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Diffusion in a potential with a time-dependent discontinuity

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Abstract
We investigate the one-dimensional diffusion of a particle in a V-shaped potential combined with a time-dependent jump at the tip. Employing the matching conditions, we calculate the exact Green function of the corresponding Smoluchowski equation. We then specialize the analysis to a harmonically oscillating height of the potential discontinuity. We calculate the particle's mean position as a function of time and study its nonlinear features. Our analysis reveals a new type of stochastic resonance. Namely, the time-asymptotic amplitude of the mean-position oscillations exhibits a maximum at an optimal value of the V-potential slope.

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1. Introduction

Diffusion over barriers is an interesting problem of great importance in a variety of fields such as physics, chemistry and engineering [1]. In recent years, the topic has been reactivated in connection with the analysis of periodically driven stochastic systems [2]. A rich variety of new effects has been analysed, the phenomenon of stochastic resonance [3] and the study of Brownian motors [4] being perhaps the most popular examples.

In a paradigmatic setting, consider a particle which diffuses in a potential well and which is driven by an external harmonic force. The mean position of the particle can be viewed as a nonlinear transformation of the input signal. However, having a time-dependent potential, the corresponding dynamical equation cannot be solved in closed form. One has to invoke an appropriate approximation, e.g. the weak-signal assumption, or one has to impose some restrictions on the external-signal frequency. In the present paper, the external driving will be mimicked by a special device which still allows for an exact analysis. Namely, we shall introduce a schematic potential which at a given space point has a step with time-dependent height. Differently speaking, the diffusing particle encounters at that point a semi-permeable boundary with externally controlled time-dependent permeability.

2. Exact Green function

To begin with, assume an overdamped Brownian test particle that moves in a general time-dependent potential. In the Brownian-motion-type notation, the Smoluchowski equation for the Green function $G(x, y; t)$ reads

$$\frac{\partial}{\partial t}G(x, y; t) = -\frac{\partial}{\partial x}\left\{-D\frac{\partial}{\partial x}G(x, y; t) - \frac{1}{\Gamma}\left[\frac{\partial U(x; t)}{\partial x}\right]G(x, y; t)\right\}. \quad (1)$$

Here $U(x; t)$ is the (time dependent) potential, i.e. $F(x; t) = -\frac{\partial}{\partial x}U(x, t)$ is the corresponding force. The curly-bracketed expression represents the probability current $J(x, y; t)$. Γ equals the particle mass times the viscous friction coefficient. The thermal-noise strength parameter D increases linearly with the temperature, $D = k_B T/\Gamma$. The initial conditions are imposed at the time $t_0 = 0$, i.e. $\lim_{t\to 0^+} G(x, y; t) = \delta(x - y)$. We assume natural boundary conditions $\lim_{x\to\pm\infty} G(x, y; t) = 0$.

As a preparatory step, consider the time-*independent* V-shaped potential $U^{(0)}(x) = F_a|x|$, with a non-negative, i.e. 'attracting', force $F_a \geqslant 0$. In this case, one possible method to calculate the relevant Green function, say $G^{(0)}(x, y; t)$, proceeds through Laplace-transforming the Smoluchowski equation and then solving the emerging ordinary differential equation. This step is performed separately in the two constant-force regions. Thereupon, one employs the matching conditions which guarantee the continuity of the probability density and of the probability current [5, 6]. Skipping details, the solution of the preparatory problem reads

$$\begin{aligned} G^{(0)}(x, y; t) = {} & \frac{\Theta(xy)}{2\sqrt{\pi Dt}}\exp\left[-\frac{(|x| - |y| + 2\alpha Dt)^2}{4Dt}\right] \\ & + \frac{\Theta(-xy)}{2\sqrt{\pi Dt}}\exp(-2\alpha|x|)\exp\left[-\frac{(|x| + |y| - 2\alpha Dt)^2}{4Dt}\right] \\ & + \frac{\alpha}{2}\exp(-2\alpha|x|)\,\mathrm{erfc}\left(\frac{|x| + |y| - 2\alpha Dt}{2\sqrt{Dt}}\right). \end{aligned} \quad (2)$$

Here the parameter $\alpha = F_a/(2k_B T) \geqslant 0$ represents the temperature-reduced attractive force, $\mathrm{erfc}(x) = 1 - \mathrm{erf}(x)$ is the complementary error function [7], and $\Theta(x)$ is the Heaviside unit-step function.

We now turn our attention to the central problem of the present work. We shall combine the potential from the preceding 'unperturbed' problem with the time-dependent jump at the origin. Thus the particle diffuses in the time-dependent potential $U(x; t) = F_a|x| + U_j(t)\Theta(x)$, where the function $U_j(t)$ controls the height of the step. Presently, the matching-conditions method meets a principal difficulty. The jump condition for the probability density assumes the form [6] $G(-\epsilon, y; t) = \xi(t)G(\epsilon, y; t)$, where $\xi(t) = \exp[U_j(t)/(k_B T)]$, and ϵ is a positive infinitesimal quantity. The condition cannot be easily Laplace-transformed and the whole calculation must be performed with the time variable. We now leave off a considerable amount of computational subtleties and focus on the final result. The exact Green function for the present problem reads

$$G(x, y; t) = G^{(0)}(x, y; t) - \int_0^t \mathrm{d}t'\, V(x; t - t')R(t')W(y; t') \quad (3)$$

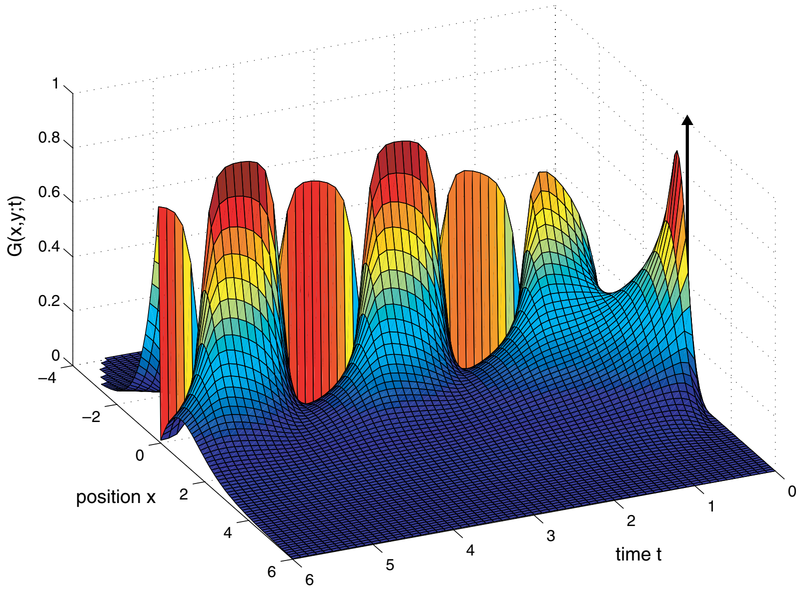

Figure 1. Time- and space-dependence of the exact Green function. Parameters used are $\alpha = 1.0$, $\kappa = 5.0$, $\omega = \pi$, and $D = 1$, in appropriate units. The initial condition $y = 2$ is indicated by the arrow.

where $G^{(0)}(x, y; t)$ is the unperturbed Green function (2) and we have introduced the following three auxiliary functions:

$$V(x; t) = \frac{x}{4Dt\sqrt{\pi Dt}} \exp\left[-\frac{(|x| + 2\alpha Dt)^2}{4Dt}\right] \tag{4}$$

$$R(t) = 2\frac{1 - \exp[U_j(t)/(k_B T)]}{1 + \exp[U_j(t)/(k_B T)]} \tag{5}$$

$$W(y; t) = \frac{\alpha}{2} \operatorname{erfc}\left(\frac{|y| - 2\alpha Dt}{2\sqrt{Dt}}\right) + \frac{1}{\sqrt{\pi Dt}} \exp\left[-\frac{(|y| - 2\alpha Dt)^2}{4Dt}\right]. \tag{6}$$

Equations (3)–(6) close up the general part of the paper. Of course, by assuming the V-shaped unperturbed potential, the concept of the time-dependent discontinuity has already been incorporated into a specific context. As a matter of fact, our method works with arbitrary shapes of (solvable) potentials at the two sides of the discontinuity.

From this point on we will be even more specific and presume harmonic oscillations of the step height. More precisely, we put $U_j(t) = U_a \cos(\omega t)$, where $U_a \geqslant 0$ is the amplitude of the input signal and ω its frequency. Substituting into equation (5), there emerges an important parameter, $\kappa = U_a/(k_B T)$. It measures the temperature-reduced amplitude of the step and can be regarded as a perturbation parameter. If $\kappa \gg 1$, one anticipates a highly nonlinear response. Figure 1 is a plot of the resulting Green function as calculated from the expressions (3)–(6), where presently $R(t) = -2\tanh\left[\frac{\kappa}{2}\cos(\omega t)\right]$.

In the adiabatic limit $\omega \to 0$, the formulae (3)–(6) describe the diffusion in the V-shaped potential superimposed with the time-independent jump at the tip. In this case, one arrives at the well-known picture: the time-asymptotic probability density for the particle's position represents the Boltzmann equilibrium state, $\pi_{\mathrm{eq}}(x) \approx \exp\{-[F_a|x| + U_a\Theta(x)]/(k_B T)\}$, and the equilibrium mean-position is shifted to the left from the origin, $\mu_{\mathrm{eq}} = -\tanh(\kappa/2)/(2\alpha)$.

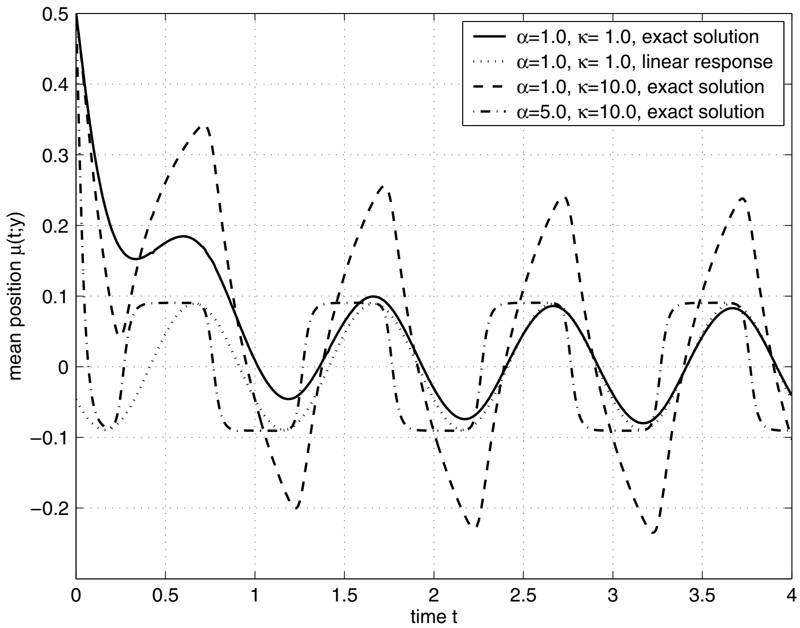

Figure 2. Time-dependence of the particle's mean position for several combinations of the parameters α and κ. The calculation is based on equations (7) and (8) (the exact results) and (9) (the linear-response regime). Other parameters used are $\omega = 2\pi$ and $D = 1.0$, in appropriate units. The initial condition was $y = 0.5$.

However, having a nonzero driving frequency, i.e. a true time-dependent discontinuity, the dynamics cannot establish a time-independent equilibrium. Instead, the time-asymptotic solution describes a stationary regime in which the probability density flows to the left (to the right) during each half period when $U_j(t) > 0 (U_j(t) < 0)$.

3. Mean position

We now proceed to discuss the particle's mean position $\mu(y;t) = \int_{-\infty}^{\infty} \mathrm{d}x\, x G(x, y; t)$. Using equation (3), we can split the expression as $\mu(y;t) = \mu^{(0)}(y;t) + \mu^{(1)}(y;t)$, where the first summand refers to the unperturbed case, and the second one shows up a time-convolution structure. After carrying out the space integrations, the final expressions read

$$\mu^{(0)}(y;t) = y - \frac{y}{|y|} 2\alpha D t + \alpha y \sqrt{D} \int_0^t \mathrm{d}t' \frac{t - t'}{t'\sqrt{\pi t'}} \exp\left[-\frac{(|y| - 2\alpha D t')^2}{4Dt'}\right] \tag{7}$$

$$\mu^{(1)}(y;t) = D \int_0^t \mathrm{d}t' \left[(1 + 2\alpha^2 D t')\,\mathrm{erfc}(\alpha\sqrt{Dt'}) - 2\alpha\sqrt{\frac{Dt'}{\pi}}\,\mathrm{e}^{-\alpha^2 D t'}\right] R(t - t') W(y; t - t') \tag{8}$$

where the functions $R(t)$ and $W(y;t)$ have been introduced in equations (5) and (6). These results are illustrated in figure 2.

In order to analyse the spectral composition of the output signal, we have performed the standard asymptotic analysis [8] based on the Laplace-transformed mean coordinate $\mu(y;z)$. In the time-asymptotic region, the unperturbed part (7) vanishes and the function (8) loses its dependence on the initial condition. The time-asymptotic output signal $\mu_s(t)$ contains the

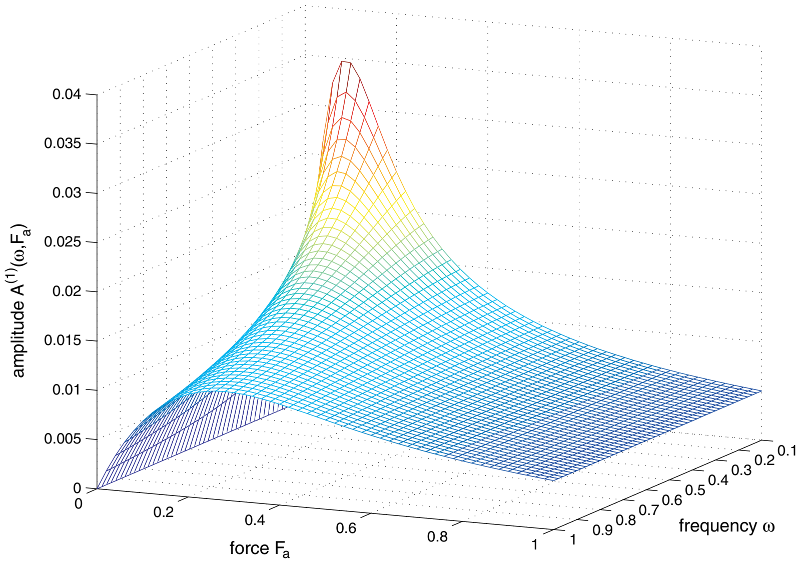

Figure 3. The linear-response amplitude as a function of the driving frequency and the potential slope. In the adiabatic limit $\omega \to 0$, the amplitude is simply $A^{(1)}(0, F_a) = U_a/(2F_a)$. In the calculation, we took $U_a = 0.01$, and $D = 0.05$, in appropriate units.

fundamental frequency and its odd harmonics. More precisely, introducing $\omega_k = (2k-1)\omega$, we have obtained

$$\mu_s(t) = \frac{1}{\alpha}\sum_{k=1}^{\infty} r_k(\kappa)\frac{\left(\rho_k^-\right)^2 + \left(\rho_k^+\right)^2}{2\Omega_k^2}\cos\left[\omega_k t - \operatorname{arctg}\frac{2\rho_k^-\rho_k^+}{\left(\rho_k^-\right)^2 - \left(\rho_k^+\right)^2}\right] \tag{9}$$

where $\Omega_k = \omega_k/(D\alpha^2)$ is the dimensionless frequency, $\rho_k^- = \left[\left(\Omega_k^2+1\right)^{1/2} - 1\right]^{1/2}$ and $\rho_k^+ = \left[\left(\Omega_k^2+1\right)^{1/2} + 1\right]^{1/2} - \sqrt{2}$. The amplitude of the kth harmonics depends on the input-signal amplitude through the function $r_k(\kappa)$. The κ-expansion of the function $r_k(\kappa)$ begins with the power κ^{2k-1}. For example, one can show $r_1(\kappa) = -\kappa + \kappa^3/16 - \kappa^5/192 + \cdots$, $r_2(\kappa) = \kappa^3/48 - \kappa^5/384 + \cdots$, etc.

Let us now focus on the linear-response regime. We keep just the first term of the series (9) and we approximate $r_1(\kappa) \approx -\kappa$ therein. Consequently, the response is harmonic at the fundamental frequency ω—cf the dotted line in figure 2. A scrutiny of the linear-response amplitude, say $A^{(1)}(\omega, F_a)$, reveals an interesting feature which is illustrated in figure 3. The amplitude exhibits a *maximum* for a specific value of the attracting force F_a. Note there is no resonance in the standard sense, the amplitude being a monotonously decreasing function of the driving frequency. Similarly, there is no maximum of the amplitude as a function of the thermal-noise intensity D.

The physical essence behind the resonance is the following. Assume first a sharp slope of the unperturbed potential. Due to the large attractive force, the particle cannot migrate far from the origin and the amplitude of its mean-position oscillations is small. Secondly, assume a flat minimum of the unperturbed potential. Then the particle performs relatively large excursions from the origin. However, the excursions occur *symmetrically* to the both sides from the origin and hence they do not contribute to the mean position. Only a small portion of the probability density in the vicinity of the origin is non-symmetrically affected by the oscillating barrier. On the whole, the amplitude of the particle's mean position is again small. In conclusion, there must exist an 'optimal' slope $F_{a,\mathrm{res}}$ for which the amplitude assumes its maximal value.

4. Discussion

To sum up, in the present paper, the price paid for the exact solution has been a somewhat simplified implementation of the external driving. Having assumed the sudden jump of the potential at the origin, the force in equation (1) exhibits a δ-function singularity. One encounters the well-known problem with an interpretation of the product $\delta(x)G(x, y; t)$. Our way of treating the potential step is effectively equivalent to accepting the Stratonovich interpretation [1] of the above product. Differently speaking, the step is considered as a limiting case of a *continuous* potential which undergoes an abrupt change in the domain $(-\Delta, \Delta)$. The limit $\Delta \to 0$ is implicitly assumed as being the last limit in the calculations.

The principal motivation for the present work has been connected with the hysteresis phenomenon [9, 10]. Hysteresis is the nonlinear and time-delayed response of a system to the harmonic variation of a control parameter, a familiar example being changes in electric displacement in response to a electric field in graded ferroelectrics [11]. Using the Landau representation of the free energy, the phenomenon can be modelled as the overdamped dynamics of a particle in a bistable asymmetric potential. It is important that the driving force cannot be assumed to be small. In our setting, the external probe is the step-hight function $U_s(t)$ and the response corresponds to the particle mean position $\mu(y; t)$. Except of the double-well shaped unperturbed potential, our approach includes all the pertinent aspects of the above problem. An analogous analysis of the diffusion dynamics in an asymmetric W-shaped potential superimposed with the time-dependent discontinuity at the central-tip coordinate is in progress and it will be reported elsewhere. In this case, we expect that the calculation would predict the experimentally observed driving-induced shift of the hysteresis loop [11] as well as an authentic stochastic resonance [3], i.e. a maximum of the mean-position amplitude as a function of the noise intensity.

Acknowledgments

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