Comments

Comment on "Short-time dynamics of noise-induced escapes and transitions in overdamped systems" by Soskin *et al.*, Semiconductor Physics, Quantum Electronics & Optoelectronics, 2022. 25, No 3. P. 262–274

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Abstract. I clarify the reasons for the observed discrepancy between the numerical simulations of noise induced escape in a quartic potential by Soskin *et al.*, and the weak noise matched asymptotic solution (MAS) of the time dependent Smoluchowski equation obtained earlier [V. Shneidman, Phys. Rev. E56, 5257 (1997)]. A minor typo – sign of a constant – is corrected and the MAS is also extended beyond the top of the barrier into the second well. Once numerics is performed for a higher barrier, the correspondence with analytics is restored.

Keywords: numerical simulations, quartic potential, matched asymptotic solution.

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In Ref. [1] Soskin *et al.* considered escape of an overdamped particle over a potential barrier. A small-time path-integral solution was discussed and direct numerical integration of a Langevin type stochastic differential equation (SDU) was performed for arbitrary times and small-to-moderate barriers. Alternatively, in Ref. [2] in the limit of a high barrier, a matched asymptotic solution (MAS) of the Smoluchowski equation was obtained, valid at intermediate and large times.

Based on comparison, the authors of Ref. [1] conclude that the MAS is "incorrect". This should be clarified since the MAS is based on combination of powerful methods of matched asymptotic expansions and Laplace transformations. In particular, a similarly constructed MAS for the problem of transient nucleation [3], on multiple occasions was later shown to be numerically accurate, though for larger barriers.

A simple examination of eqs. (13a) and (13b) of Ref. [2] shows that there should be a "–" sign in front of the term τC in eq. (13a). [In a similarly structured incubation time in the nucleation problem, eq. (A.9) [3], the sign of the constant is right]. Otherwise, the general results of Ref. [2] appear correct. For verification, the quartic potential [1] $U(x) = -x^2/2 + x^4/4$ is considered with stable points at $x_S = \pm 1$ and the barrier at $x_* = 0$; the particle is initially placed at the left stable point $x = -1$.

Equation (17) of Ref. [2] gives the time dependence of the flux

$$j(x,t) = I_K \int_0^\infty \mathrm{d}y \exp\left\{-y - \frac{e^{-\alpha u}}{y^\alpha}\right\}. \qquad (1)$$

Here I_K is the quasi steady state (Kramers) flux, and for the quartic potential at $x = x_*$ one has $\alpha = 2$ and $u = 2\left(t - t_i^*\right)$. The "incubation time" is now given by

$$t_i^* = \frac{3}{4}\ln\frac{1}{D} - \ln 2\ . \qquad (2)$$

Note the "–" in front of ln 2; the asterisk is added to indicate the top of the barrier. As shown below later, eq. (1) with different α and u is also valid beyond the barrier, sufficiently deep into the second well.

Before comparing the above to numerics, note that away from equilibrium points the small expansion parameter of MAS is the inverse of the barrier, and for barriers of several tens accuracy of the leading approximation can be sufficient. On the other hand, near the equilibrium points the expansion parameter is the inverse *root* of the barrier see, *e.g.* Ref. [3] or [4]. Here, for a reliable comparison either higher order corrections are to be included in the MAS (as for the Laplace transform [4] and for the time-dependence of the critical flux [5] in the nucleation problem) or, alternatively numerics has to be performed for a really high barrier. In the framework of the present Comment, I select the numerical option. Also, however the MAS will be extended beyond the top of the barrier, with less demands on the barrier height.

For numerical solution, the Smoluchowski equation was written in terms of reduced $w(x,t) = P(x,t)/P_{eq}(x)$ with $P_{eq}(x) \sim \exp(-U/D)$ being the (quasi) equilibrium probability density. (This is suggested by the MAS – unlike the non-reduced probability density $P(x, t)$ which changes with x exponentially fast in the first well, the reduced $w(x, t)$ changes with x more moderately.) Then, the flux is determined by $j(x,t) = -DP_{eq}(x)\partial w(x,t)/\partial x$. A reflecting and absorbing boundaries were placed at $x = -2$ and $x = +1$, respectively, and for initial density a numerical approximation of a δ-function by $P(x,0) = \left(\sqrt{\pi}/\epsilon\right)\exp\left[-(x+1)^2/\epsilon^2\right]$ with $\epsilon << \sqrt{D}$ was used, with typical $\epsilon = 0.001$. Numerical solution was then obtained using the standard 'NDSolve' command in *Mathematica 12*.

Numerical results are shown by dashed lines in Fig. 1. For a relatively small barrier of 6.25 corresponding to $D = 0.04$ (left) this dashed line appears to be in correspondence with the numerical data of Ref. [1] (not shown, see Fig. 1 of Ref. [1]) based on a SDU, save for inevitable scatter of the latter. The strong shift between numerics and analytics noted in Ref. [1] has been corrected, although the correspondence of transient shapes is still not perfect. This is not surprising since for such a low barrier even the quasi steady state (Kramers) limit is not achieved too accurately – note that the numerical curve does not saturate to 1. The difference between numerics and analytics is significantly reduced with increase of the barrier (the dashed and solid lines on the right), but as mention above, for the flux on top of the barrier to be accurate in the leading order of MAS, the barrier has to be really high.

To extend the MAS beyond the barrier, I follow the major steps of Ref. [3]. First, I switch from $w(x, t)$ which decays with x exponentially fast, to the flux $j(x, t)$ which changes more smoothly in the region $0 < x < 1$. The Laplace transform of this flux to the right of the barrier (the "right outer solution") has the structure $J(x, p) \sim \exp\left(-p\int dx/v\right)$, where p is the Laplace index. Matching this with the inner solution near $x = x_*$ [2] gives the proportionality constant in the outer solution. After inversion of the Laplace transform using the same asymptotic technique as described in Ref. [2], one obtains an expression which is similar in structure to eq. (1) but with $\alpha = 4$ and $u = t - t_i(x)$. The new "incubation time" is given by

$$t_i(x) = \frac{5}{4}\ln\frac{1}{D} + \frac{1}{2}\log\left(\frac{x^2}{2(1-x^2)}\right). \tag{3}$$

The result is valid almost everywhere in the domain $0 < x < 1$, except for the boundary layers of the order $\sqrt{D}$ which are located respectively, near unstable $x_* = 0$ and the second stable $x_S = 1$ equilibrium points. Due to relatively large $\alpha = 4$ in the off-barrier domain, for practical purposes eq. (1) can be approximated by its limiting form

$$j(x,t) \approx I_K \exp\left(-e^{-u}\right), \tag{4}$$

which is typical for the nucleation problem [3] and which in the present case results in an elementary function of both x and t.

Comparison with numerics at x = 1/2 is shown in Fig. 2 for a small, intermediate and large barriers, respectively. Note that accuracy of the MAS (solid lines) is much better at x = 1/2 than at $x = 0$, the top of the

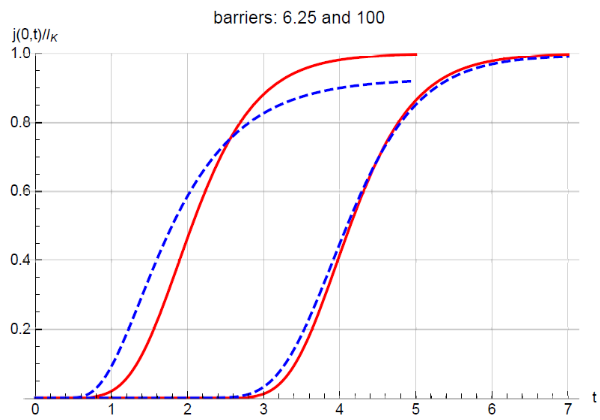

Fig. 1. Reduced transient flux at the top of the barrier (x = 0) for a small barrier $1/4D$ = 6.25 (left) and for a large barrier $1/4D$ = 100 (right). Solid lines – eqs. (1), (2) with α = 2 and $u = 2\left(t - t_i^*\right)$, dashed lines – numerics. I_K is the Kramers flux.

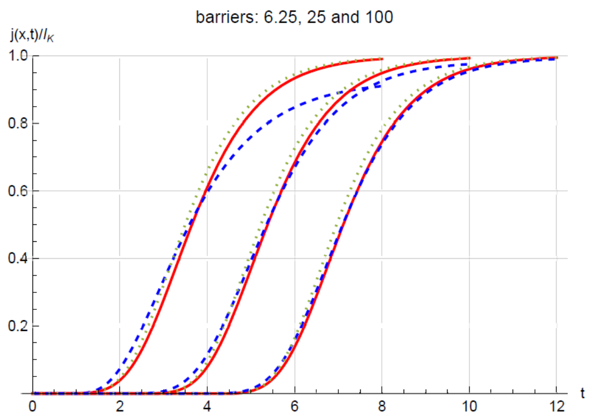

Fig. 2. The reduced transient flux $j(x, t)/I_K$ at $x = 1/2$ (off the barrier top) for three values of the barrier height; from left to right: $1/4D$ = 6.25, 25 and 100, respectively. Solid lines – eqs. (1), (3) with α = 4 and $u = t - t_i(x)$, dashed lines – numerics, dotted – elementary approximation, Eqs. (3), (4).

barrier (Fig. 1). For the smallest barrier (left) the difference between the leading MAS and numerics (dashed line in Fig. 2) is inevitable since at large time the former converges to Kramers flux, while the latter does not. Accuracy rapidly increases with increasing barrier, as for $1/4D = 25$ and 100. For all barriers, the MAS in this region can be reasonably approximated by the elementary double exponential eq. (4) – large α limit, shown by the dotted line.

In summary, the status of the leading part of time-dependent matched asymptotic solution (MAS) of the Smoluchowski equation has been restored. While there remain technical issues of including higher order corrections into the MAS for lower barriers (especially near the barrier top), as well as a more carefull assessment of the standard numerics when the barrier is very large, currently analytics and numerics appear in good correspondence, with the difference wanishing with the increase of the barrier height.

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Анотація. Я пояснюю причини спостережуваної невідповідності між результатами чисельного моделювання виходу, викликаного шумом, у квартичному потенціалі за Соскіним та ін., та асимптотикою зі слабким шумом (MAS) залежного від часу рівняння Смолуховського, отриманого раніше [V. Shneidman, Phys. Rev. E56, 5257 (1997)]. Незначну друкарську помилку – знак константи – виправлено, і MAS також поширено за верхню частину бар’єра в другу яму. Оскільки числові значення для вищого бар’єра отримано, відповідність з аналітикою відновлено.

Ключові слова: чисельне моделювання, квартичний потенціал, асимптотика зі слабким шумом.