Fokker-Planck equation for bistable potential in the optimized expansion

Anna Okopińska

Institute of Physics, Pedagogical University, Konopnickiej 15, 25-406 Kielce, Poland
and Institute für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

The optimized expansion is used to formulate a systematic approximation scheme to the probability distribution of a stochastic system. The first-order approximation for the one-dimensional system driven by noise in an anharmonic potential is shown to agree well with the exact solution of the Fokker-Planck equation. Even for a bistable system the whole period of evolution to equilibrium is correctly described at various noise intensities.

Introduction. The Fokker-Planck (FP) equation is widely used to describe nonequilibrium systems in physics, chemistry, and biology [1]. The stochastic approach consists in representing the most relevant degrees of freedom of the system by the variable x driven by noise and deterministic interaction potential $U(x,t)$. The time development of the probability distribution $W(x,t)$ is given by a partial differential equation

$$(\partial/\partial t)\, W(x,t) = L_{FP}W(x,t):$$
$$= \partial/\partial x\,[U'(x,t)W(x,t) + D\,\partial^2/\partial x^2\, W(x,t)] \tag{1}$$

with the diffusion coefficient D representing a noise intensity, and the drift coefficient $U'(x,t)$ being a derivative of the interaction potential with respect to x. The Green's function of the FP equation $P(x,t|x',t')$ that fulfills the initial condition $P(x,t|x',t') = \delta(x,x')$, is called the transition probability (conditional probability), since it describes the probability density evolution, $W(x,t) = \int P(x,t|x',t')W(x',t')dx'$, from time t' to t. For a time-independent potential $U(x)$ the separation ansatz

$$W(x,t) = \Phi(x)e^{-\kappa t} \tag{2}$$

reduces the time-dependent FP equation (1) to the stationary eigenfunction equation,

$$L_{FP}\Phi(x) = \frac{\partial U'(x)\Phi(x)}{\partial x} + D\frac{\partial^2 \Phi(x)}{\partial x^2} = -\kappa\Phi(x). \tag{3}$$

The lowest eigenvalue of L_{FP} is identically zero, $\kappa = 0$, and the corresponding eigenfunction can be found exactly, yielding the stationary probability distribution $W_{st}(x) = \Phi_0(x) = Ne^{-U(x)/D}$, where the normalization constant $N = (\int_{-\infty}^{\infty} e^{-U(x)/D}dx)^{-1}$. For an arbitrary $U(x)$ the higher eigenfunctions and the nonstationary probability distribution cannot be found exactly. For developing approximation methods it is convenient to transform the FP operator to the Hermitian form by the transformation $\Psi(x) = e^{U(x)/2D}\Phi(x)$. This brings the FP equation to the pseudo-Schrödinger equation,

$$[D\, d^2/dx^2 - V(x)]\Psi(x) = \lambda\Psi(x) \tag{4}$$

for the particle of the mass $M = \hbar/2D$ in the potential,

$$V(x) = [U'(x)]^2/4D - U''(x)/2. \tag{5}$$

By Eq. (2) the wave function Ψ evolves in imaginary time $-i\hbar t$; the transition probability, $P(x,t|x',t')$, being the Green's function of the original FP equation (1), is thus related to the imaginary time evolution amplitude of the pseudo-Schrödinger equation (4). The evolution amplitude can be represented by a path integral

$$K(x,t|x',t') = \int_{x(t')=x'}^{x(t)=x} Dx \exp\left(-\int_{t'}^{t} L[x]dt\right) \tag{6}$$

over all functions that begin at $x(t')=x'$ and end at $x(t)=x$, where the Lagrangian $L[x] = M\dot{x}^2/2 + V(x)$. Both $U(x)$ and $V(x)$ being time independent, the evolution depends only on time difference, $T = t - t'$, and we have

$$P(x,x',T) = e^{[U(x')-U(x)]/2D}K(x,x',T), \tag{7}$$

where $K(x,x',T) = K(x,t;x',t')$ and $P(x,x',T) = P(x,t|x',t')$. We study a stochastic system in an anharmonic potential

$$U(x) = \gamma x^2/2 + \lambda x^4, \tag{8}$$

when the pseudo-Schrödinger potential (5) takes the form

$$V(x) = g_0 + g_2 x^2 + g_4 x^4 + g_6 x^6, \tag{9}$$

with $g_0 = -\gamma/2$; $g_2 = (\gamma^2/4D - 6\lambda)$; $g_4 = 2\lambda\gamma/D$; and $g_6 = 4\lambda^2/D$.

For vanishing λ the problem reduces to the Ornstein-Uhlenbeck process in the potential $U(x) = \gamma x^2/2$. The pseudo-Schrödinger potential is also quadratic, $V(x) = -\gamma/2 + (\gamma^2/4D)x^2$, and the path integral (6) yields

$$K_\gamma(x,x',T) = \sqrt{\frac{\gamma}{2\pi D(1-e^{-2\gamma T})}}\exp\left\{\frac{\gamma}{4D\,\sinh\gamma T}\right.$$
$$\left.\times[(x^2+x'^2)\cosh\gamma T - 2xx']\right\}. \tag{10}$$

By Eq. (7) this leads to an exact expression for the transition probability of the Ornstein-Uhlenbeck process

$$P_\gamma(x,x',T) = \sqrt{\frac{\gamma}{2\pi D(1-e^{-2\gamma T})}} \exp\left(-\frac{\gamma(x-x'e^{-\gamma T})^2}{2D(1-e^{-2\gamma T})}\right).$$

(11)

In the presence of anharmonicity ($\lambda \neq 0$) the path integral cannot be performed exactly, but various approximation methods are developed. Perturbative calculations of $P(x,x',T)$ in powers of λ are possible only if $\gamma>0$. In this case the first-order approximation describes well the evolution of the system approaching the stationary distribution in the long time limit. For double-well potential ($\gamma<0$) the transition probability is non-normalizable and perturbative approximations give a wrong description of the time evolution, since the maxima of the transition probability escape to $x = \pm\infty$.

A few years ago we formulated the optimized expansion (OE) scheme for the Schrödinger evolution amplitude [2], which is more powerful than the perturbative approach. The aim of this paper is an extension of the OE to stochastic processes. The efficiency of the method will be shown on the example of a bistable system driven by noise in the double-well potential. Such a system attracts much attention in non-linear optics, solid-state physics and chemistry. The solution of the FP equation, which describes the evolution from an unstable to the stationary state is of special interest; however, in all studies the evolution process is divided into few steps and different approximations are used in each time sector [3]. Our approximation has the advantage of being uniform in the whole period of stochastic evolution.

The optimized expansion. OE has been formulated to generate nonperturbative approximations for the effective action in quantum field theory [4]. The method consists in calculating the effective action as a series in ϵ, by splitting the Lagrangian into $L = L_0 + \epsilon(L - L_0)$, where the unperturbed part contains arbitrary parameters, to be optimized in every order calculation. The method is equivalent to a systematic resummation of the perturbation series and gives the Hartree-Fock-Bogoliubov approximation in the leading order. A similar idea has been applied to calculate other physical quantities in a number of works [5,6] under different names (self-similar perturbation theory, δ expansion, variational perturbation theory, optimized perturbation theory, etc.). In the application to the quantum mechanical particle the classical Lagrangian in Eq. (6) is modified to the form

$$L_\omega[x] + \epsilon V_{int}[x] = \frac{M\dot{x}^2}{2} + \frac{M\omega^2 x^2}{2} + \epsilon\left(V(x) - \frac{M\omega^2 x^2}{2}\right),$$

(12)

where the harmonic oscillator of the mass M and an arbitrary frequency ω is chosen as the unperturbed system. The imaginary time evolution amplitude

$$K(x,x',T) = e^{W(x,x',T)}$$

(13)

can be calculated [2,7] with the cumulant expansion

$$W(x,x',T) = W_\omega(x,x',T) - \epsilon\langle V_{int}(x)\rangle_\omega$$
$$+ (\epsilon^2/2)(\langle V_{int}^2(x)\rangle_\omega$$
$$- \langle V_{int}(x)\rangle_\omega\langle V_{int}(x)\rangle_\omega) - \cdots,$$

(14)

where by Eq. (10)

$$W_\omega(x,x',T)$$
$$= \ln K_\omega(x,x',T)$$
$$= \tfrac{1}{2}\ln[\omega/(4\pi D \sinh \omega T)]$$
$$- \{\omega[(x^2+x'^2)\cosh \omega T - 2xx']\}/(4D \sinh \omega T)$$

(15)

for the particle of the mass $\hbar/2D$ and the expectation values are calculated for the unperturbed Lagrangian

$$\langle\cdots\rangle_\omega = \int_{x(t')=x'}^{x(t)=x} Dx \cdots \exp\left(-\int_{t'}^t L_\omega[x]dt\right).$$

(16)

The Nth-order approximation $W^{(N)}(x,x',T)$ is obtained after setting $\epsilon = 1$, since only in this case does the modified Lagrangian agree with the classical one. The exact result, being a sum of an infinite series, would not depend on an arbitrary frequency, ω, but a finite order truncation shows such a dependence. We fix, therefore, the value of ω by requiring

$$\delta W^{(N)}/\delta\omega = 0,$$

(17)

to make the given order approximant as insensitive as possible to small variation of ω. The optimization condition (17) determines ω as a function of x, x', and T, which changes from order to order, improving the convergence properties of the approximation scheme.

In the case of polynomial potential the expectation values (16) are given by Gaussian functional integrals, yielding an analytic expression for $W^{(N)}$. The first-order result for a quartic oscillator, obtained in Ref. [2], provides a satisfactory approximation to the evolution amplitude and particle density. For a sextic potential (9) the first-order result reads

$$W^{(1)}(x,x',T) = -g_0 T + W_\omega(x,x',T) + (\omega^2/4D - g_2)\langle x^2\rangle_\omega$$
$$- g_4\langle x^4\rangle_\omega - g_6\langle x^6\rangle_\omega,$$

(18)

where $\langle x^2\rangle_\omega = \int_{t'}^t [L^2(\tau) + K(\tau)]d\tau$, $\langle x^4\rangle_\omega = \int_{t'}^t [L^4(\tau) + 6L^2(\tau)K(\tau) + 3K^2(\tau)]d\tau$, $\langle x^6\rangle_\omega = \int_{t'}^t [L^6(\tau) + 15K(\tau)L^4(\tau) + 45K^2(\tau)L(\tau)^2 + 15K^3(\tau)]d\tau$ with $L(\tau) = [x\sinh\omega(\tau-t') + x_b\sinh\omega(t-\tau)]/[\sinh\omega(t-t')]$ and $K(\tau) = [2D\sinh\omega(\tau-t')\sinh\omega(t-\tau)]/[\omega\sinh\omega(t-t')]$. Upon performing the integrals we obtain

$$\langle x^2\rangle_\omega = \frac{1}{4\omega^2\sinh^2 T\omega}[2D - 2T\omega^2 x^2 - 2T\omega^2 x'^2$$
$$+ 4T\omega^2 xx'\cosh T\omega - 2D\cosh 2T\omega$$
$$- 4\omega xx'\sinh T\omega + \omega(2DT + x^2 + x'^2)\sinh 2T\omega],$$

$$\langle x^4 \rangle_\omega = \frac{1}{32\omega^3 \sinh^4 T\omega} [36D^2 T\omega + 54D\omega x^2 - 12T\omega^3 x^4 + 54D\omega x'^2 - 48T\omega^3 x^2 x'^2 - 12T\omega^3 x'^4$$

$$+ 24\omega x x'(2T\omega^2 x^2 + 2T\omega^2 x'^2 - 3D)\cosh T\omega - 24\omega(2Dx^2 + 2Dx'^2 + D^2 T + \omega^2 x^2 x'^2 T)\cosh 2T\omega$$

$$+ 72D\omega x x' \cosh 3T\omega - 6D\omega(2DT + x^2 + x'^2)\cosh 4T\omega - 36\omega^2 x x'(4DT + x^2 + x'^2)\sinh T\omega$$

$$+ 4(18DT\omega^2 x^2 + 2\omega^2 x^4 + 18DT\omega^2 x'^2 + 9\omega^2 x^2 x'^2 + 2\omega^2 x'^4 - 9D^2)\sinh 2T\omega - 4\omega^2 x x'(12DT + x^2$$

$$+ x'^2)\sinh 3T\omega + (18D^2 - \omega^2 x^4 - \omega^2 x'^4)\sinh 4T\omega],$$

$$\langle x^6 \rangle_\omega = \frac{1}{384\omega^4 \sinh^6 T\omega}[60(35D^3 - 72D^2 T\omega^2 x^2 - 20D\omega^2 x^4 + 2T\omega^4 x^6 - 72D^2 T\omega^2 x'^2 - 81D\omega^2 x^2 x'^2 + 18T\omega^4 x^4 x'^2$$

$$- 20D\omega^2 x'^4 + 18T\omega^4 x^2 x'^4 + 2T\omega^4 x'^6) + 240\omega^2 x x'(36D^2 T + 14Dx^2 - 3T\omega^2 x^4 + 14Dx'^2 - 9T\omega^2 x^2 x'^2$$

$$- 3T\omega^2 x'^4)\cosh T\omega - 15(150D^3 - 144D^2 T\omega^2 x^2 - 65D\omega^2 x^4 - 144D^2 T\omega^2 x'^2 - 192D\omega^2 x^2 x'^2 - 48T\omega^4 x^4 x'^2$$

$$- 65D\omega^2 x'^4 - 48T\omega^4 x^2 x'^4)\cosh 2T\omega - 120\omega^2 x x'(63D^2 T + 27Dx^2 + 27Dx'^2 + 2T\omega^2 x^2 x'^2)\cosh 3T\omega$$

$$- 120\omega^2 x x'(63D^2 T + 27Dx^2 + 27Dx'^2 + 2T\omega^2 x^2 x'^2)\cosh 4T\omega - 120D\omega^2 x x'(9DT + x^2 + x'^2)\cosh 5T\omega$$

$$+ 15D(22D^2 - \omega^2 x^4 - \omega^2 x'^4)\cosh 6T\omega - 120\omega x x'(105D^2 - 48DT\omega^2 x^2 - 4\omega^2 x^4 - 48DT\omega^2 x'^2 - 9\omega^2 x^2 x'^2$$

$$- 4\omega^2 x'^4)\sinh T\omega - 15(150D^3 - 144D^2 T\omega^2 x^2 - 65D\omega^2 x^4 - 144D^2 T\omega^2 x'^2 - 192D\omega^2 x^2 x'^2 - 48T\omega^4 x^4 x'^2$$

$$- 65D\omega^2 x'^4 - 48T\omega^4 x^2 x'^4)\sinh 2T\omega - 120\omega^2 x x'(63D^2 T + 27Dx^2 + 27Dx'^2 + 2T\omega^2 x^2 x'^2)\sinh 3T\omega$$

$$- 120\omega^2 x x'(63D^2 T + 27Dx^2 + 27Dx'^2 + 2T\omega^2 x^2 x'^2)\sinh 4T\omega - 120D\omega^2 x x'(9DT + x^2 + x'^2)\sinh 5T\omega + 15D(22D^2$$

$$- \omega^2 x^4 - \omega^2 x'^4)\sinh 6T\omega].$$

The imaginary time evolution amplitude for the quantum mechanical particle in the sextic potential (9) is obtained by taking

$$K^{(1)}(x,x',T) = e^{W^{(1)}(x,x',T)}. \qquad (19)$$

This approximate solution of the Schrödinger equation defines, by Eq. (7), an approximation to the transition probability of the stochastic process in a quartic potential (8) to be given by

$$P^{(1)}(x,x',T) = e^{[U(x') - U(x)]/2D} e^{W^{(1)}(x,x',T)}. \qquad (20)$$

The value of ω for considered values of x, x', and T is obtained by solving the optimization condition $[\delta W^{(1)}(x,x',T)]/\delta\omega = 0$.

   Results and conclusions. The first-order OE (20) provides a good approximation to the transition probability, when the interaction potential is convex ($\gamma > 0$); however, for larger anharmonicity the total probability decreases in time. A similar problem appears in the variational perturbation calculation [8], where the total probability increases in time. The spoiling of the normalization by optimization is a general feature of perturbative schemes with variational parameters and can be cured by normalizing each order result by hand. Upon normalization a good agreement with the exact solu-

tion of the FP equation is obtained in the whole period of evolution. Here we show the results in the most demanding case of double-well interaction potential ($\gamma < 0$), when the pseudo-Schrödinger potential has a multiple-well structure. The critical value of the diffusion coefficient ($D_{cr} = \gamma^2/24\lambda$), distinguishes two cases: the pseudo-Schrödinger potential of double-well shape (large noise, $D > D_{cr}$), and of triple-well shape (small noise).

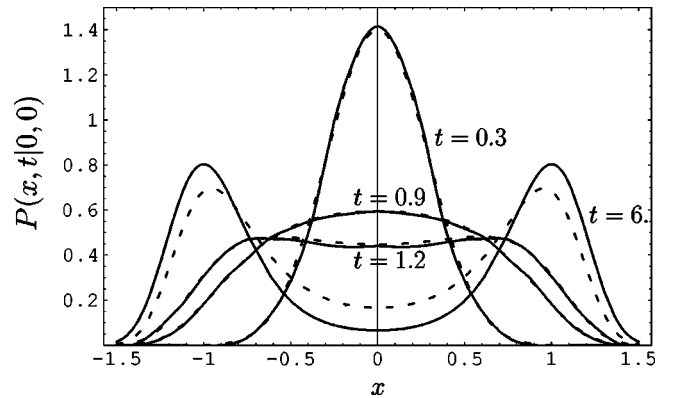   We compare our approximation to the transition probabil-

FIG. 1. The transition probability $P(x,t|0,0)$ for bistable potential $U(x) = -x^2/2 + x^4$ at $D = 0.1$ in the first order of the OE (*dashed line*) at the time $t = 0.3$, $t = 0.9$, $t = 1.2$, and $t = 6$, compared with the exact results [9] (*solid line*).

FIG. 2. Same as in Fig. 1, but for $D=0.05$ at $t=0.9$, $t=1.5$, and $t=6$, compared with the exact results [3] (*solid line*).
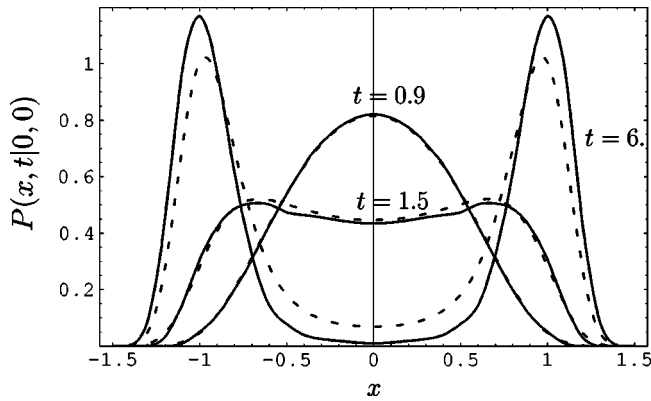

FIG. 3. Same as in Fig. 1, but for $D=0.01$ at $t=1.2$, $t=2.2$ and $t=6$, compared with the exact results [3] (*solid line*).

ity, $P(x,t|0,0)$, with the exact results calculated numerically [3,9] for the interaction potential $U(x)=-\frac{1}{2}x^2+\frac{1}{4}x^4$ in the most demanding case of small noise, $(D<D_{cr}=\frac{1}{6})$. The evolution of the transition probability at noise intensity $D=0.1$ is shown in Fig. 1, and the results at $D=0.05$ and $D=0.01$, in Figs. 2 and 3, respectively. The transition probability for the system being initially in the unstable state $[P(x,0|0,0)=\delta(x-0)]$ is presented at different times: the first value is in the initial region, next ones are in the intermediary region, and the time when the stationary distribution is already achieved. It is remarkable that a good description of the evolution from the unstable configuration to the stable one is obtained already in the first order of the OE, even in the difficult case of small noise. This is due to optimization of the variational parameter ω. The description is uniform, since the optimization condition (21) has a solution for all the values of x during the whole period of evolution. For $D=0.05$ and $D=0.01$ our approximation is of similar quality as the two- or three-stage approximations based on Ω expansion [3], and also a good description is obtained for $D=0.1$, when the approximation discussed by Hu becomes inaccurate as observed in Ref. [9].

After completing this work we learned that approximate solutions of the FP equation in an anharmonic potential have been also studied by directly improving the perturbative expansion of the transition probability, using a drift coefficient as a variational parameter [8]. The variational expressions substantially differ from 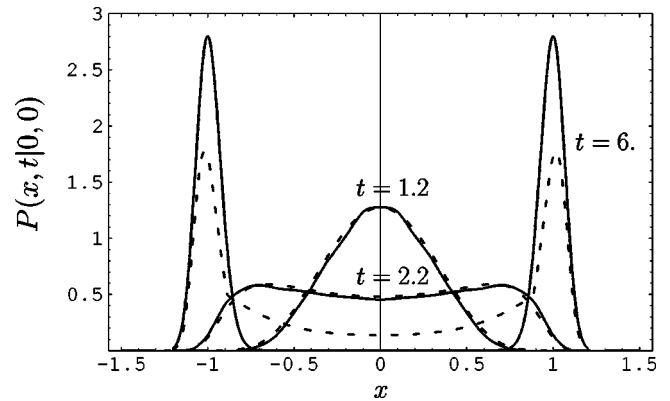ours, because the sextic term of the pseudo-Schrödinger potential (9) does not contribute to the first order of their method. In the case of single-well potential the variational parameter is uniquely determined by extremum condition, in analogy to our optimization condition, and numerical results for the transition probability are similar to ours. In the case of bistable system the extremum condition has a solution only in the early stage of evolution, and different criteria of the variational parameter fixing have to be invoked for larger times. In this manner a very good description of the final stage of evolution is obtained, but the intermediate stage is described badly. This is in difference with our approximation that is continuous in time, even for bistable system. With a unique criterium of optimization in the whole period of evolution our method provides a very good approximation of the initial and intermediate stage, discrepancies appear only in the final stage of evolution.

One has to note that the accuracy of our approximation can be improved by higher-order calculation in a systematic way. An extension of our approach to higher-dimensional systems is possible. Also the dynamics of stochastic systems driven by time-dependent forces can be studied in the OE. The influence of a periodic force on the bistable system, which is a topic of current interest because of the phenomenon of stochastic resonance, will be discussed in a future publication.

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