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Modification of the Potential Function of a Mechanical System Caused by Periodic Action

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With 1 Figure

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Summary

The motion of a particle in the field of potential forces under conditions of large friction that has a component which is nonlinear with respect to the velocity is studied. It is shown that a periodic external force of small period results, under certain circumstances, in a modification of the initial potential function a term linear with respect to the deflection is added. Possible implications of this result for problems in physico-chemical biology are discussed.

1. Introduction

We suppose that a mechanical system consists of separate parts connected by potential forces. The relative motion of the parts processes in a very viscous fluid so that natural vibrations in any given potential wells are overdamped. This model is used in physico-chemical biology to describe the mechanical properties of globular proteins [1], [2], [3]. There the set of local minima of the potential function (called conformational states) and the ability of the system to proceed from one minimum to another are the most important characteristics that define the functioning of globular protein. It is necessary to elucidate how the comformational properties (the position of the minima and their relative depths) change if we apply to a part of the system a periodic force of a small period and without constant component. Such a problem arises when we describe theoretically the mechanism by which periodic electric fields effect globular proteins and other biopolymers.

In the present paper we give a qualitative answer to the question posed. For this purpose we consider the simplest situation when there is only one degree of freedom. The equation of motion then coincides with the equation of an anharmonic oscillator with a potential of several minima placed in a non-Newtonian viscous fluid (the non-Newtonian character of biological fluids is a fact known in reology); in such a case the friction force depends nonlineary on the velocity. The behaviour of the trajectories of such a system is investigated in this paper. It is shown that every trajectory either goes to infinity or attains a final stage where the deflection moves within a fixed small interval whose position may be quite different from that of a local minimum of the initial potential function. When the motion is considered on a rough scale (the presence of a hierarchy of scales is characteristic to internal motions in globular proteins [1], [2], [3]), and when the size of the region under consideration is negligibly small, we can speak of a new local minimum of the potential function. Consistent study enables us to conclude that an external periodic action results in a modification of the potential function by an additional term linear with respect to the deflection. A set of conformational states can either deform (change in the position and depth of the minima) or rearrange qualitatively (individual minima may disappear and/or new minima may appear).

2. Basic Equation

The equation of motion of an anharmonic oscillator with a nonlinear friction and periodic driving force has the following (dimensional) form

$$\begin{gathered} m \frac{d}{d\tau} V(\tau) + \Lambda V(\tau) - Eg\left(\frac{V(\tau)}{V_0}\right) = F_0 f\left(\frac{\tau}{T}\right) - \Phi_0 \varphi\left(\frac{X(\tau)}{X_0}\right), \\ \frac{d}{d\tau} X(\tau) = V(\tau) \end{gathered} \tag{1}$$

where the notations are used: X coordinate, V velocity, m mass of the oscillator, Λ coefficient of linear friction; E, V_0 and the non-dimensional function g characterize a nonlinear friction; Φ, X_0 and the non-dimensional function φ characterize the force produced by an anharmonic potential; F_0, T and the non-dimensional function f characterize the driving force (of period T). The constants F_0, $\Phi_0 \geqq 0$ are chosen so that the functions f, φ do not exceed one in absolute value. The function g should be odd from physical considerations. It is assumed that g and φ satisfy a Lipshits condition with constants g^* and φ^*, respectively. We also assume that the inequalities

$$Eg^*/(\Lambda V_0) < 1/2, \tag{2}$$

$$\Lambda T/m \ll 1, \tag{3}$$

$$m\varphi^*\Phi_0/(\Lambda^2 X_0) \ll 1 \tag{4}$$

are valid.

The inequality (2) means that the nonlinear friction is small compared to the linear one, (4) means that the natural vibrations are overdamped. The inequality (3) is valid if the period of the driving force is small enough.

In non-dimensional variables $t = \tau/T$, $x = X/(V_0 T)$, $v = V/V_0$ the Eq. (1) gets the form

$$\dot{v}(t) + \lambda v(t) - \varepsilon g(v(t)) = f_0 f(t) - \varphi_0 \varphi(k_0 x(t)), \qquad \dot{x}(t) = v(t). \tag{5}$$

3. Auxiliary Equations

Consider the auxiliary equation

$$\dot{v} + \lambda v - \varepsilon g(v) = h(t), \tag{6}$$

where $\|h\| \equiv \sup_{t \geqq 0} |h(t)| < \infty$. The influence of the righthand side perturbation on the unique solution of the Eq. (6) is given by (see [4], [5])

$$\|\delta v\| \leqq (\lambda - \varepsilon g^*)^{-1} \|\delta h\|. \tag{7}$$

Consider the equation

$$\dot{v} + \lambda v - \varepsilon g(v) = f_0 f(t) + d, \tag{8}$$

where $f(t)$ is a 1-periodic that has no constant component: $\langle f \rangle \equiv \int_0^1 f(t)\, dt = 0$.

The Eq. (8) has a unique periodic solution $V_d^*(t)$ which is globally asymptotically stable. The speed of transition from an arbitrary solution $V(t)$ of (8) to $V_d^*(t)$ can be estimated by

$$|V_d^*(t + \delta t) - V(t + \delta t)| \leqq \exp\big((\varepsilon g^* - \lambda)\, \delta t\big)\, |V_d^*(t) - V(t)|. \tag{9}$$

Definition. A constant d_0 such that $V_{d_0}^*$ satisfies the relation $\langle V_{d_0}^* \rangle = 0$ is called a stopping force for the driving force $f_0 f(t)$ which has no constant component.

Theorem. The stopping force exists, is unique and satisfies the estimate

$$|d_0| < f_0. \tag{10}$$

The proof is obtained by going over to an integral equation for $V_d^*(t)$. The impossibility to improve the estimate (10) follows from the following example.

Example. Assume that only a dry friction exists, $\lambda v - \varepsilon g(v) = F \cdot \mathrm{sign}\,(v)$, and the periodic function $f_0 f(t)$ has the following form

$$f_0 f(t) = \begin{cases} f_0^+ & \text{if} \quad t \in [0; \alpha[\\ -f_0^- & \text{if} \quad t \in [\alpha; 1[, \end{cases} \qquad f(t+1) = f(t), \qquad t \in R^1,$$

where $\alpha < 1/2$, $f_0^+ > F$, $f_0^- < F$. Then the condition $\langle f_0 f \rangle = 0$ requires $f_0^- = \alpha/(1-\alpha) \cdot f_0^+$. One can find the stopping force value starting from the condition that the whole momentum which is transferred to an oscillator during one period by the periodic force and the stopping force must be equal to zero. At the internal $[0; \alpha[$ the momentum transferred is equal to $\Delta P_1 = (f_0^+ - F + d_0)\alpha$, and at the interval $[\alpha; 1[$ $\Delta P_2 = -(f_0^- - F - d_0) \cdot (1 - \alpha)$.

From the condition $\Delta P_1 + \Delta P_2 = 0$ we get $d_0/f_0^+ = -(1 - 2\alpha) F/f_0^+$. If here $F/f_0^+ \approx 1$, $2\alpha \ll 1$, the ratio $|d_0/f_0^+|$ $(= |d_0/f_0|)$ may be made as close to unity as desired. So the stopping force value may, practically, be equal to the driving force amplitude. Unfortunately, in less trivial situations it may be found only by numerical methods.

From the definition and the theorem it follow, if in (8) $d = d_0 + b$, $b \neq 0$, the velocity in a stable regime of motion has a constant component. It satisfies the relation

$$\langle V^*_{d_0+b} \rangle = b\big(1 + W(b)\big)/\lambda, \tag{11}$$

where

$$|W(b)| \leqq \varepsilon g^*/(\lambda - \varepsilon g^*). \tag{12}$$

Consider the equation

$$\dot{v} + \lambda v - \varepsilon g(v) = f_0 f(t) + b(t), \tag{13}$$

where $f(t)$ is the above periodic function and $b(t)$ is a nonperiodic one; also

$$\sup_{t \geqq 0} |\dot{b}(t)| \leqq b^*. \tag{14}$$

The Eq. (13) has a unique solution $V(t)$ for an arbitrary initial condition. We shall say that the motion with velocity $V(t)$ undergoes a drift to the right (left) over the interval $[t_0; t_1]$, $(t_1 - t_0 \gg 1)$, if for all $n \in [t_0; t_1]$ $\int_0^1 V(t + n)\, dt > 0$ (< 0). We use the function $b(t)$ to define a piecewise constant function $\tilde{b}(t)$ in the following way: $t \in [n; n + 1[\Rightarrow \tilde{b}(t) = b(n)$, $n \in N$. Consider the equation

$$\dot{\tilde{v}} + \lambda \tilde{v} - \varepsilon g(\tilde{v}) = f_0 f(t) + \tilde{b}(t). \tag{15}$$

From (7), (14) we get the estimate

$$\|v - \tilde{v}\| \leqq b^*/(\lambda - \varepsilon g^*), \tag{16}$$

where $v, \tilde{v}$ are the solutions to the Eqs. (13), (15), respectively, with equal initial conditions.

For an arbitrary function $d(t)$ we define the function $v^*_{d(t)}(t)$ as the periodic solution to Eq. (8) for the "frozen" value $d = d(t)$.

At every interval $t \in [n; n + 1[$ (15) coincides in form with (8). Therefore, from the estimates (3), (7), (9), (16) we get the estimate.

$$|v(t) - v^*_{\tilde{b}(t)}(t)| \leqq b^*/(\lambda - \varepsilon g^*)^2, \tag{17}$$

where $v(t)$ is that solution to Eq. (13) which is valid for times when the initial velocity is "forgotten" (when the effect of the initial velocity has disappeared).

Transition to dimensional quantities enables us to conclude that the accuracy, characterized by the inequality (17), of the approximate to Eq. (13) by a family of periodic solutions of the Eq. (8) is controlled by great values of friction coefficient Λ.

4. Steady Motion

The Eqs. (1), (5) have a unique solution for all $t \geqq 0$ (see [4]). The presence of a great friction Λ in (1) makes it possible to conclude from energy considerations that high initial velocities will damp rapidly and, beginning from some time t_0, the effect of an initial velocity may be neglected. The motion at this stage will be called steady. For a steady motion we get from (7) the estimate

$$\sup_{t \geqq t_0} |v(t)| \leqq (f_0 + \varphi_0)/(\lambda - \varepsilon g^*), \tag{18}$$

where $v(t)$ is the solution to Eq. (5). Considering (5) as equation of the form (13) with $b(t) = -\varphi_0\varphi(k_0 x(t))$, we get from (17), (18) the estimate

$$|v(t) - \overset{*}{v}_{b(t)}(t)| \leqq (f_0 + \varphi_0)\, \varphi_0 \varphi^* k_0 (\lambda - \varepsilon g^*)^{-3}, \tag{19}$$

where $v(t)$ is the solution of Eq. (5) which is valid for a steady regime of motion. By writing (19) in dimensional from we can see that its accuracy is provided by a large friction (Λ) and a "soft" potential function (with small values of its two first derivatives).

5. Final Motion

The presence of a large friction in (1) allows us to assume that after some transients have disappeared, the effect of an initial deflection may be neglected "in the small"[1]. The motion at this stage will be called final (a final solution).

We now put a question: In what region will the final motion be concentrated when a constant external force is introduced on the right-hand side of (5)? When no periodic force is acting ($f_0 = 0$), the final solution will be characterized by zero velocity and a deflection x that satisfies the equation $\varphi_0\varphi(k_0 x) - d = 0$, i.e. the external force d is neutralized by the potential force $\varphi_0\varphi(k_0 x)$ at a point (points) x. It is possible to determine a complete function $\varphi_0\varphi(k_0 x)$ by finding all such points for various d.

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[1] I.e. a sufficiently small perturbation of an initial deflection does not effect the solution. In general, Eq. (5) (not (8)) may have several periodic solutions (see [6]) and each of them is available as a terminal one. The situation is controlled by the initial conditions.

When $f_0 \neq 0$, we rewrite Eq. (5) (with "diagnostic" force d) in the form

$$\dot{v} + \lambda v - \varepsilon g(v) = f_0 f(t) + d_0 - \big(\varphi_0 \varphi(k_0 x(t)) + d_0 - d\big), \qquad \dot{x} = v, \tag{20}$$

where d_0 is a stopping force for $f_0 f(t)$. For the solution $v(t)$ of the Eq. (20) in a steady regime we have again the estimate (19),

$$|v(t) - v^*_{b(t)}(t)| \leqq (\varphi_0 + |d_0 - d|)\, \varphi^* k_0 (f_0 + d_0 + \varphi_0 + |d_0 - d|)/(\lambda - \varepsilon g^*)^3, \tag{21}$$

with

$$b(t) = -\big(\varphi_0 \varphi(k_0 x(t) + d_0 - d)\big). \tag{22}$$

From Sect. 3, 4 and (21) it follows, if the function $b(t)$ given by the formula (22) is sufficiently different from zero during the time interval nesessary to attain a steady regime of motion, the motion with velocity $v(t)$ satisfying (20) will undergo a drift. Indeed, according to (11), (12), (21) for the velocity $v(t)$ to have a constant component it is sufficient that the following inequality holds: $\big|\varphi_0 \varphi\big(k_0 x(t)\big) - d + d_0\big| > \delta$ where $\delta = (\varphi_0 + |d_0 - d|)\,(f_0 + \varphi_0 + d_0 + |d_0 - d|) \times \varphi^* k_0/(1 - 2\varepsilon g^*/\lambda)/(\lambda - \varepsilon g^*)^2$. We define the shifted equilibrium positions x^* in the following way

$$\varphi_0 \varphi(k_0 x^*) + d_0 - d = 0, \qquad \varphi'(k_0 x^*) > 0. \tag{23}$$

Thus, we can conclude that in a final regime of motion the trajectory $x(t)$ satisfying (20) will be concentrated in the neighbourhood of one of the points x^* defined by the inequality

$$|\varphi_0 \varphi(k_0 x) + d_0 - d| \leqq \delta. \tag{24}$$

6. Modified Potential Function

A physically interesting case is characterized by the inequalities $f_0 < \varphi_0$, $|d - d_0| < \varphi_0$. Writing down the dimensional version (24), we can see that δ has an order Λ^{-2} and the smallness of δ is ensured by (4). At the same time d_0 has zero order in Λ. A situation when $\delta \ll d_0$ is therefore natural. It then follows from (24), if an anharmonic oscillator acted upon by a periodic force of a small period will be effected by a constant force d, the trajectory of final motion will be concentrated in a region away from the equilibrium positions x_0 defined by the relations

$$\varphi_0 \varphi(k_0 x_0) - d = 0, \qquad \varphi'(k_0 x_0) > 0. \tag{25}$$

If the motion is observed to a scale when the size of the region (24) is negligibly small, the evolution in a final regime of motion may be regarded as an equilibrium in the position x^* defined by (23). Comparing (23) and (25) we can conclude that in terms of large-scale observations the oscillator acted upon by a periodic

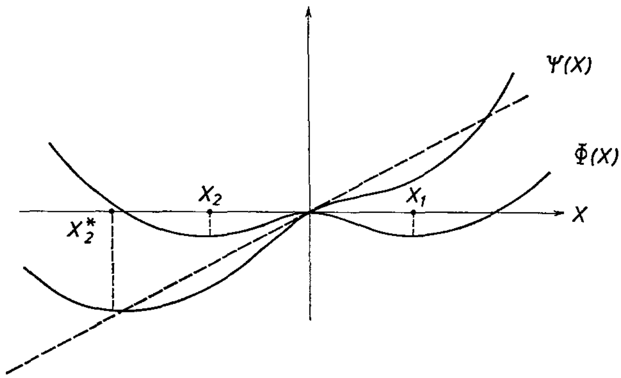

Fig. 1

force behaves so (considering stable equilibrium positions) that the force field $\Phi_0\varphi(X/X_0)$ is replaced by a new force field $\Phi_0\varphi(X/X_0) + D_0$ (where $D_0 = d_0 m V_0/T$). The initial potential function $\Phi(X)$ thus transforms to the modified potential function

$$\Psi(X) = \Phi(X) - D_0 X. \tag{26}$$

Example. Let the original potential function $\Phi(X)$ has the form

$$\Phi(X) = \Phi_0 \left(\left(\frac{X}{X_0} \right)^4 - \alpha \left(\frac{X}{X_0} \right)^2 \right),$$

where $\alpha > 0$, $\Phi_0 > 0$. Two points $X_1 = X_0 \sqrt{\frac{\alpha}{2}}$ and $X_2 = -X_1$ satisfy cond. (25) in this case (see Fig. 1). The modified potential function has the form

$$\Psi(X) = \Phi(X) - D_0 X$$

and there is one or two points X^* which satisfy cond. (23), depending on the absolute value of a stopping force D_0.

7. Discussion

For the effect of a periodic force to be described adequately in terms of the modified potential function it is necessary, according to (4), that the coupling should be soft, and the viscosity large. A physically substantiated possibility to neglect small-scale motions against the background of large-scale ones is also needed. All these requirements are satisfied for internal motions in globular proteins [1], [2], [3].

The value of a modifying effect is determined, according to (26), by the value of a stopping force D_0 which, in the model considered, may be different from zero if the friction law is nonlinear. (The arguments for the nonlinearity of the friction law in globular proteins are given in [7]). Moreover, the absolute value of D_0 can be close to the amplitude of driving force F_0. In general, the value of D_0 is intricately dependent on the form of the signal, $F_0 f(\tau/T)$, by the amplitudes and the phases of its individual harmonics, i.e. by its informational content. Thus, we are dealing with a system which reacts sensitively to the information content of an action. Such behavior is characteristic of nonlinear systems.

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