER-RAMAN SPECTRUM OF A DAVYDOV SOLITON

A recent survey of laser-Raman spectroscopy of living cells (Webb, 1980) reveals, among many others, the following facts: i) At 300°K a Raman spectrum is observed only when cells are metabolically active, ii) The intensity ratios of Stokes to anti-Stokes lines indicate that the Raman active states are produced *in vivo* by non-thermal means, and iii) Spectral lines below 300 cm^{-1} shift to lower frequencies as the cells progress through their life cycles. A particular spectrum of *E. coli* [taken from Fig. 7 of (Webb, 1980)] shows the following lines between 30 and 200 cm^{-1}:

TABLE I

Line #	cm^{-1}
1	45
2	52
3	63
4	85
5	90
6	108
7	123
8	152
9	182

Previous numerical studies (Hyman, et al., 1981) have shown that the anharmonic character of a real alpha-helix has the proper order of magnitude to support Davydov solitons. Recently this numerical model has been made more precise through the following modifications: i) Ten additional dipole-dipole coupling terms have been included to make the threshold for soliton formation insensitive to the number of such terms, ii) The dynamical equations were modified to reflect the true helical symmetry, and iii) The linear restoring force of the longitudinal hydrogen bonds was taken to be the value (21 newtons/meter) obtained by Kuprievich and Kudritskaja from SCF calculations (private communication). The critical nonlinear parameter in the model is χ_1, the change in energy of an Amide-I bond per unit extension of a corresponding longitudinal hydrogen bond.

A summary of numerical results is displayed in Fig. 1. Here the ordinate ("BOND ENERGY") is the amide-I occupation probability plotted against unit cell number at a particular value of time for various values of χ_1 between 0 and $0.8\text{x}10^{-10}$ newtons. It is interesting to note that a soliton forms at just the value ($\chi_1 = .34\text{x}10^{-10}$ newtons) that Kuprievich and Kudritskaja have computed. To appreciate the internal dynamics of a soliton consider Fig. 2. Here, in addition to total amide-I occupation probability at each unit cell, is plotted also components along the three "spines" (etc. N-C=0---N-C=0---etc.) that run longitudinally along the helix. An interspine oscillation is clearly observed with a period which corresponds to a physical time, $T_1 = 2\text{x}10^{-12}$ seconds. A shorter oscillation, also seen from Fig. 2, is caused by interaction of the soliton with the fundamental periodicity of the unit cell. The period of this oscillation is $T_2 = \frac{8}{3}\,\text{x}10^{-13}$ seconds. Raman lines should be expected at energies

$$E_1 = 17 \text{ cm}^{-1}$$
$$E_2 = 125 \text{ cm}^{-1}$$

corresponding to these two periods and their sums and differences. Thus the following table is readily constructed.

TABLE II

Line #	Structure	cm^{-1}
1	$2E_1$	34
2	$3E_1$	51
3	$4E_1$	68
4	$5E_1$	85
5	E_2-2E_1	91
6	E_2-E_1	108
7	E_2	125
8	E_2+2E_1	159
9	E_2+3E_1	176

Comparison of the measured lines in Table I with those calculated in Table II reveals a striking similarity. It should be emphasized that the periods T_1 and T_2 were computed before the present author was aware of the measurements recorded in Table I. Furthermore the tendency of such spectral lines to shift to lower wave numbers as cells progress through their life cycles is gracefully explained by assuming that solitons move more slowly as a cell ages.

CONCLUSION

Laser-Raman spectroscopy of metabolically active cells provides evidence that alpha-helix solitons play a functional role in life processes (Scott, 1981).

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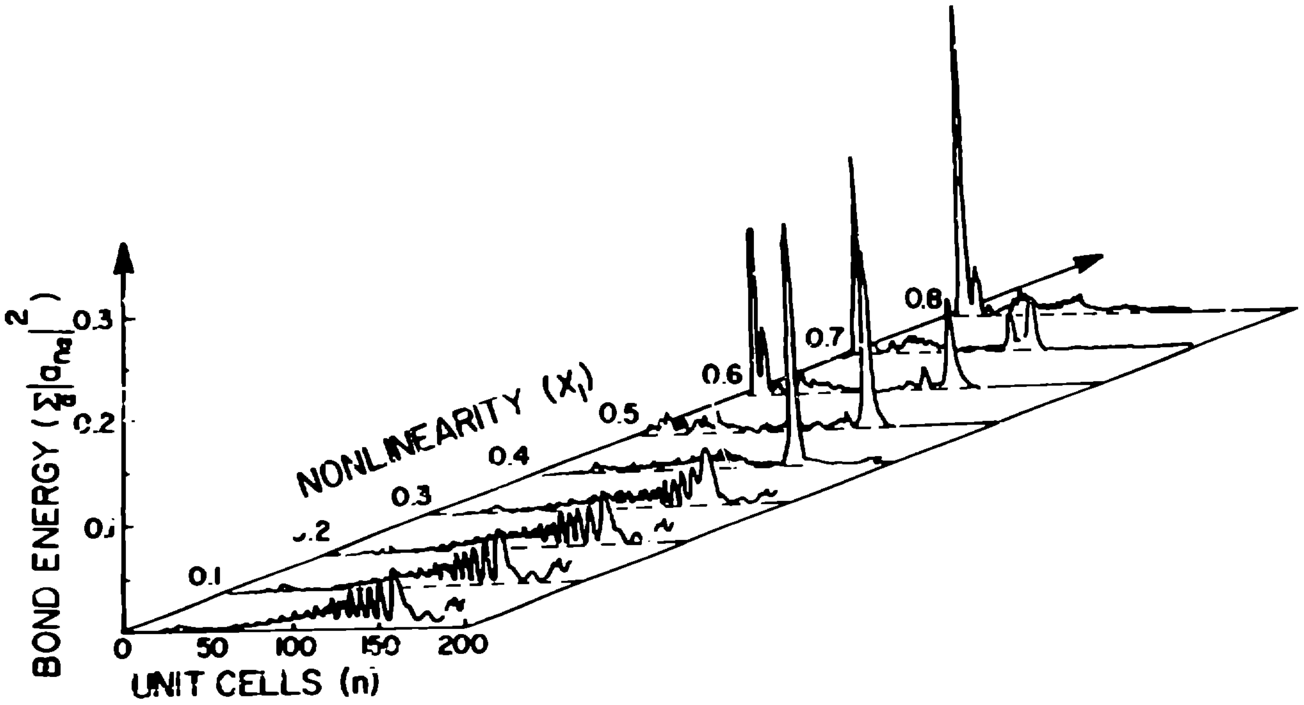

Fig. 1. Plots of bond occupation probability vs. unit cell for several values of the nonlinearity parameter χ_1 ($\times 10^{-10}$ newtons) at computer time $\tau=400$. The computation was begun with one quantum in each of the first two unit cells at $\tau=0$

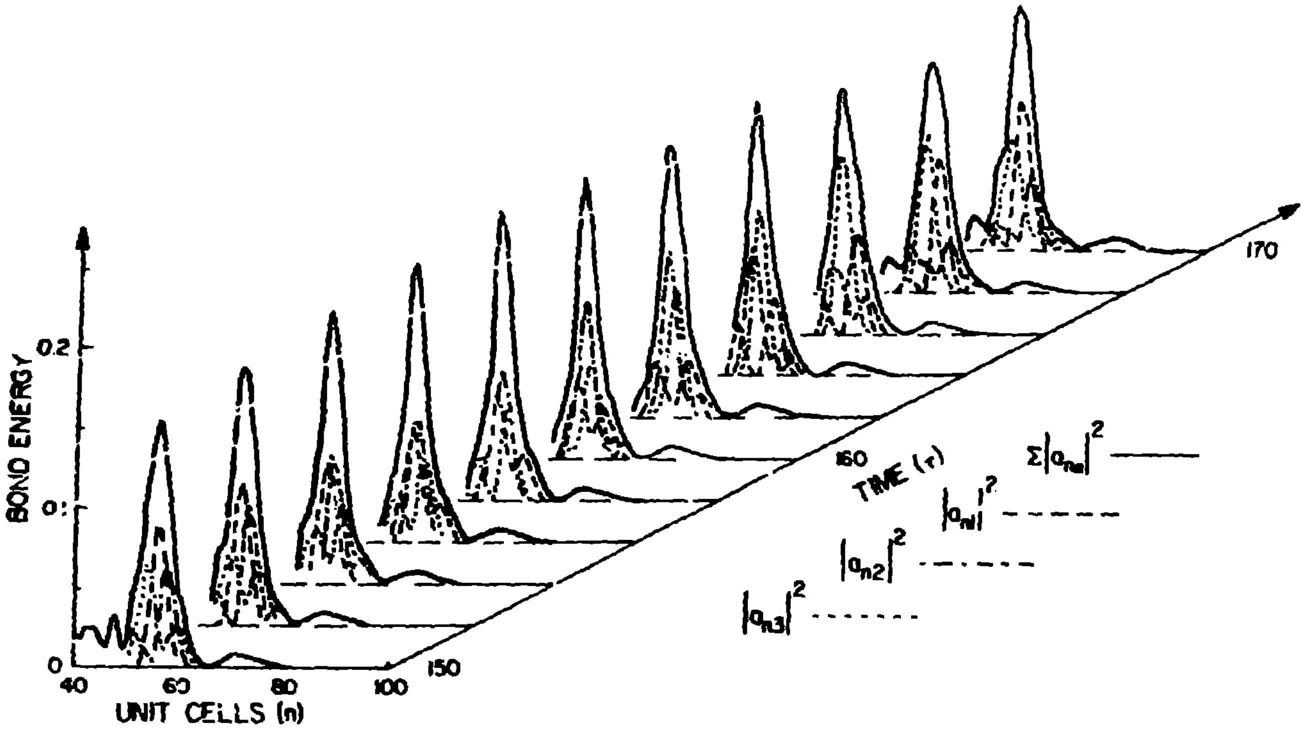

Fig. 2. Sketch of numerical calculations showing the internal dynamics of an alpha soliton. The initial conditions are as in Fig. 1 and $\chi_1 = 0.4 \times 10^{-10}$ newtons.