Method for numerical simulation of two-term exponentially correlated colored noise

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A method for numerical simulation of two-term exponentially correlated colored noise is proposed. The method is an extension of traditional method for one-term exponentially correlated colored noise. The validity of the algorithm is tested by comparing numerical simulations with analytical results in two physical applications.

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I. INTRODUCTION

In many fields of physics, for instance transport processes in condensed matter physics, activation processes in chemical reactions, thermal fission and fusion reactions in nuclear physics, and stochastic resonance phenomenon and biophysics, generalized Langevin approach of relevant variables provides a very useful framework for theoretical description of the reactions under consideration [1–10]. In such a description, evolutions of the relevant variables are determined, in general, by non-Markovian stochastic differential equations, which involve memory dependent dissipation and correlated random forces. For example, in a linear coupling with the intrinsic degrees of freedom, the temporal evolution of a single relevant variable is determined by a generalized Langevin equation given by Eqs. (46) and (47) below in Sec. IV. In this equation $\epsilon(t)$ denotes a Gaussian c-number quantum noise with a correlation function given by [1,2,11]

$$\langle \epsilon(t)\epsilon(t')\rangle = \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi} e^{-i\omega(t-t')} \frac{\hbar\omega}{2T} \coth\left(\frac{\hbar\omega}{2T}\right) 2D(\omega), \quad (1)$$

where $D(\omega)$ represents the spectral density of the intrinsic degrees of freedom. Except in the linear regime analytical solutions of stochastic differential equations are not possible, therefore, probability distribution of the relevant variables are obtained by numerically generating a sufficient number of solutions of the equation of motion. At sufficiently high temperature, memory effects can be ignored and random force is usually treated within the Markovian approximation as a Gaussian white (δ correlated) noise. In this case, the algorithm for numerical simulations of the Langevin equation is well known [12].

On the other hand, at low temperatures, often we are faced with a correlated noise with long correlation time induced by the quantum statistical fluctuations. Therefore, it is of great interest to develop algorithm to simulate non-Markovian stochastic processes with correlated noise. In Refs. [13,14] an algorithm was presented for numerical simulation of exponentially correlated colored noise. This procedure was later extended for a correlated noise of linear superposition of several exponential terms with all positive coefficients [15], see also [16]. However, as in the linear coupling model presented in Eq. (1), due to quantum statistical effects, the correlation function of the noise may develop a pronounced negative portion and hence it cannot be represented as a superposition of positive exponential terms alone [11,17]. This can be seen by employing a Lorentzian profile for the spectral distribution of intrinsic degrees of freedom $D(\omega)$. The ω integration in Eq. (1) can be carried out by the residue method. As a result, the correlation function can be expressed as a superposition of exponential terms with positive and negative coefficients. An extension of the implementation procedure to superposition of exponential terms with positive and negative coefficients may provide a powerful tool for numerical simulations of quantum noise of the form given by Eq. (1). In the present work, we restrict our treatment to a two-term exponential form and propose an algorithm for simulation of the correlated noise which is given as a superposition of two exponential terms with positive and negative coefficients. The proposed algorithm allows numerical simulations for a wide class of stochastic processes with correlated noise that exhibits a negative portion.

In Secs. II and III, we explain the formalism and the simulation algorithm for two-term exponential correlated noise with positive and negative coefficients. In Sec. IV, we present applications of the proposed algorithm to free diffusion in momentum space and diffusion over one dimensional parabolic barrier. The conclusions are given in Sec. V.

II. FORMALISM OF TWO-TERM EXPONENTIALLY CORRELATED COLORED NOISE

For simplicity, we consider a stochastic equation with a single variable

$$\dot{x} = f(x) + \epsilon(t), \quad (2)$$

where $f(x)$ is a driving force and ϵ denotes a correlated Gaussian random noise with zero mean value, $\langle\epsilon(t)\rangle=0$, and correlation given by a linear combinations of two exponentials

$$\langle \epsilon(t)\epsilon(t')\rangle = D_1\lambda_1 e^{-\lambda_1|t-t'|} + D_2\lambda_2 e^{-\lambda_2|t-t'|}. \tag{3}$$

Here, $\langle\cdots\rangle$ denotes the average taken over the ensemble generated by the equation. D_1 and D_2 are the noise strengths of the two terms in the right hand side of Eq. (3), respectively. λ_1 and λ_2 are the inverse of the correlation times of respective terms. In this case, as an extension of the method in [13], it is possible to develop an algorithm for numerical simulation of the exponentially correlated colored noise by introducing two auxiliary stochastic variables as $\epsilon(t)=\epsilon_1(t)+\epsilon_2(t)$, and Eq. (2) is replaced by a set of three equations [15]

$$\dot{x} = f(x) + \epsilon(t), \tag{4}$$

$$\dot{\epsilon}_1 = -\lambda_1\epsilon_1 + \lambda_1 g_1, \tag{5}$$

$$\dot{\epsilon}_2 = -\lambda_2\epsilon_2 + \lambda_2 g_2. \tag{6}$$

In these equations, let the stochastic sources g_1 and g_2 represent Gaussian random white noises with zero mean and second moments determined by

$$\langle g_1(t)g_1(t')\rangle = 2D_1'\delta(t-t'), \tag{7a}$$

$$\langle g_2(t)g_2(t')\rangle = 2D_2'\delta(t-t'), \tag{7b}$$

$$\langle g_1(t)g_2(t')\rangle = 2D_{12}'\delta(t-t'), \tag{7c}$$

where D_1', D_2', and D_{12}' are parameters to be determined by the correlation function Eq. (3). When both coefficients D_1 and D_2 are positive, ϵ_1 and ϵ_2 behave as independent random numbers and therefore the mixed diffusion coefficient can be taken to be zero, $D_{12}'=0$. On the other hand, when one of the coefficients, D_1 or D_2, is negative, the mixed diffusion coefficient D_{12}' must take a finite negative value. As discussed in Sec. III, the range of diffusion coefficients is determined in terms of the input parameters D_1, D_2, λ_1, and λ_2.

As shown in the Appendix, solutions of Eqs. (5) and (6) lead to the two-term exponentially correlated colored noise

$$\{\langle \epsilon(t)\rangle\} = 0, \tag{8a}$$

$$\{\langle \epsilon(t)\epsilon(t')\rangle\} = (\widetilde{D}_1+\widetilde{D}_{12})e^{-\lambda_1|t-t'|} + (\widetilde{D}_2+\widetilde{D}_{12})e^{-\lambda_2|t-t'|}, \tag{8b}$$

where in addition to the ensemble averaging $\langle\cdots\rangle$, an average $\{\cdots\}$ over the initial ϵ values must be carried out with a Gaussian distribution

$$P[\epsilon(0)] = \frac{1}{2\pi\sqrt{\Delta}}\exp\left\{-\frac{1}{2\Delta}[\epsilon_1^2(0)\widetilde{D}_1 + 2\epsilon_1(0)\epsilon_2(0)\widetilde{D}_{12} + \epsilon_2^2(0)\widetilde{D}_2]\right\}, \tag{9}$$

with $\widetilde{D}_1=D_1'\lambda_1$, $\widetilde{D}_2=D_2'\lambda_2$, $\widetilde{D}_{12}=D_{12}'\frac{2\lambda_1\lambda_2}{\lambda_1+\lambda_2}$, and $\Delta=\widetilde{D}_1\widetilde{D}_2-\widetilde{D}_{12}^2$.

The time evolution of the random variables ϵ_1 and ϵ_2 is found by integrating Eqs. (5) and (6). The integration is performed by splitting the interval into small time steps Δt and using one of the following methods: Euler method [12], integral method [13] and stochastic Runge-Kutta method [14]. In our calculations, we choose to use the integral algorithm which is highly accurate. Then using the results Eqs. (A1) and (A2), we obtain

$$\epsilon_1(t+\Delta t) = e^{-\lambda_1\Delta t}\epsilon_1(t) + h_1(t,\Delta t), \tag{10}$$

$$\epsilon_2(t+\Delta t) = e^{-\lambda_2\Delta t}\epsilon_2(t) + h_2(t,\Delta t), \tag{11}$$

where

$$h_1(t,\Delta t) = \lambda_1\int_t^{t+\Delta t} e^{-\lambda_1(t+\Delta t-s)}g_1(s)ds, \tag{12}$$

$$h_2(t,\Delta t) = \lambda_2\int_t^{t+\Delta t} e^{-\lambda_2(t+\Delta t-s)}g_2(s)ds. \tag{13}$$

The first and second moments of the h functions are determined by

$$\langle h_1(t,\Delta t)\rangle = 0, \tag{14a}$$

$$\langle h_2(t,\Delta t)\rangle = 0, \tag{14b}$$

$$\langle h_1^2(t,\Delta t)\rangle = \widetilde{D}_1(1-e^{-2\lambda_1\Delta t}), \tag{14c}$$

$$\langle h_2^2(t,\Delta t)\rangle = \widetilde{D}_2(1-e^{-2\lambda_2\Delta t}), \tag{14d}$$

$$\langle h_1(t,\Delta t)h_2(t,\Delta t)\rangle = \widetilde{D}_{12}(1-e^{-(\lambda_1+\lambda_2)\Delta t}). \tag{14e}$$

III. INTEGRAL ALGORITHM FOR TWO-TERM EXPONENTIALLY CORRELATED COLORED NOISE

The initial ϵ values satisfying the distribution Eq. (9) can be simulated as

$$\epsilon_1(0) = C_{11}\omega_1, \tag{15}$$

$$\epsilon_2(0) = C_{21}\omega_1 + C_{22}\omega_2, \tag{16}$$

where ω_1 and ω_2 are Gaussian random numbers satisfying

$$\langle \omega_i\rangle = 0, \tag{17}$$

$$\langle \omega_i\omega_j\rangle = \delta_{ij}, \quad i=1,2, \quad j=1,2. \tag{18}$$

Using the correlation properties of $\epsilon_1(0)$ and $\epsilon_2(0)$ given by Eqs. (A11)–(A13), the coefficients C_{11}, C_{21}, and C_{22} are found as

$$C_{11} = \widetilde{D}_1^{1/2}, \tag{19}$$

$$C_{21} = \frac{\widetilde{D}_{12}}{\widetilde{D}_1^{1/2}}, \tag{20}$$

$$C_{22} = (\widetilde{D}_2 - C_{21}^2)^{1/2}. \tag{21}$$

The time evolution of ϵ values given by Eqs. (10) and (11) and satisfying Eqs. (14) can be simulated according to

$$\epsilon_1(t+\Delta t)=\epsilon_1(t)e^{-\lambda_1\Delta t}+F_{11}\omega_3, \tag{22}$$

$$\epsilon_2(t+\Delta t)=\epsilon_2(t)e^{-\lambda_2\Delta t}+F_{21}\omega_3+F_{22}\omega_4. \tag{23}$$

In these expressions, ω_3 and ω_4 are again uncorrelated Gaussian random numbers with zero mean and unit variances, and the coefficients are given by

$$F_{11}=[\tilde{D}_1(1-e^{-2\lambda_1\Delta t})]^{1/2}, \tag{24}$$

$$F_{21}=\frac{\tilde{D}_{12}}{[\tilde{D}_1(1-e^{-2\lambda_1\Delta t})]^{1/2}}(1-e^{-(\lambda_1+\lambda_2)\Delta t}), \tag{25}$$

$$F_{22}=[\tilde{D}_2(1-e^{-2\lambda_2\Delta t})-F_{21}^2]^{1/2}. \tag{26}$$

Equations (19), (21), and (26) impose certain conditions on the magnitude of diffusion coefficients, which can be expressed as

$$\tilde{D}_1>0, \tag{27}$$

$$\tilde{D}_2>0, \tag{28}$$

$$\frac{\tilde{D}_{12}^2}{\tilde{D}_1\tilde{D}_2}<1, \tag{29}$$

$$\frac{\tilde{D}_{12}^2}{\tilde{D}_1\tilde{D}_2}<\frac{(1-e^{-2\lambda_1\Delta t})(1-e^{-2\lambda_2\Delta t})}{(1-e^{-(\lambda_1+\lambda_2)\Delta t})^2}. \tag{30}$$

The first two conditions are also necessary for the validity of the autocorrelation functions (7a) and (7b) at $t=t'$. Since the right hand side of Eq. (30) is less than one, we can discard the third condition Eq. (29). The right hand side of Eq. (30) is also rapidly decreasing function of the time step Δt and approaches its asymptotic value as

$$\lim_{\Delta t\to 0}\frac{(1-e^{-2\lambda_1\Delta t})(1-e^{-2\lambda_2\Delta t})}{(1-e^{-(\lambda_1+\lambda_2)\Delta t})^2}=\frac{4\lambda_1\lambda_2}{(\lambda_1+\lambda_2)^2}, \tag{31}$$

which is a stronger condition. Finally, besides the conditions Eqs. (27) and (28), we have

$$\frac{\tilde{D}_{12}^2}{\tilde{D}_1\tilde{D}_2}\leqslant\frac{4\lambda_1\lambda_2}{(\lambda_1+\lambda_2)^2}. \tag{32}$$

With these conditions in mind, we turn our attention in expressing the diffusion coefficients $\tilde{D}_1$, $\tilde{D}_2$, and $\tilde{D}_{12}$ in terms of the given parameters D_1, D_2, λ_1, and λ_2. Equating the Eq. (3) to Eq. (8b), we have

$$D_1\lambda_1=\tilde{D}_1+\tilde{D}_{12}, \tag{33}$$

$$D_2\lambda_2=\tilde{D}_2+\tilde{D}_{12}. \tag{34}$$

Here, we have two equations but three unknown parameters $\tilde{D}_1$, $\tilde{D}_2$, and $\tilde{D}_{12}$ which means that one of these parameters is free and can be fixed in several ways. We choose to fix $\tilde{D}_{12}$ by convention. Then using these two equations, the condition Eq. (32) can be written as

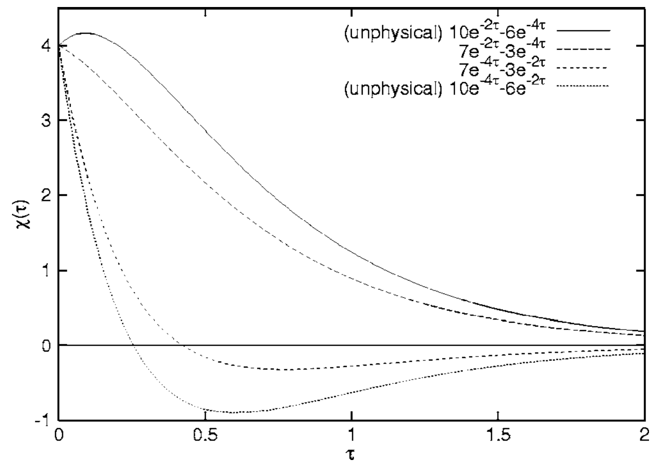

FIG. 1. Four examples of the correlation function, Eq. (3) with $D_1D_2<0$ are indicated. Two of the examples are unphysical due to violation of one of the conditions, Eqs. (38)–(40).

$$f(\tilde{D}_{12})=-\frac{(\lambda_1-\lambda_2)^2}{4\lambda_1\lambda_2}\tilde{D}_{12}^2-(D_1\lambda_1+D_2\lambda_2)\tilde{D}_{12}+D_1\lambda_1D_2\lambda_2 \geqslant 0. \tag{35}$$

If both the parameters D_1 and D_2 are positive, the inequality above will always be valid for $\tilde{D}_{12}=0$. Hence the algorithm reduces to the superposition method [15]. If $D_1D_2<0$, we have a more interesting case, in which the correlation function may have a negative portion, see Fig. 1. Then the maximum of the function $f(\tilde{D}_{12})$ is given by

$$f(\tilde{D}_{12}^{(max)})=\frac{\lambda_1\lambda_2}{(\lambda_1-\lambda_2)^2}(D_1\lambda_1+D_2\lambda_2)^2+D_1\lambda_1D_2\lambda_2\geqslant 0, \tag{36}$$

where

$$\tilde{D}_{12}^{(max)}=-\frac{2\lambda_1\lambda_2}{(\lambda_1-\lambda_2)^2}(D_1\lambda_1+D_2\lambda_2). \tag{37}$$

Once the inequality (36) is satisfied, we have at least one solution for $\tilde{D}_{12}$, namely Eq. (37). The validity of correlation function Eq. (3) at $t=t'$ as well as the condition (36) impose certain restrictions on the given parameters as

$$D_1+D_2>0, \tag{38}$$

$$D_1\lambda_1+D_2\lambda_2>0, \tag{39}$$

$$D_1\lambda_1^2+D_2\lambda_2^2\geqslant 0. \tag{40}$$

Even though the conditions above seem to be restrictions only due to the algorithm, they are indeed also physical restrictions. For any multiexponential correlation function of the form

$$\chi(|t-t'|) = \langle \epsilon(t)\epsilon(t')\rangle = \sum_i D_i\lambda_i e^{-\lambda_i|t-t'|}, \tag{41}$$

there are three physical restrictions:

(1) $\Sigma_i D_i\lambda_i > 0$. This is for the consistency of the correlation function at $t=t'$.

(2) $\Sigma_i D_i > 0$. In the classical (Markovian) limit, that is all $\lambda_i \to \infty$, the correlation function reduces to the form $2\Sigma_i D_i \delta(t-t')$. And again for consistency in the classical limit one needs this condition.

(3) $\Sigma_i D_i \lambda_i^2 \geqslant 0$. The time derivative of the correlation function at $t=t'$ must be negative or zero indicating the initial decrease of the correlation function. The equality case corresponds to Gaussian-like correlation functions where the roots of Eq. (35) are equal and given by Eq. (37).

The correlated algorithm incorporates these physical restrictions naturally. The four possible shapes of the correlation function with two exponential terms satisfying the conditions $D_1D_2 < 0$ and Eq. (39) are shown in Fig. 1 for four arbitrary examples. Two of the examples are unphysical due to violation of one of the conditions.

For a given correlation function in the form Eq. (3), which can be corresponding to a specific physical system or can be a fit of a correlation function, one must fix the value of $\widetilde{D}_{12}$ which in general can assume any value between the roots of Eq. (35). The numerical computations show that among these values the choice of $\widetilde{D}_{12}$ is not very affective, hence it is appropriate to fix it as in Eq. (37). Then, the simulation algorithm to the first order follows as

$$x(t+\Delta t) = x(t) + [f(x) + \epsilon_1(t) + \epsilon_2(t)]\Delta t, \tag{42}$$

where $\epsilon_1(t+\Delta t)$ and $\epsilon_2(t+\Delta t)$ are given by Eqs. (22) and (23) with the initial values determined by Eqs. (15) and (16).

IV. TEST AND APPLICATION OF THE CORRELATED ALGORITHM

A. Test of the algorithm

In order to test the accuracy of the algorithm, we apply it to the free diffusing particle in momentum space with the two-term exponentially correlated noise where the analytic solution can be easily obtained. The corresponding simple stochastic differential equation is given by

$$\dot{p} = \epsilon(t), \tag{43}$$

where $\epsilon(t)$ is a mean-zero Gaussian random number with the correlation Eq. (3). The average value of p does not change in time and remains equal to the initial value, $\langle p(t)\rangle = p(0)$, and the variance can be easily calculated to give

$$\sigma_p^2(t) = -2\left[\frac{D_1}{\lambda_1}(1 - e^{-\lambda_1 t} - \lambda_1 t) + \frac{D_2}{\lambda_2}(1 - e^{-\lambda_2 t} - \lambda_2 t)\right]. \tag{44}$$

In the simulations, we consider a correlation function of the form

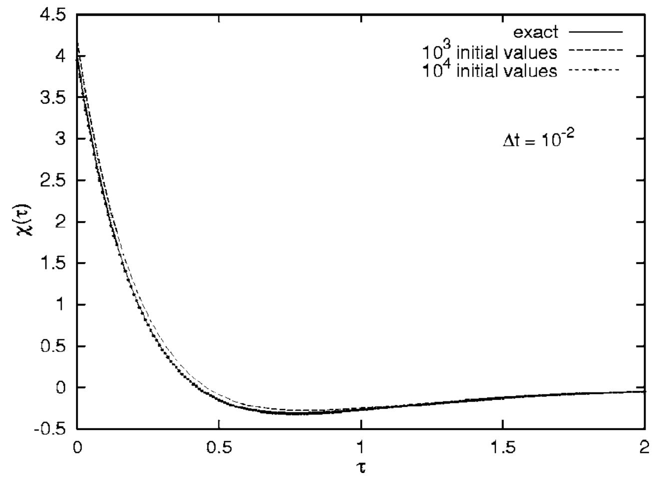

FIG. 2. The comparison of the exact correlation function with simulated ones (dashed line with 10^3 initial values and dotted line with 10^4 initial values).

$$\chi(t) = \langle \epsilon(t+s)\epsilon(s)\rangle = 7e^{-4|t|} - 3e^{-2|t|}. \tag{45}$$

We fix the mixed diffusion coefficient to be $\widetilde{D}_{12} = -16$, take the time step as $\Delta t = 10^{-2}$ and the sharp initial value $p(0) = 5$. Figure 2 shows a comparison of exact correlation function (solid line) with simulations (dashed line with 10^3 initial values and dotted line with 10^4 initial values). Figures 3 and 4 show a comparison of the analytical results for the mean value and the variance of the variable p with simulations. Simulations carried out with 10^4 and 10^5 realizations are indicated by dashed lines and dotted lines respectively. As seen from the figures, already with 10^5 realization, the simulations provide a perfect agreement with the analytical results.

B. Application to generalized Langevin equation

Now, let us consider a more realistic system where a particle undergoes a diffusion over a parabolic barrier, then the

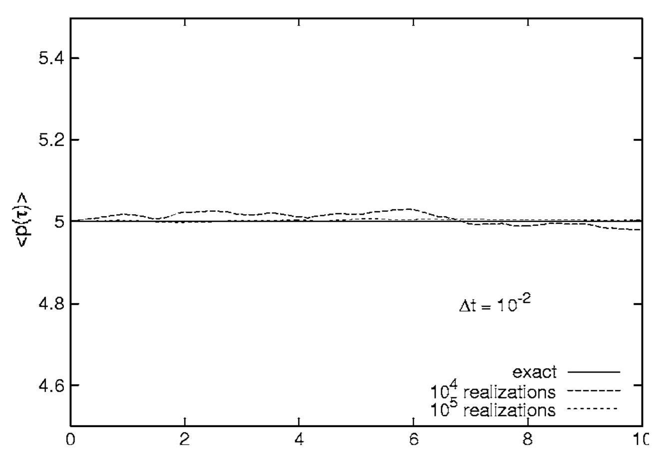

FIG. 3. The comparison of the exact average of p with simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations).

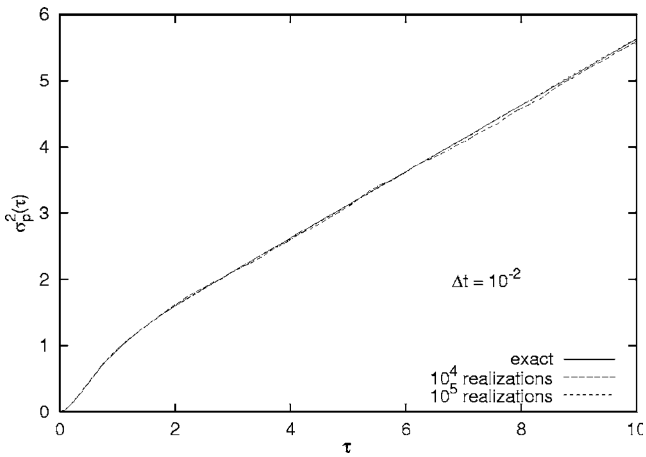

FIG. 4. The comparison of the exact variance of p and simulated ones (dashed line with 10^4 realizations of the algorithm and dotted line with 10^5 realizations).

system can be described by the following generalized Langevin equation (GLE)

$$\dot{q}(t) = p(t), \tag{46}$$

$$\dot{p}(t) = -\frac{\partial V}{\partial q} - \int_0^t \chi(t-t')p(t')dt' + \epsilon(t), \tag{47}$$

where

$$\chi(t) = D_1\lambda_1 e^{-\lambda_1 t} + D_2\lambda_2 e^{-\lambda_2 t} \tag{48}$$

and the potential is

$$V(q) = \tfrac{1}{2}[q_0^2 - q^2(t)]. \tag{49}$$

Here, we assume that the memory kernel has a two-term exponential form. From the fluctuation-dissipation theorem, we have

$$\langle \epsilon(t) \rangle = 0, \tag{50}$$

$$\langle \epsilon(t)\epsilon(t') \rangle = \chi(|t-t'|). \tag{51}$$

The mass of the particle as well as the temperature is chosen to be unity for convenience. Equation (47) can be written as

$$\dot{p} = -\frac{\partial V}{\partial q} + \tilde{\epsilon}_1 + \tilde{\epsilon}_2, \tag{52}$$

$$\dot{\tilde{\epsilon}}_1 = -\lambda_1\tilde{\epsilon}_1 - D_1\lambda_1 p + \lambda_1 g_1, \tag{53}$$

$$\dot{\tilde{\epsilon}}_2 = -\lambda_2\tilde{\epsilon}_2 - D_2\lambda_2 p + \lambda_2 g_2, \tag{54}$$

where g_1 and g_2 are the correlated white noises Eqs. (7) and

$$\tilde{\epsilon}_1(t) = \epsilon_1(t) - D_1\lambda_1\int_0^t e^{-\lambda_1(t-t')}p(t')dt', \tag{55}$$

$$\tilde{\epsilon}_2(t) = \epsilon_2(t) - D_2\lambda_2\int_0^t e^{-\lambda_2(t-t')}p(t')dt'. \tag{56}$$

Here ϵ_1 and ϵ_2 are given by Eqs. (A1) and (A2). Note that the initial values of both $\tilde{\epsilon}_i$ and ϵ_i are the same $(i=1,2)$. With this knowledge, the time evolution of the system to the first order follows as

$$q(t+\Delta t) = q(t) + p(t)\Delta t, \tag{57}$$

$$p(t+\Delta t) = p(t) + \left(-\frac{\partial V}{\partial q} + \tilde{\epsilon}_1(t) + \tilde{\epsilon}_2(t)\right)\Delta t, \tag{58}$$

$$\tilde{\epsilon}_1(t+\Delta t) = \tilde{\epsilon}_1(t)e^{-\lambda_1\Delta t} - D_1 p(t)(1-e^{-\lambda_1\Delta t}) + F_{11}\omega_3, \tag{59}$$

$$\tilde{\epsilon}_2(t+\Delta t) = \tilde{\epsilon}_2(t)e^{-\lambda_2\Delta t} - D_2 p(t)(1-e^{-\lambda_2\Delta t}) + F_{21}\omega_3 + F_{22}\omega_4, \tag{60}$$

where the F functions are the ones given in Eqs. (24)–(26).

By extending the approach of [18] to two-term exponential correlation, it is possible to obtain an analytical solution to the given GLE, Eq. (47), that is, to find the mean values, $\langle p(t)\rangle$ and $\langle q(t)\rangle$ and the variances, $\sigma_q^2(t)$, $\sigma_p^2(t)$, and $\sigma_{pq}^2(t)$ [19]. The joint probability distribution of $p(t)$ and $q(t)$ is a two dimensional Gaussian determined by the mean values and the variances. The analytical expression for passing probability over the parabolic barrier is given by [20,21]

$$P(t,q_0,p_0) = \int_0^\infty \frac{1}{\sqrt{2\pi\sigma_q^2(t)}}\exp\left(-\frac{[q-\langle q(t)\rangle]^2}{2\sigma_q^2(t)}\right)dq = \frac{1}{2}\operatorname{erfc}\left(-\frac{\langle q(t)\rangle}{\sqrt{2}\sigma_q(t)}\right), \tag{61}$$

where $\langle q(t)\rangle$ and $\sigma_q^2(t)$ denotes the mean value and variance of the variable q. The analytical expressions for these quantities are given by

$$\langle q(t)\rangle = R(t)q_0 + Q(t)p_0, \tag{62}$$

where

$$R(t) = \sum_{i=1}^{4}\frac{s_i(s_i+\lambda_1)(s_i+\lambda_2) + D_1\lambda_1(s+a_2) + D_2\lambda_2(s_i+\lambda_1)}{\prod_{n\neq i}(s_i-s_n)}e^{s_i t}, \tag{63}$$

$$Q(t) = \sum_{i=1}^{4}\frac{(s_i+\lambda_1)(s_i+\lambda_2)}{\prod_{n\neq i}(s_i-s_n)}e^{s_i t}, \tag{64}$$

and

$$\sigma_q^2(t) = \sum_{i,j=1}^{4} \frac{(s_i+\lambda_1)(s_i+\lambda_2)(s_j+\lambda_1)(s_j+\lambda_2)}{\prod_{n\neq i}(s_i-s_n)\prod_{m\neq j}(s_j-s_m)}[D_1\lambda_1 A(t,\lambda_1) + D_2\lambda_2 A(t,\lambda_2)], \quad (65)$$

where

$$A(t,\lambda) = \frac{1}{s_i+s_j}\left[\frac{1}{s_i+\lambda}+\frac{1}{s_j+\lambda}\right]e^{(s_i+s_j)t} - \left[\frac{e^{(s_i-\lambda)t}}{(s_i-\lambda)(s_j+\lambda)} + \frac{e^{(s_j-\lambda)t}}{(s_i+\lambda)(s_j-\lambda)}\right] + \frac{1}{s_i+s_j}\left[\frac{1}{s_i-\lambda}+\frac{1}{s_j-\lambda}\right]. \quad (66)$$

In these expressions s_i $(i=1,2,3,4)$, denote the roots of the secular equation

$$s^4 + (\lambda_1+\lambda_2)s^3 + (\lambda_1\lambda_2 + D_1\lambda_1 + D_2\lambda_2 - 1)s^2 + [\lambda_1\lambda_2(D_1+D_2) - (\lambda_1+\lambda_2)]s - \lambda_1\lambda_2 = 0, \quad (67)$$

which is the denominator of the Laplace transform of $q(t)$ derived from the given GLE.

The passing probability over the parabolic barrier can be numerically calculated by generating sufficiently large number of events where Eqs. (57)–(60) are used for each event, counting the number of events for which the particle diffused over the barrier and dividing this number by the total number of events. On the other hand, the analytical result of the overpassing probability can be obtained by using Eq. (61) which, for large times, approaches an asymptotic value that can be written as a function of the initial kinetic energy $K=\frac{1}{2}p_0^2$ and the barrier height $B=\frac{1}{2}q_0^2$.

For the computations, we choose the correlation function as in Eq. (45) again and take sharp initial values for q and p as $q_0=-2$ and $p_0=(2K)^{1/2}$ where K is the initial kinetic energy. The numerical computations (simulations) are obtained with the time step $\Delta t=10^{-2}$, the mixed diffusion coefficient $\tilde{D}_{12}=-16$ which is found from Eq. (37), 10^4 realizations of the algorithm and time iteration up to $t=10$ which is enough for the probability to reach its asymptotic value. The numerical (dashed line) and analytical (solid line) results are shown in Fig. 5 where the passing probability is plotted as a function of the initial kinetic energy. The results are in a good agreement with each other.

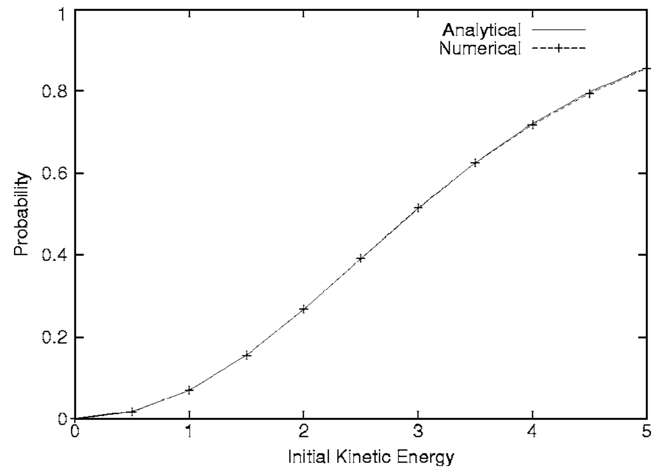

FIG. 5. The passing probability over the barrier is plotted versus the initial kinetic energy in arbitrary units. The analytical and numerical results (dashed line) are shown for the correlation $\chi(t)=7e^{-4|t|}-3e^{-2|t|}$. The numerical computations are done with the time step, $\Delta t=10^{-2}$ and 10^4 realizations.

V. CONCLUSION

In a previous work [15], a method is proposed for simulation of the general Langevin equation with a correlated noise. However, applicability of this method is restricted to the situation in which the correlation function of the noise is expressed as a linear combination of positive exponential terms. In certain situations, for example, in a linear coupling of the relevant degrees with the intrinsic modes of the system, the quantum noise may exhibit a pronounced negative portion. In such cases, the method cannot be applied to simulate generalized Langevin equation. In this paper, we propose an extension of this method that can be applied for numerical simulation of general Langevin equation in which quantum noise can be approximated by a linear combination of exponential terms with positive and negative coefficients. We describe an explicit description of the numerical algorithm and present two different application in order to test the accuracy of the proposed algorithm. Comparison of the numerical simulations with the analytic results verify the accuracy of the proposed algorithm.

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APPENDIX

The solution of Eqs. (5) and (6) are given by

$$\epsilon_1(t) = e^{-\lambda_1 t}\epsilon_1(0) + \lambda_1\int_0^t e^{-\lambda_1(t-s)}g_1(s)ds, \quad (A1)$$

$$\epsilon_2(t) = e^{-\lambda_2 t}\epsilon_2(0) + \lambda_2\int_0^t e^{-\lambda_2(t-s)}g_2(s)ds. \quad (A2)$$

Since $\epsilon(t)=\epsilon_1(t)+\epsilon_2(t)$, we have

$$\langle\epsilon(t)\rangle = e^{-\lambda_1 t}\langle\epsilon_1(0)\rangle + e^{-\lambda_2 t}\langle\epsilon_2(0)\rangle. \quad (A3)$$

Let $\epsilon_1(0)$ and $\epsilon_2(0)$ be mean-zero Gaussian random numbers, then averaging over these random numbers we find

$$\{\langle\epsilon(t)\rangle\} = 0. \quad (A4)$$

By using the Eqs. (7), the correlations of ϵ_1 and ϵ_2 can be found as

$$\langle \epsilon_1(t)\epsilon_1(t')\rangle = \widetilde{D}_1 e^{-\lambda_1|t-t'|} + [\langle \epsilon_1^2(0)\rangle - \widetilde{D}_1]e^{-\lambda_1(t+t')}, \tag{A5}$$

$$\langle \epsilon_2(t)\epsilon_2(t')\rangle = \widetilde{D}_2 e^{-\lambda_2|t-t'|} + [\langle \epsilon_2^2(0)\rangle - \widetilde{D}_2]e^{-\lambda_2(t+t')}, \tag{A6}$$

$$\langle \epsilon_1(t)\epsilon_2(t')\rangle = \widetilde{D}_{12} e^{-\lambda_{12}|t-t'|} + [\langle \epsilon_1(0)\epsilon_2(0)\rangle - \widetilde{D}_{12}]e^{-(\lambda_1 t+\lambda_2 t')}, \tag{A7}$$

where $\lambda_{12}=\lambda_1$ for $t>t'$ and $\lambda_{12}=\lambda_2$ for $t'>t$. Again averaging over the random numbers $\epsilon_1(0)$ and $\epsilon_2(0)$ we find

$$\{\langle \epsilon_1(t)\epsilon_1(t')\rangle\} = \widetilde{D}_1 e^{-\lambda_1|t-t'|}, \tag{A8}$$

$$\{\langle \epsilon_2(t)\epsilon_2(t')\rangle\} = \widetilde{D}_2 e^{-\lambda_2|t-t'|}, \tag{A9}$$

$$\{\langle \epsilon_1(t)\epsilon_2(t')\rangle\} = \widetilde{D}_{12} e^{-\lambda_{12}|t-t'|}, \tag{A10}$$

once these random numbers satisfy the following equations

$$\{\langle \epsilon_1^2(0)\rangle\} = \widetilde{D}_1, \tag{A11}$$

$$\{\langle \epsilon_2^2(0)\rangle\} = \widetilde{D}_2, \tag{A12}$$

$$\{\langle \epsilon_1(0)\epsilon_2(0)\rangle\} = \widetilde{D}_{12}. \tag{A13}$$

Now we have enough information to build the autocorrelation of $\epsilon(t)$ and it is found to be

$$\{\langle \epsilon(t)\epsilon(t')\rangle\} = (\widetilde{D}_1 + \widetilde{D}_{12})e^{-\lambda_1|t-t'|} + (\widetilde{D}_2 + \widetilde{D}_{12})e^{-\lambda_2|t-t'|}. \tag{A14}$$

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