Self-organized digital disorder of Davydov’s beta kink

Haret C. Rosu
Instituto de Física de la Universidad de Guanajuato, Apdo Postal E-143, León, Guanajuato, México

I discuss the digital disorder introduced by Rosu and Canessa [Phys. Rev. E 47, R3818 (1993)] in the Davydov model of energy diffusion along α-helix protein chains. The digitally disordered Davydov beta kinks display self-organized features, i.e., power law correlations both in time and space, that may be attributed to incipient dynamic structural changes of the protein chain as a consequence of coarse-graining the fluctuations due to microscopic degrees of freedom. In this paper, I provide a simple semiconductor model for the flicker noise and also comment on the multifractality that one may associate with the protein chains by means of digital disorder.

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I. INTRODUCTION

In a previous paper [1], Canessa and the present author, stimulated by the findings of Voss concerning 1/f noise in long samples of DNA sequences from GenBank [2], obtained that type of noise in the Davydov’s model [3] through a simple digital dynamics of α-helix chains. I recall that digital dynamics/disorder, i.e., dynamics in digital time can also lead to other types of complex behavior, as for example to broken symmetries, oscillations, and chaos [4]. The aim of the paper is to present possible interpretations of the chain dynamics as affected by the simple digital dynamics of [1] and discuss in a heuristic manner the emerging physical picture.

The outline of the paper is as follows. After reviewing the Davydov model and solutions and shortly discussing the digital noise of the so-called β-kink in the next section, I provide in section 3 a simple physical picture for the flicker noise in terms of a partial site-trapping of the Davydov model and solutions and shortly discussing the emerging physical picture.

II. DAVIDOV MODEL

The α-helix is the most common secondary structure of proteins entailing three spines in the longitudinal z-direction that we consider infinite in extent and having the peptide sequence (−−−H − N − C = O)n, n = ∞, where the dashed lines represent hydrogen bonds. There are side radicals and their order is characteristic to each protein. The 3 spines are weaved together in a sort of incommensurate quasi-one dimensional structure, but here we shall consider only the simple one-spine chain, containing the peptide groups as molecular units.

In the Davydov model the main assumption is that a substantial part of the chemical energy (ε = 0.422 eV) released in the hydrolysis of adenosine triphosphate (ATP) turns into vibrational energy (ε0 = 0.205 eV) of the self-trapped amide-I (C=O stretching) mode of the peptide unit. The amplitude of the amide mode is self-trapped in the form of a sech- envelope soliton whenever there is a balance between the dipolar nearest-neighbour interaction and an admittedly quite strong nonlinear amide-phonon interaction. The energy transfer in the standard Davydov model is through the nonradiative resonant dipole- dipole interaction and a rather ambiguous vibrational-acoustic coherent state, the so-called D1 ansatz. It is a mixture of quantum and classical Hamiltonian methods that has been deeply scrutinized in the literature [5]. Davydov Hamiltonian can be written in the form

\[ H_D = H_{C=O} + H_{ph} + H_{int} \]  
\[ H_{C=O} = \sum_n \epsilon_0 B_{n}^{1}B_{n} - J(B_{n}^{1}B_{n+1}^{1} + B_{n+1}^{1}B_{n}) \]  
\[ H_{ph} = \sum_q \hbar \Omega_q (b_q^\dagger b_q + \frac{1}{2}) \]  
\[ H_{int} = \frac{1}{\sqrt{N}} \sum_{q,n} \chi(q) e^{i q n R} B_n^1 B_n (b_q + b_{-q}^\dagger) \]

The capital and small operators are vibrational and phonon ones, respectively. Brown [6] has shown in a clear way that Davydov Hamiltonian is a particular case of the general Fröhlich Hamiltonian of polaronic systems [7]

\[ H_F = \sum_{m} J_{mn} a_m^\dagger a_n + \sum_{q} \hbar \omega_q b_q^\dagger b_q + \sum_{q,n} \hbar \omega_q (\chi_q^a b_q^\dagger + \chi_q^b b_q) a_n^\dagger a_n \]
with $D_1$ states satisfying the Schrödinger equation of the Fröhlich Hamiltonian in the limit $J_{mn} = 0$ and another $D_2$ ansatz valid for Schrödinger evolution in the limit $\chi^2 = 0$.

The continuous limit, nonlinear Schrödinger (NLS) subsonic soliton solutions of the energy transport coming out from the Davydov model are

$$\alpha(\xi) = \sqrt{\mu/2} e^{-(\chi^2/2J^2) - E_0} \cosh^{-1}(\mu R/\xi)$$

$$\rho(\xi) = \frac{\chi^2}{w} \text{sech}^{-2}(\mu R/\xi)$$

$$\beta(\xi) = \frac{\chi^2}{w} (1 - \tanh(Q\xi))$$

where $\xi = x - v_s t$ is the moving frame coordinate, $J$ is the hopping (dipole-dipole) constant, $\chi$ is the nonlinear dipole-phonon coupling parameter, $\gamma_s = 1/\sqrt{1 - s^2}$ ($s = v_s/v_a$) is the soliton 'relativistic' factor, $w$ is the elasticity constant of the chain, $\mu = \chi^2/2Jw$, $Q = MR^2\gamma_s/2\hbar^2$, $E_0 = \epsilon_0 - 2J + \hbar^2 v_s^2/4JR^2 - J\mu^2/3$, and $\epsilon_0 \approx 0.205eV$, the quantum energy of the amide dipole oscillator. The first soliton is the vibrational soliton in which one may remark the soliton energy $E_s$, self-trapped by the carrier wave. The second solution is related to the local deformation produced by the vibrational soliton in the lattice. The $\beta$-kink is a domain-wall configuration of the displacements of the peptide groups from their equilibrium positions. It has an enhanced stability of topological origin since all the peptide groups from the right side of the kink ($\xi > 0$) are in nondisplaced positions whereas all the peptide groups at the left ($\xi < 0$) are displaced by the same amount $\beta_0 = 2\gamma_s^2/\nu_0$. In order to destroy the domain wall configuration, one should first turn the left peptide groups to their initial position. We think of the Davydov $\beta$-kink as an interphase boundary for the non-equilibrium transition from the Davydov dynamical regime of the polypeptide chain to a dynamic ‘ferroelectric’ phase of the chain. In the literature on ferroelectricity it is common to consider the interfacial boundary as the kink solution of a time-dependent Ginsburg-Landau (GL) equation. Our interpretation is based on the fact that for low subsonic regime ($s^2 \ll 1$) the Davydov kink is just the complement of the GL kink (i.e., $K_D \propto (1 - K_{GL})$). Since we are in a non-equilibrium situation the more precise terminology for these kinks is dynamic interphase boundaries or interfacial patterns. One would like to study their morphology during the growth. This is a difficult task since we are in a more complicated case as compared to the simple solid on solid model, or the kinetic Ising model, where the width of the interface is given in terms of the nearest neighbor exchange interaction $J$, corresponding to the $J$ parameter in the Davydov model. The width of the $\beta$-kink is determined by two parameters, namely the $J$ of nearest neighbors and the $\chi$ parameter of the nonlinear interaction, controlling the interfacial morphology.

Perhaps, one should notice the formal analogy between the form of the Davydov kink and the Glauber transition rate in one-dimensional spin chains. The message of this analogy is that the kink is just a step structural function which is required by a Hamiltonian evolution and by a detailed balance condition in the spatial coordinate.

The digital disorder introduced in $[\text{1}]$ is due to small random displacements of the instantaneous kink position, which $a\ priori$ may appear to be equivalent to small fluctuations of the kink velocity. The procedure is as follows. The centre of mass of the kink in the moving frame is taken as the spatial origin and small random excursions $\Delta x$ are allowed between $\pm 1$. The time correlations of such fluctuations are estimated by means of the dimensionless noise power spectrum, which usually characterize random processes of the quantity chosen as probability density, in our case the $\beta$- kink function. Thus the temporal correlations at the scale $0 < t < \tau \approx 1/f$ are measured by $[\text{2}]$

$$S_\beta(f) \propto \frac{1}{\tau} \int_0^\tau \beta(\xi) e^{2\pi i f t} dt |^2$$

When calculated with a standard fast Fourier transform (FFT) algorithm, $S_\beta(f)$ displayed clearly $1/f$ noise $[\text{1}]$. Moreover, the fact that the hyperbolic tangent is the solution of the GL equation with real coefficients leads to power law correlations in the space domain through a multifractal formalism. But power law correlations both in time and space are necessary requisites of self-organized criticality (SOC) $[\text{10}]$. The digital noise has its origin in the removed microscopic degrees of freedom, for instance the type of lattice, when one is passing to the continuous NLS limit. In this sense, the digital noise is an internal one in the terminology of the SOC literature $[\text{11}]$, while the disorders coming from varying the parameters in the Davydov model, which were studied some time ago by Förner $[\text{12}]$, belong to the class of external noises. Díaz-Guilera $[\text{11}]$ showed that the two types of noises can be considered as different limits of an Ornstein-Uhlenbeck stochastic process. Actually, the digital noise is very close to a proposal of Cruziero-Hansson $[\text{13}]$, who has argued that the thermal destabilization of the Davydov soliton at low temperatures starts through a cascade of disordered states in the displacements, of intermediate energy between the soliton and the exciton states. At higher (biological) temperatures, the disorder in the displacements is transmitted to the vibrational soliton which in this way is destroyed, although the states populated in the decay preserve the localization of the amide I excitation $[\text{14}]$. As a matter of fact, experimental evidence provided by optical calorimetry shows that phonons and vibrations heat up at different rates $[\text{3}]$. 

\[2\]
III. MODEL FOR THE FLICKER NOISE OF THE $\beta$-KINK

A simple interpretation of 1/f noise may be given in terms of a partial site-trapping of the $\beta$-kink. This trapping modulates the mobility of the domain wall and is correlated with the carrier-wave self-trapping. The toy model is adapted from semiconductor physics [16]. We shall consider the $\alpha$-chain to be at a slightly non-zero temperature, say $T \leq 11K$ [17], where the Davydov system is still not washed out by thermal effects. Let us suppose a sort of site-trapping changing the kink mobility by rectangular pulses, whose duration $\tau$ is the trapping time. Furthermore, all pulses can be considered statistically independent and thus their distribution is Poisson valid for $\tau_p$ series of rectangular pulses with the same duration.

We have obtained a shot-noise power spectrum between two limiting energies $E_1$ and $E_2$. From the thermal assumption one obtains

$$P(\tau_0) = \frac{1}{\log(\tau_2/\tau_1)} \cdot \frac{1}{\tau_0}$$

valid for $\tau_1 < \tau_0 < \tau_2$, where $\tau_1 = K \exp(-E_1/kT)$ and $\tau_2 = \exp(-E_2/kT)$. The power spectrum of a time series of rectangular pulses with the same duration $\tau$ and Poisson distributed, was obtained long ago by Gisolf [18]

$$S_g = \text{const} \cdot \tau \left( \frac{\sin(\omega \tau/2)}{\omega \tau/2} \right)^2$$

By combining $g(\tau)$ with Eq.(1), Van der Ziel [10] obtained a shot-noise power spectrum

$$S'_g = \text{const} \cdot \frac{\tau_0}{1 + \omega^2 \tau_0^2}$$

One gets the 1/f noise by averaging the shot spectrum with the square distribution of the trapping times $\tau$ as

$$S_{\text{flicker}} = \frac{kT}{E_2 - E_1} \frac{1}{\omega} \left[ \arctan(\omega \tau_2) - \arctan(\omega \tau_1) \right]$$

Of course, the simple flicker mechanism we have used here was more for illustrative purposes, and further work is required to clarify the nature of such noise in protein chains. For example, the flicker noise can be explained alternatively by means of a scaled Langevin equation as introduced by Kogama and Hara [19]. For that, it is sufficient to consider the same scaling parameter both in the Langevin variable and in the attached noise as was shown in their paper.

IV. MULTIFRACTALITY OF $\beta$-KINKS

The implicit occurrence of the GL kink in the Davydov $\beta$ displacements is essential for discussing the multifractal issue. Previously, Brax [20] showed the equivalence of the GL equation with real coefficients under random initial conditions and the linear heat equation with Gaussian random potential and made a multifractal analysis of the problem of direct relevance for our study. As is well-known the GL equation, which is a cubic reaction-diffusion equation, describes phenomenologically the evolution of the order parameter in superconductive phase transitions, and models also spatial and time fluctuations of systems near Hopf bifurcations. In 1972, Scalapino, Sears and Ferrell [21] studied in detail the statistical mechanics of one-dimensional GL fields. They remarked that such fields can describe the dynamical behaviour of nearly-ordered systems which are not undergoing sharp phase transitions, and conjectured that the real-field case may have application in some organic chain systems. Our approach is just a further confirmation of that idea. As a matter of fact, in the D’Alambert variable ($\xi = x - vt$), the GL kink $K_{GL}$ is the solution of a GL equation of the type

$$\frac{\partial K_{GL}}{\partial t} = \frac{\partial^2 K_{GL}}{\partial x^2} + p_1 K_{GL} - p_3 K_{GL}^3$$

with real $p_1$ and $p_3$ coefficients. Such GL equations are typical for the structural phase-transitions in equilibrium situations, but they can be used also in nonequilibrium/ driven systems. Moreover, in Eq.(8) one can recognize the complement of the GL kink (i.e., the Davydov $\beta$-kink) playing the role of the probability density distribution $P$. Following Brax, one can develop a multifractal formalism if the kink probabilistic distribution function is identified with the $\tau$- function of the multifractal formalism

$$\mathcal{G}(\xi_2) - \mathcal{G}(\xi_1) \approx \int_{\xi_1}^{\xi_2} \beta(\xi') d\xi' \equiv -\tau(\xi)$$

I recall that in the multifractal formalism the function $\tau q$ is the cumulant generating function. The derivative of this function with respect to $q$ is denoted by $\alpha$ and via the Lagrange multipliers procedure of statistical thermodynamics, one obtains the function $f(\alpha)$ which is the density of a measure, and could be interpreted as a fractal dimension when it is positive, and related to instabilities for negative values. The equations $\alpha = \delta \tau/\delta q$ and $f(\alpha) = q_0 - \tau$ represent the basis of the multifractal formalism [23]. Formally, $q$ is the inverse temperature, $\tau$
is the Gibbs free energy, and $f$ is the entropy. One can plot the second derivative of the $\tau$-function (the ‘specific heat’) and find out intervals of the ‘temperature’ variable, within which the plot clearly displays features of a phase transition, that is a peak in the ‘specific heat’ at a certain value of the ‘temperature’ variable [22].

V. CONCLUDING REMARKS

The digitally disordered Davydov beta kinks can display features characteristic to self-organized criticality. Here, I considered the digital noise of Davydov kinks as a reflection of hidden microscopic degrees of freedom of the protein chain. It is an internal noise in the SOC terminology, representing the dynamics of a self-organized state of the chain, therefore not destroying the soliton solution all over the scaling region.

I ascribed the $1/f$ noise to carrier trapping and so to some sort of short-distance thermal activation physics, rather than to coherence effects. This would be more in the standard spirit of solid state physics. In general $1/f$ mesoscopic noise can have many interpretations and it would be helpful to disentangle its real origin. At the level of vibrational degrees of freedom it will be of interest to see if the vibrational soliton possesses self-organized features as well, and to investigate the connection with the kink digital disorder.

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