COMMENTS

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Comment on "Brownian motion of two interacting particles under a square-well potential"

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We present the exact solution of the Fokker-Planck equation for a particle escaping from the square-well potential under the influence of white noise. The mean-square displacement obeys the Einstein relation, in contrast to the conclusion of the recent article by Akio Morita [Phys. Rev. E **49**, 3697 (1994)].

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Diffusion over potential barriers is an old problem of great importance in physics, the simplest model for such a problem being the escape of a particle from a square well of depth V_0 and width u (Fig. 1) under the influence of white noise. The Fokker-Planck equation for the probability distribution function $\rho(x,t)$ for the position x of a particle at time t reads [2]

$$\partial_t \rho = \partial_x[\partial_x \rho + A\delta(x-u)\rho]. \tag{1}$$

Here $A = V_0/T$, where the temperature T is measured in units of energy and the time is measured in units of length squared (the diffusion coefficient is chosen equal to unity). The initial condition is assumed to be a δ function,

$$\rho(x, t=0) = \delta(x - x_0). \tag{2}$$

The wall at $x = 0$ was taken as a reflective boundary, i.e., the boundary condition at $x = 0$, along with finiteness of ρ at $x \to \infty$, is

$$\partial_x \rho = 0 \text{ at } x = 0 \ , \ \rho \text{ is finite at } x \to \infty. \tag{3}$$

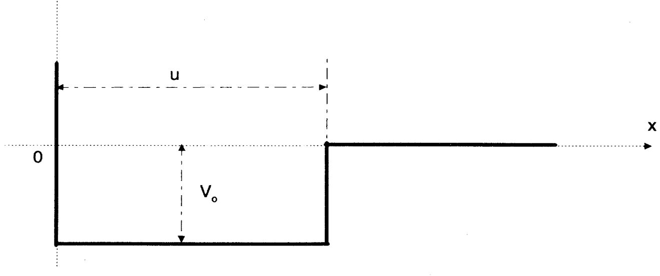

FIG. 1. Square-well potential $V(x)$.

A quite sophisticated analysis of (1)–(3) was performed in Ref. [1] which includes, in particular, the different asymptotic forms of the confluent hypergeometric functions, leading to a very strange result for the asymptotic expansion of the mean-square displacement $\langle x^2 \rangle$. Indeed, it was found [1] that the Einstein relation does not hold ($x^2 \not\approx 2t$ at $t \to \infty$) and the diffusion is anomalous ($x^2 \sim t^n$ with $n > 1$). A similar result was obtained in Ref. [1] for the escape from a three-dimensional spherically symmetric potential well. However, we believe the analysis in Ref. [1] is flawed because of the incorrect use of the Laplace transform of Eq. (1); namely, the author of Ref. [1] ignored the existense of the branch point in inverting the Laplace transform. We present here the exact solution of (1)–(3), first for the simple case $x_0 = u$, i.e., $\rho(x, t=0) = \delta(x-u)$ (initially a particle is located at the right end of the barrier), and then for the general case (2). It is self-evident that the asymptotic results will not depend on the precise initial position of the particle inside a well. In contrast to Ref. [1], we solve Eq. (1) in two regions, $0 < x < u$ and $u < x < \infty$, and then match the solutions obtained at $x = u$. In each of these regions, Eq. (1) does not contain a δ function. Let us perform the Laplace transform, $\hat{\rho}(s) = \int_0^\infty \rho(t) e^{-st} dt$:

$$\partial_x^2 \hat{\rho} = s\hat{\rho} - \rho(x,0) = s\hat{\rho} - \delta(x-u), \tag{4}$$

where the initial condition $\rho(x, t=0) = \delta(x-u)$ has been used. The solutions of Eq. (4) in the two regions of interest are

$$\hat{\rho}_1 = C_1 \cosh(\sqrt{s}x) \ , \ 0 < x < u,$$
$$\hat{\rho}_2 = C_2 \exp^{-\sqrt{s}x} \ , \ u < x < \infty. \tag{5}$$

The boundary conditions (3) were used to obtain (5). Turning now to the matching conditions at $x = u$, one has to take into account the jump of $\rho(x,t)$ at this point, namely [2], $\rho(u+\epsilon,t)e^A = \rho(u-\epsilon,t)$, and the continuity of the current. The latter is assured by integrating (4) over the x region $(u-\epsilon, u+\epsilon)$ with an infinitesimal ϵ. This procedure gives

$$\partial_x \hat{\rho}_2|_{x=u+\epsilon} - \partial_x \hat{\rho}_1|_{x=u-\epsilon} = -1. \tag{6}$$

The two matching conditions for ρ and $\partial_x \rho$ at $x = u$ lead to the following values for the constants C_1 and C_2 :

$$C_1 = \frac{1}{\sqrt{s}[\sinh(\sqrt{s}u) + e^{-A}\cosh(\sqrt{s}u)]} ;$$
$$C_2 = \frac{e^{\sqrt{s}u - A}\cosh(\sqrt{s}u)}{\sqrt{s}[\sinh(\sqrt{s}u) + e^{-A}\cosh(\sqrt{s}u)]}. \tag{7}$$

Equations (5) and (7) yield a complete solution of the time-dependent problem (1) in the Laplace-transformed form. For a comparision with Ref. [1], we restrict ourselves to the calculations performed in Ref. [1]. The Laplace transform of $\langle x^2 \rangle$ becomes

$$\mathcal{L}\{\langle x^2\rangle\} = \frac{2}{s^2} + \frac{u^2}{s} + \frac{2u\sqrt{s}\cosh(\sqrt{s}u)(1-e^A)}{s^2[e^A\sinh(\sqrt{s}u) + \cosh(\sqrt{s}u)]}. \tag{8}$$

Expanding the hyperbolic functions in (8) in terms of negative exponentials and then in a series by the binomial theorem, one can perform the Laplace transform exactly [3]:

$$\langle x^2\rangle = 2t + u^2 - \frac{4u}{\sqrt{\pi}}\sum_{n=0}^{\infty}\left(\frac{e^A-1}{e^A+1}\right)^{n+1}\left\{\sqrt{t}\left[\exp\left(\frac{-u^2(n+1)^2}{t}\right) + \exp\left(\frac{-u^2(n)^2}{t}\right)\right] - \sqrt{\pi}u(n+1)\mathrm{erfc}\left(\frac{u(n+1)}{\sqrt{t}}\right) - \sqrt{\pi}un\,\mathrm{erfc}\left(\frac{un}{\sqrt{t}}\right)\right\}. \tag{9}$$

For $A = 0$, (9) reduces to the well-known field-free result $\langle x^2\rangle = 2t + u^2$. Using the asymptotic expansion of erfc(z) for small z, erfc$(z) \cong 1 - 2z/\sqrt{\pi}$, leads to the following asymptotic expansion for $t \to \infty$:

$$\langle x^2\rangle|_{t\to\infty} = u^2 - 2e^Au^2 + 2(e^A)^2u^2 + 2t - \frac{4u(e^A-1)}{\sqrt{\pi}}\sqrt{t} + O\left(\frac{1}{\sqrt{t}}\right). \tag{10}$$

If one considers the general initial condition (2), the result (10) remains unchanged except that one has to replace u^2 in the first term of the right-hand side of (10) by x_0^2. In addition to $\langle x^2\rangle$, we also calculated the time-dependent probability $P(t)$ to remain inside the well. The solution (5) and (7) yields for the Laplace transform of $P(t)$

$$\mathcal{L}\{P(t)\} = \int_0^u \hat{\rho}_1(x,s)dx = \frac{\sinh(\sqrt{s}u)}{s[\sinh(\sqrt{s}u) + e^{-A}\cosh(\sqrt{s}u)]}. \tag{11}$$

The inverse Laplace transform of (11) is then

$$P(t) = \frac{e^A}{e^A+1}\sum_{n=0}^{\infty}\left(\frac{e^A-1}{e^A+1}\right)^n\left[\mathrm{erfc}\left(\frac{un}{\sqrt{t}}\right) - \mathrm{erfc}\left(\frac{u(n+1)}{\sqrt{t}}\right)\right], \tag{12}$$

which has the following asymptotic form for $t \to \infty$:

$$P(t)|_{t\to\infty} \approx \frac{ue^A}{\sqrt{\pi t}}. \tag{13}$$

The same limiting form is obtained for the initial condition (2). Finally, in contrast to Ref. [1], we have found that the Einstein relation does hold for a particle escaping from the potential well shown in Fig. 1, as one would expect for obvious physical reasons.

[1] A. Morita, Phys. Rev. E **49**, 3697 (1994).
[2] H. Risken, *The Fokker-Planck Equation* (Springer-Verlag, Berlin, 1984).
[3] G. Roberts and H. Kaufman, *Table of Laplace Transforms* (Saunders, Philadelphia, 1966).