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Local Conformational Perturbations of the DNA Molecule in the SG-Model

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Abstract. Within the formalism of the Fokker–Planck equation, the influence of nonstationary external force, random force, and dissipation effects on dynamics local conformational perturbations (kink) propagating along the DNA molecule is investigated. Such waves have an important role in the regulation of important biological processes in living systems at the molecular level. As a dynamic model of DNA was used a modified sine-Gordon equation, simulating the rotational oscillations of bases in one of the chains DNA. The equation of evolution of the kink momentum is obtained in the form of the stochastic differential equation in the Stratonovich sense within the framework of the well-known McLaughlin and Scott energy approach. The corresponding Fokker–Planck equation for the momentum distribution function coincides with the equation describing the Ornstein–Uhlenbek process with a regular nonstationary external force. The influence of the nonlinear stochastic effects on the kink dynamics is considered with the help of the Fokker–Planck nonlinear equation with the shift coefficient dependent on the first moment of the kink momentum distribution function. Expressions are derived for average value and variance of the momentum. Examples are considered which demonstrate the influence of the external regular and random forces on the evolution of the average value and variance of the kink momentum. Within the formalism of the Fokker–Planck equation, the influence of nonstationary external force, random force, and dissipation effects on the kink dynamics is investigated in the sine–Gordon model. The equation of evolution of the kink momentum is obtained in the form of the stochastic differential equation in the Stratonovich sense within the framework of the well-known McLaughlin and Scott energy approach. The corresponding Fokker–Planck equation for the momentum distribution function coincides with the equation describing the Ornstein–Uhlenbek process with a regular nonstationary external force. The influence of the nonlinear stochastic effects on the kink dynamics is considered with the help of the Fokker–Planck nonlinear equation with the shift coefficient dependent on the first moment of the kink momentum distribution function. Expressions are derived for average value and variance of the momentum. Examples are considered which demonstrate the influence of the external regular and random forces on the evolution of the average value and variance of the kink momentum.

INTRODUCTION

The sine–Gordon equation with random parameters is used to construct models of propagation of ultrashort optical pulses [1], in physics of condensed state [2], and also in a number of other areas of nonlinear physics [3, 4]. The influence of weak fluctuations on the kink dynamics (one-soliton solutions of the sine–Gordon equation) with dissipation was first investigated in [5, 6]. Nonlinear Waves (kink) propagating along a DNA molecule, considered as one of the elements of the transmission mechanism of structural changes and information material in the functioning of the molecule. Within the McLaughlin and Scott energy approach [7], the stochastic dynamic equations for the kink momentum, velocity, and center of mass were derived with allowance for the influence of weak random perturbations and dissipation effects. The evolution of the average values and variances was investigated with the help of the distribution functions of these values obtained by solving the Fokker–Planck equation. The investigations started in [5, 6] were then continued in [8], and the influence of large-scale random perturbations on the kink dynamics was modeled numerically. The results obtained were used to investigate the statistical properties of quasi–one-dimensional magnetic components. The equations describing the kink dynamic

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characteristics in a random medium were obtained in [9] by the inverse scattering transform method [10]. The kink acceleration was investigated in [11] under the influence of random nonlinear perturbations (the nonlinearity coefficient in the sine–Gordon equation was set to be a random function of time) in the context of the theory of soliton perturbations. The influence of stochastic processes on the kink dynamics was investigated in [12] in the approximation of dominant dissipation. The contributions of the first and second orders to the diffusion coefficient were calculated, and the kink dynamics was modeled numerically with the use of the method of perturbation theory. The joint influence of the nonstationary external force, random force, and dissipation effects on the kink velocity in the sine–Gordon model is studied in the present work following [5–7] within the formalism of the Fokker–Planck equation. In the present work, the influence of the nonlinear random effects (processes with a stochastic feedback) on the kink dynamics is investigated on the basis of the Fokker–Planck nonlinear equation. The evolution of the average momentum and its variance is analyzed.

FOKKER–PLANCK EQUATION FOR THE KINK MOMENTUM DISTRIBUTION FUNCTION

Let us write down the sine–Gordon equation with additional terms in the dimensionless form:

$$\phi_{tt} - \phi_{zz} + \sin\phi = -\alpha\phi_t + \widetilde{f}(t) + \sqrt{\widetilde{D}}\,\xi(t)\,. \quad (1)$$

Here α is the dissipation coefficient, $\widetilde{f}(t)$ is the nonstationary regular external force, $\widetilde{D}$ is the diffusion coefficient, and the random force $\xi(t)$ is chosen in the form of the Gaussian white noise with average value $\langle \xi(t) \rangle = 0$ and correlation $\langle \xi(t)\xi(t') \rangle = \delta(t-t')$.

For $\alpha = \widetilde{f}(t) = \widetilde{D} = 0$, Eq. (1) has the one-soliton solution (kink) of the following form:

$$\phi_{(k)}(z,t) = 4\arctan\left\{\exp\left[\frac{z - \upsilon t - z_0}{\sqrt{1-\upsilon^2}}\right]\right\}. \quad (2)$$

Here υ is the kink velocity, and the coordinate z_0 characterizes the initial position of the kink.

Let us write down Eq. (1) for (ϕ_t, ϕ) at $\alpha = \widetilde{f}(t) = \widetilde{D} = 0$ in the Hamiltonian form. The Hamiltonian of the sine–Gordon equation $H^{SG}(\phi)$ is the functional [7, 10, 13]

$$H^{SG}(\phi) = \int_{-\infty}^{\infty}\left[\frac{1}{2}\phi_t^2 + \frac{1}{2}\phi_z^2 + (1-\cos\phi)\right]dz\,. \quad (3)$$

Substituting Eq. (3) into Eq. (2), we obtain the expression for the kink energy [14]:

$$H^{SG}(\phi_{(k)}) = 8(1-\upsilon^2)^{-1/2}. \quad (4)$$

Following the energy analysis algorithm [7], we obtain the well-known equation of evolution of the kink velocity for Eq. (1). Let ϕ be an arbitrary solution of Eq. (1) for $\alpha,\ \widetilde{f}(t),\ \widetilde{D} \neq 0$ then from Eqs. (1) and (3), we have

$$\frac{d\,H^{SG}(\phi)}{d\,t} = \int_{-\infty}^{\infty}\left(-\alpha\phi_t^2 + (\widetilde{f}(t) + \sqrt{\widetilde{D}}\xi(t))\phi_t\right)dz\,. \quad (5)$$

Substitution of Eq. (2) into Eq. (5) yields

$$\frac{d\,H^{SG}(\phi_{(k)})}{d\,t} = \int_{-\infty}^{\infty}\left(-\alpha(\phi_{(k)_t})^2 + (\widetilde{f}(t) + \sqrt{\widetilde{D}}\,\xi(t))\phi_{(k)_t}\right)dz = -8\alpha\frac{\upsilon^2}{\sqrt{1-\upsilon^2}} + 2\pi\upsilon(\widetilde{f}(t) + \sqrt{\widetilde{D}}\,\xi(t))\,. \quad (6)$$

On the other hand, assuming that the kink velocity υ depends on time $\upsilon = \upsilon(t)$, we differentiate Eq. (4) with respect to time *t*; as a result, we obtain

$$\frac{d\,H^{SG}(\phi_{(k)})}{d\,t} = 8\left(1-\upsilon(t)^2\right)^{-3/2}\upsilon(t)\frac{d\,\upsilon(t)}{d\,t}\,. \quad (7)$$

From Eqs. (6) and (7), we find the sought-after equation for the kink velocity $\upsilon(t)$ in the following form:

$$\frac{d\upsilon(t)}{dt} = -\alpha\upsilon(t)\left(1-\upsilon^2(t)\right) + \left(f(t) + \sqrt{D}\,\xi(t)\right)\cdot\left(1-\upsilon^2(t)\right)^{3/2}. \tag{8}$$

where $f(t) = \frac{\pi}{4}\tilde{f}(t)$, $D = \frac{\pi^2}{16}\tilde{D}$.

Replacing the variable υ according to the formula

$$\upsilon = \frac{x}{\sqrt{1+x^2}}. \tag{9}$$

we reduce Eq. (8) to the form

$$\frac{dx}{dt} = -\alpha\, x + f(t) + \sqrt{D}\,\xi(t). \tag{10}$$

The variable x is related to the kink momentum P as follows: $x = P/8$, $P = \frac{8\upsilon}{\sqrt{1-\upsilon^2}}$.

We consider Eq. (10) with random force $\sqrt{D}\,\xi(t)$ to be the stochastic differential equation in the Stratonovich sense [5, 6], for which the Fokker–Planck equation for the probability density function $W(x,t)$ in designations [15] is written in the form

$$\frac{\partial W(x,t)}{\partial t} = \partial_x\left(\alpha\, x - f(t)\right)W(x,t) + \frac{D}{2}\partial_{xx}W(x,t). \tag{11}$$

Following [16], we replace the sought-after function in Eq. (12)

$$W(x,t) = U(x-\varphi(t),t), \tag{12}$$

where we determine the function $\varphi(t)$ below. Substituting Eq. (12) into Eq. (14), we obtain

$$\partial_t U(y,t) - \dot{\varphi}(t)\partial_y U(y,t) = \partial_y\left(\alpha(y+\varphi(t)) - f(t)\right)U(y,t) + \frac{D}{2}\partial_{yy}U(y,t). \tag{13}$$

where $y = x - \varphi(t)$. Assuming that the function $\varphi(t)$ satisfies the condition

$$\dot{\varphi}(t) + \alpha\varphi(t) - f(t) = 0 \tag{14}$$

we reduce Eq. (14) to the form

$$\partial_t U(y,t) = \partial_y(\alpha y)U(y,t) + \frac{D}{2}\partial_{yy}U(y,t) \tag{15}$$

Equation (16) describes the well-known Ornstein–Uhlenbek process [17]. From condition (15), we obtain

$$\varphi(t) = \exp(-\alpha(t-t_0))\left[\varphi(t_0) + \int_{t_0}^{t} f(\tau)\exp(\alpha(\tau-t_0))\,d\tau\right] \tag{16}$$

here $\varphi(t_0)$ is an integration constant.

The Fourier transform

$$\tilde{U}(s,t) = \int_{-\infty}^{+\infty}\exp(isy)\,U(y,t)\,dy \tag{17}$$

reduces Eq. (16) to the form

$$\partial_t\tilde{U} + \alpha\, s\partial_s\tilde{U} = -\frac{1}{2}Ds^2\tilde{U} \tag{18}$$

Using the method of characteristics, we write down the general solution of Eq. (18) in the form

$$\tilde{U}(s,t,t_0) = \exp\left[-\frac{Ds^2}{4\alpha}\right]g(s\exp(-\alpha(t-t_0))) \tag{19}$$

Here, $g(u)$ denotes an arbitrary function of the variable u.

We now find the distribution function specified by Eq. (15) from the condition

$$U(y,t_0\,|\,y_0,t_0)=\delta(y-y_0) \tag{20}$$

Its Fourier transform is

$$\widetilde{U}(s,t_0)=\exp(iy_0 s) \tag{21}$$

From Eqs. (21) and Eq. (19), we obtain

$$g(s)=\exp\left[\frac{Ds^2}{4\alpha}+iy_0 s\right] \tag{22}$$

Correspondingly,

$$\widetilde{U}(s,y_0,t,t_0)=\exp\left[-\frac{Ds^2}{4\alpha}(1-e^{-2\alpha(t-t_0)})+isy_0e^{-\alpha(t-t_0)}\right] \tag{23}$$

The inverse Fourier transform of identity (24), $U(y,t|y_0,t_0)=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-isy}\widetilde{U}(s,y_0,t,t_0)ds$ yields

$$U(y,t|y_0,t_0)=\frac{\sqrt{\alpha}}{\sqrt{D\pi(1-e^{-2\alpha(t-t_0)})}}\exp\left[-\frac{\alpha}{D(1-e^{-2\alpha(t-t_0)})}(y-y_0e^{-\alpha(t-t_0)})^2\right] \tag{24}$$

Returning to the variable $x=y+\varphi(t)$ in identity (24), we derive the solution of Eq. (11) in the form

$$W(x,t|x_0,t_0)=\frac{\sqrt{\alpha}}{\sqrt{D\pi(1-e^{-2\alpha(t-t_0)})}}\exp\left[-\frac{\alpha}{D(1-e^{-2\alpha(t-t_0)})}(x-\varphi(t)-(x_0-\varphi(t_0))e^{-\alpha(t-t_0)})^2\right]. \tag{25}$$

We note that $W(x,t_0|x_0,t_0)=\delta(x-x_0)$. Expression (25) has the meaning of the probability density function for x at the moment of time t, given that $x=x_0$ at $t=t_0$.

For the kink momentum $P=8x$, from Eq. (25) it follows that

$$W(P,t|P_0,t_0)=\frac{\sqrt{\alpha}}{8\sqrt{D\pi(1-e^{-2\alpha(t-t_0)})}}\exp\left[-\frac{\alpha}{D(1-e^{-2\alpha(t-t_0)})}\left(\frac{P}{8}-\varphi(t)-\left(\frac{P_0}{8}-\varphi(t_0)\right)e^{-\alpha(t-t_0)}\right)^2\right] \tag{26}$$

The average value of the kink momentum for distribution function (26) is found in the following form:

$$\langle P\rangle(t,t_0)=\int_{-\infty}^{+\infty}PW(P,t|P_0,t_0)\,dP=P_0\exp(-\alpha(t-t_0))+8\left[\int_{t_0}^{t}f(\tau)\exp(-\alpha(t-\tau))\,d\tau\right] \tag{27}$$

The variance $\sigma(t,t_0)$ is given by the expression

$$\sigma(t,t_0)=\langle P^2\rangle(t,t_0)-\langle P\rangle^2(t,t_0)=\frac{4\pi^2}{\alpha}\widetilde{D}(1-e^{-2\alpha(t-t_0)}) \tag{28}$$

where $\langle P^2\rangle(t,t_0)=\int_{-\infty}^{+\infty}P^2W(P,t|P_0,t_0)\,dP$ Equation (27) demonstrates that P_0 has the meaning of the average value of the kink momentum for $t=t_0$.

It can be easily seen that the average value of the kink momentum given by Eq. (27) coincides with the solution of Eq. (11) without random force $\xi(t)=0$. This is in agreement with the results obtained in [14], where the kink dynamics under the action of external regular force $f(t)$ was considered. The variance $\sigma(t,t_0)$ given by Eq. (28) depends on the diffusion coefficient $\widetilde{D}$ and is independent of the regular external force $f(t)$. Fig. 1 shows the time dependence of the kink momentum variance; from the figure, it can be seen that $\sigma(t_0,t_0)=0$. This corresponds to a certain value of the momentum P_0 at $t = t_0$. The variance increases with time asymptotically approaching to $4\widetilde{D}\pi^2/\alpha$. Dependence (28) coincides with the results of numerical calculations presented in [5]. For the kink rootmean square velocity in the nonrelativistic case ($\upsilon << 1$, $P = 8\upsilon$) we obtain $\left\langle \upsilon^2 \right\rangle(t,t_0) = \frac{\pi^2}{16\alpha}\widetilde{D}(1 - e^{-2\alpha(t-t_0)})$ from formula (26) for $\left\langle \upsilon_0 \right\rangle = 0$ and $f(t) = 0$ This is also in agreement with the results presented in [5].

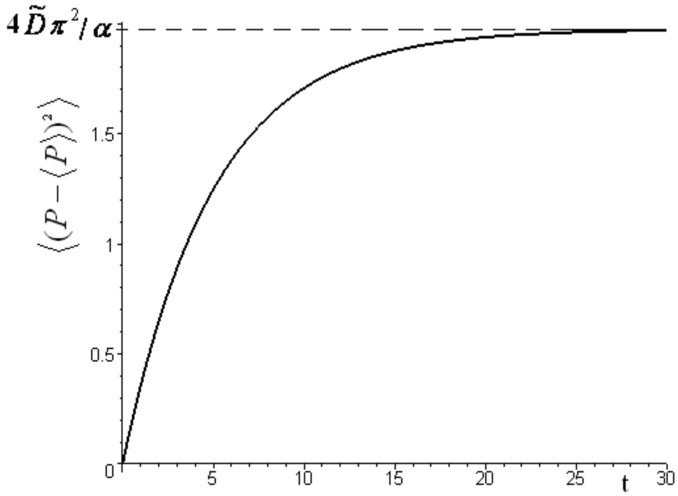

FIGURE 1. Root-mean-square value of the kink momentum for α=0.1, $\widetilde{D}$=0.01, t_0=0

CONCLUSIONS

The joint influence of the nonstationary external force, random δ-correlated force, and dissipation effects on the evolution the kink momentum in the sine–Gordon model within the formalism of the Fokker–Planck equation has been investigated in this work. The equation of evolution for the kink momentum was derived with the help of the wellknown McLaughlin and Scott energy approach; it has the form of the stochastic differential equation in the Stratonovich sense. The corresponding Fokker–Planck equation for the probability density function of the kink momentum has the form of the equation describing the Ornstein–Uhlenbek process whose evolution operator is written with the help of the Green's function. The obtained expressions for the kink average momentum (27) and variance (28) demonstrated that the average value of the kink momentum depends on the external regular force and is independent of the diffusion coefficient $\widetilde{D}$, whereas the variance is determined by this coefficient and monotonically increases with time, asymptotically approaching $4\widetilde{D}\pi^2/\alpha$.

This peculiarity of the kink dynamics under the action of the nonlinear random force with stochastic feedback can be used to control the kink motion, successively switching on and off the random force. The above-indicated peculiarities of the kink dynamics are important from the viewpoint of the study of general laws of interaction between the stochasticity and nonlinearity.

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