Diffusion over a saddle with a Langevin equation

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The diffusion problem over a saddle is studied using a multidimensional Langevin equation. An analytical solution is derived for a quadratic potential and the probability to pass over the barrier deduced. A very simple solution is given for the one-dimensional problem and a general scheme is shown for higher dimensions.

I. INTRODUCTION

The Langevin equation [1] has been applied to most fields of physics. It was solved several times for parabolic potential wells, see, e.g., Refs. [2–4]. As analytical solutions can be derived for quadratic potentials only, it has really rather become widely used in numerical simulations.

Our purpose is to establish an analytical expression for the diffusion over a potential barrier. In order to have a solvable problem, we assume that, around the saddle point, the potential can be approximated by quadratic functions. Some very simple expressions are obtained in one dimension. Because many processes obviously involve more than one coordinate, we extend our analysis to multidimensional cases. We thus derive an analytic expression for the distribution function of the Langevin equation, valid for multidimensional models, and then study the probability to overpass the barrier.

Our approach is only valid for classical diffusion satisfying the dissipation-fluctuation theorem. A solution for the one dimension Langevin equation in the overdamped limit is derived in Ref. [5] for Lévy flights [6], but it cannot be simply extended to multidimensional Langevin equations.

The interest of our approach will be shown in the case of heavy-ion fusion problems, for which Langevin equation type simulations have been used by several groups [7–9]. The very small cross section of such a mechanism makes numerical simulations very difficult, because very large statistics have to be computed. Our analytical expressions, though using somewhat crude approximations, could be useful to extract some general trends. The problematics of realistic calculations is out of the scope of this paper, where we only discuss general considerations concerning the Langevin formalism.

II. LANGEVIN EQUATION

A. Introduction

To study the diffusion over a one-dimensional (1D) parabolic potential barrier, $V(q_1) = -m_1\omega_1^2 q_1^2/2$ with a given initial condition $q_{10} < 0$ and $p_{10} > 0$, the Langevin equation reads

$$\ddot{q}_1 + \beta_1\dot{q}_1 - \omega_1^2 q_1 = r_1(t), \qquad (1)$$

where $r_1(t)$ is a Gaussian stochastic force. As discussed in Appendix B, we rule out any anomalous diffusion process. The first two moments of this force are

$$\langle r_1(t)\rangle = 0 \quad \text{and} \quad \langle r_1(t)r_1(t')\rangle = \frac{2T\beta_1}{m_1}\delta(t-t'), \quad (2)$$

in agreement with the dissipation-fluctuation theorem. In the previous equations, T, m_1, and β_1 denote the temperature, the mass, and the reduced friction, respectively. All these parameters are assumed to be time, position, and velocity independent, or at most very slowly varying, in the vicinity of the saddle. The angle brackets indicate an ensemble average.

For any n-dimensional problem, one can generalize the previous approach, replacing the $(q_1, \dot{q}_1)$ variables by vectors $(Q, \dot{Q})$,

$$\ddot{Q} + \beta\dot{Q} - \Omega^2 Q = R(t). \qquad (3)$$

Such a canonical form of the problem results from two successive, very standard manipulations: (i) change the representation by transforming all tensors $\mathcal{T}$, such as the friction tensor and the spring tensor, into a form $M^{-1/2}\mathcal{T}M^{-1/2}$, where M is the usual mass tensor, naturally, (ii) change again the representation so that the spring tensor becomes diagonal.

More precisely, assume some initial representation with a vector of degrees of freedom $Z \equiv \{z_1, \ldots z_n\}$, driven by a constant, symmetric mass tensor M, a constant, symmetric friction tensor $\mathcal{G}$, a constant, symmetric spring tensor $\mathcal{S}$ and a random vector force $\mathcal{F}$. The initial dynamical equation reads

$$M\ddot{Z} + \mathcal{G}\dot{Z} - \mathcal{S}Z = \mathcal{F}(t). \qquad (4)$$

This is equivalent to

$$M^{1/2}\ddot{Z} + M^{-1/2}\mathcal{G}M^{-1/2}M^{1/2}\dot{Z} - M^{-1/2}\mathcal{S}M^{-1/2}M^{1/2}Z$$
$$= M^{-1/2}\mathcal{F}(t). \qquad (5)$$

Now let U be that orthogonal matrix which lists the right eigenvectors of $M^{-1/2}\mathcal{S}M^{-1/2}$ as columns. Accordingly, $M^{-1/2}\mathcal{S}M^{-1/2} = U\mathcal{D}U^{-1}$, where $\mathcal{D}$ is diagonal. (Throughout this argument we rule out, naturally, those very exceptional

cases where diagonalizations and/or inversions are singular.) Then the dynamical equation reads as well,

$$U^{-1}M^{1/2}\ddot{Z}+U^{-1}M^{-1/2}\mathcal{G}M^{-1/2}UU^{-1}M^{1/2}\dot{Z}-\Omega^2 U^{-1}M^{1/2}Z$$
$$=U^{-1}M^{-1/2}\mathcal{F}(t). \tag{6}$$

With the definitions, $Q\equiv U^{-1}M^{1/2}Z$, $\beta\equiv U^{-1}M^{-1/2}\times\mathcal{G}M^{-1/2}U$, and $R(t)=U^{-1}M^{-1/2}\mathcal{F}(t)$, this is nothing but the canonical form, Eq. (3).

For 2D, for instance, we may obtain the first final degree of freedom as a ''valley'' direction to the saddle and the other final degree as a ''confining'' direction

$$Q=\begin{bmatrix} q_1 \\ q_2 \end{bmatrix}, \quad \Omega^2=\begin{bmatrix} \omega_1^2 & 0 \\ 0 & -\omega_2^2 \end{bmatrix}, \quad \beta=\begin{bmatrix} \beta_1 & \beta_{12} \\ \beta_{12} & \beta_2 \end{bmatrix}, \tag{7}$$

and $R(t)$ is a random force with two components. Such two components are correlated when β is nondiagonal but can be related, through a suitable matrix Γ, to a vector of independent random numbers

$$R(t)=\Gamma\begin{bmatrix} \nu_1(t) \\ \nu_2(t) \end{bmatrix}, \tag{8}$$

with

$$\langle \nu_1(t)\nu_1(t')\rangle=\delta(t-t'), \quad \langle \nu_2(t)\nu_2(t')\rangle=\delta(t-t'),$$
$$\text{and} \quad \langle \nu_1(t)\nu_2(t)\rangle=0. \tag{9}$$

The matrix Γ is real, but usually not symmetric. The fluctuation-dissipation theorem, incidentally, which is easy to derive from the initial form, Eq. (4), states that $\Gamma\Gamma^T=2T\beta$, where T is the temperature and where the superscript T indicates transposition. All necessary details are found in Appendix A.

It will be stressed again here that the matrices β, Ω^2, and Γ take into account an overall multiplication of motion equations by the inverse of the (square root of the) mass tensor. It is easy to prove that this manipulation does not change the signs of the eigenvalues of the resulting matrices, and that such resulting matrices are usually non diagonal. In turn, the final spring tensor Ω^2 can be made diagonal by the additional manipulation (ii). The generalization to n dimensions is trivial.

B. Analytical solution

Defining $P=\dot{Q}$, it is easy to transform Eq. (3) into a first-order differential equation, in a $(2n)$-dimensional space,

$$\frac{d}{dt}\begin{bmatrix} Q \\ P \end{bmatrix}=\begin{bmatrix} 0 & 1 \\ \Omega^2 & -\beta \end{bmatrix}\begin{bmatrix} Q \\ P \end{bmatrix}+\begin{bmatrix} 0 \\ R \end{bmatrix}. \tag{10}$$

In the following we call the block matrix

$$D=\begin{bmatrix} 0 & 1 \\ \Omega^2 & -\beta \end{bmatrix}$$

appearing in Eq. (10) the drift matrix (DM). In the upper-left and upper-right corners of this $2n\times 2n$ matrix, the symbols 0 and 1 denote, respectively, the null and the unit $n\times n$ matri-

ces, naturally. Whenever this DM can be diagonalized, and in the limit where the time and space derivatives of all physical parameters such as masses, drifts, frequencies, etc., can be neglected, the previous system can be transformed into

$$\frac{d}{dt}\begin{bmatrix} X_1 \\ \vdots \\ X_{2n} \end{bmatrix}=D\begin{bmatrix} X_1 \\ \vdots \\ X_{2n} \end{bmatrix}+\theta^{-1}\begin{bmatrix} 0 \\ R \end{bmatrix}, \tag{11}$$

where D is the diagonal drift matrix (DDM),

$$D=\theta^{-1}D\theta=\begin{bmatrix} a_1 & 0 & 0 \\ 0 & \cdots & 0 \\ 0 & 0 & a_{2n} \end{bmatrix}, \tag{12}$$

and θ is the ''rotation'' matrix,

$$\begin{bmatrix} q_1 \\ \vdots \\ q_n \\ p_1 \\ \vdots \\ p_n \end{bmatrix}=\theta\begin{bmatrix} X_1 \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ X_{2n} \end{bmatrix}. \tag{13}$$

This matrix θ is the matrix of right (column) eigenvectors of the DM. Any normalization may be chosen for such eigenvectors.

It can be stressed here that the eigenmodes X_i are linear combinations of both positions and momenta, hence the saddle dynamics should be visualized in phase space rather than coordinate space only. All such eigenmodes are expected to decay exponentially with time, except just one, corresponding to a resulting preferred direction along the valley, in phase space.

In that same limit where the derivatives of the physical parameters (masses, etc.) can be neglected, such first order differential equations can be formally integrated into

$$x_i(t)\equiv X_i e^{-a_i t}-X_{io}$$
$$=\int_0^t d\tau e^{-a_i\tau}[\alpha_{i1}\nu_1(\tau)+\cdots+\alpha_{in}\nu_n(\tau)],$$
$$i=1,2,\ldots,2n. \tag{14}$$

Here the α_{ij}'s are defined from the effects of both θ^{-1} and Γ matrices (in matrix notation, $\alpha=\theta^{-1}\begin{bmatrix} 0 \\ \Gamma \end{bmatrix}$, where α is a $2n\times n$ matrix, and 0 and Γ are $n\times n$ ones) and the ν_i's are uncorrelated white random numbers, extending Eqs. (9) to n dimensions. Then, the Euler type variables $(x_1,\ldots,x_{2n})$ should have the same statistical properties as those of

$$\left(\int_0^t d\tau e^{-a_1\tau}[\alpha_{11}\nu_1(\tau)+\cdots+\alpha_{1n}\nu_n(\tau)],\ldots,\right.$$
$$\left.\int_0^t d\tau e^{-a_{2n}\tau}[\alpha_{(2n)1}\nu_1(\tau)+\cdots+\alpha_{(2n)n}\nu_n(\tau)]\right). \tag{15}$$

These are Gaussian random numbers whose correlations are easily evaluated from those of the ν_i's,

$$A_{ij}(t)=\langle x_i(t)x_j(t)\rangle$$

$$=\int_0^t d\tau\, e^{-(a_i+a_j)\tau}(\alpha_{i1}\alpha_{j1}+\cdots+\alpha_{in}\alpha_{jn})$$

$$=\frac{1-e^{-t(a_i+a_j)}}{a_i+a_j}\sum_{k=1}^n \alpha_{ik}\alpha_{jk}. \tag{16}$$

In a more compact matrix notation,

$$A=\int_0^t d\tau\, e^{-\tau D}\alpha\alpha^T e^{-\tau D}. \tag{17}$$

Notice the occurrence of the matrix

$$\alpha\alpha^T=\theta^{-1}\begin{bmatrix}0 & 0\\ 0 & 2T\beta\end{bmatrix}(\theta^T)^{-1},$$

which is trivially positive definite if θ is real.

Using functional integral techniques, the full distribution function can then be easily evaluated (see Appendix B for details) and reads

$$W(x_1,\ldots,x_{2n},t;X_{10},\ldots,X_{(2n)0})$$

$$=\frac{1}{(2\pi)^n}\frac{1}{\sqrt{\det A}}\exp\left(-\frac{1}{2}[x_1,\ldots,x_{2n}]A^{-1}\begin{bmatrix}x_1\\ \vdots\\ x_{2n}\end{bmatrix}\right), \tag{18}$$

where the matrix elements of A are those defined by Eq. (16). This makes also a Gaussian distribution, naturally. If necessary, it is then easy to return to the original variables $(q_1,\ldots,q_n;p_1,\ldots,p_n)$. Since

$$\begin{bmatrix}q_1\\ \vdots\\ q_n\\ p_1\\ \vdots\\ p_n\end{bmatrix}=\theta\begin{bmatrix}x_1 e^{a_1 t}\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ x_{2n}e^{a_{2n}t}\end{bmatrix}+\theta\begin{bmatrix}X_{10}e^{a_1 t}\\ \vdots\\ \vdots\\ \vdots\\ \vdots\\ X_{2n0}e^{a_{2n}t}\end{bmatrix}, \tag{19}$$

where the second term of the right-hand side is the average trajectory and the first one is the diffusion part, it is obvious that

$$\begin{bmatrix}\langle q_1(t)\rangle\\ \vdots\\ \langle q_n(t)\rangle\\ \langle p_1(t)\rangle\\ \vdots\\ \langle p_n(t)\rangle\end{bmatrix}=e^{tD}\begin{bmatrix}q_{10}\\ \vdots\\ q_{n0}\\ p_{10}\\ \vdots\\ p_{n0}\end{bmatrix}, \tag{20}$$

and

$$\mathcal{A}(t)=\left\langle\begin{bmatrix}q_1-\langle q_1(t)\rangle\\ \vdots\\ q_n-\langle q_n(t)\rangle\\ p_1-\langle p_1(t)\rangle\\ \vdots\\ p_n-\langle p_n(t)\rangle\end{bmatrix}[q_1-\langle q_1(t)\rangle,\ldots,q_n-\langle q_n(t)\rangle,p_1-\langle p_1(t)\rangle,\ldots,p_n-\langle p_n(t)\rangle]\right\rangle \tag{21}$$

$$=\theta e^{tD}A(t)e^{tD}\theta^T=2T\int_0^t d\tau\, e^{(t-\tau)\mathcal{D}}\begin{bmatrix}0 & 0\\ 0 & \beta\end{bmatrix}e^{(t-\tau)\mathcal{D}^T}. \tag{22}$$

Eventually, the full distribution function reads

$$W(q_1,\ldots,p_n,t;q_{10},\ldots,p_{n0})=\frac{1}{(2\pi)^n}\frac{1}{\sqrt{\det\mathcal{A}(t)}}\exp\left(-\frac{1}{2}[q_1-\langle q_1(t)\rangle,\ldots,p_n-\langle p_n(t)\rangle]\mathcal{A}^{-1}(t)\begin{bmatrix}q_1-\langle q_1(t)\rangle\\ \vdots\\ p_n-\langle p_n(t)\rangle\end{bmatrix}\right), \tag{23}$$

after renormalization with the Jacobian. This result is well known; see, e.g., [2].

C. Probability of passing over the saddle

To evaluate the probability of passing over the barrier, we are interested in the ''reduced'' distribution obtained when all degrees of freedom but q_1 are integrated out. It is also necessarily a Gaussian distribution

$$W(q_1,t;q_{10},\ldots,q_{n0},p_{10},\ldots,p_{n0})$$

$$=\frac{1}{\sqrt{2\pi}\sigma_{q_1}(t)}\exp\left[-\frac{(q_1-\langle q_1(t)\rangle)^2}{2\,\sigma_{q_1}^2(t)}\right]. \tag{24}$$

The only remaining task is then to evaluate $\langle q_1(t)\rangle$ and $\sigma_{q_1}(t)$. From Eqs. (20), (22) one gets

$$\langle q_1(t)\rangle = \theta_{11}X_{10}e^{a_1t} + \cdots + \theta_{1(2n)}X_{(2n)0}e^{a_{2n}t} \quad (25)$$

and

$$\sigma_{q_1}^2(t) = \langle(\theta_{11}x_1e^{a_1t} + \cdots + \theta_{1(2n)}x_{2n}e^{a_{2n}t})^2\rangle \quad (26)$$

$$= \sum_{i=1}^{2n}\sum_{j=1}^{2n}\theta_{1i}\theta_{1j}A_{ij}(t)e^{(a_i+a_j)t}$$

$$= \sum_{i=1}^{2n}\sum_{j=1}^{2n}\theta_{1i}\frac{e^{(a_i+a_j)t}-1}{a_i+a_j}\theta_{1j}(\alpha\alpha^T)_{ij} \quad (27)$$

$$= 2T\sum_{i=1}^{2n}\sum_{j=1}^{2n}\theta_{1i}\frac{e^{(a_i+a_j)t}-1}{a_i+a_j}$$

$$\times \theta_{1j}\sum_{v=1}^{n}\sum_{w=1}^{n}(\theta^{-1})_{i,n+v}\beta_{vw}(\theta^{-1})_{i,n+w}. \quad (28)$$

To go further and do more physics, one needs the eigenvalues and the eigenvectors of the DM. This is not always feasible analytically for any dimension. However, the previous scheme can be applied to particular problems where the drift matrix is explicitly known. Let us first consider the 1D and the 2D cases, for which some general features will be shown.

III. ONE DIMENSION PROBLEM

The 1D approach is interesting because of its simplicity. Intuitively, choosing as unique variable, the valley one and averaging all over the others should be enough in a first approximation. In this approach, the DM can be easily diagonalized and the diffusion energetical condition, time, and probability can be easily calculated.

A. Solution of the Langevin equation

There are only one mass and one random force, m_1 and R_1, respectively. The latter is related to one random number ν_1, normalized according to Eq. (9). The corresponding matrix Γ boils down to one number only, which, according to the fluctuation-dissipation theorem, reads $\Gamma=(2\beta_1T/m_1)^{-1/2}$. The eigenvalues of the DM are $a=(\beta_1'-\beta_1)/2$ and $b=-(\beta_1'+\beta_1)/2$, with $\beta_1'=(\beta_1^2+4\omega_1^2)^{1/2}$. Note that $a>0$ and $b<0$. The matrix θ and its inverse read

$$\theta=(\beta_1')^{-1}\begin{bmatrix}1 & -1\\ (\beta_1'-\beta_1)/2 & (\beta_1'+\beta_1)/2\end{bmatrix},$$

$$\theta^{-1}=\begin{bmatrix}(\beta_1'+\beta_1)/2 & 1\\ (\beta_1-\beta_1')/2 & 1\end{bmatrix}. \quad (29)$$

The matrix $\alpha=\theta^{-1}\begin{bmatrix}0\\\Gamma\end{bmatrix}$ is thus

$$\alpha=(2T\beta_1/m_1)^{1/2}\begin{bmatrix}1\\1\end{bmatrix}. \quad (30)$$

The eigencoordinates read, with $p_1=\dot{q}_1$

$$\begin{bmatrix}X\\Y\end{bmatrix}=\begin{bmatrix}(\beta_1'+\beta_1)/2 & 1\\ (\beta_1-\beta_1')/2 & 1\end{bmatrix}\begin{bmatrix}q_1\\p_1\end{bmatrix}. \quad (31)$$

The Euler type variables, x and y, are then defined as

$$x(t)=Xe^{-at}-X_0,$$
$$y(t)=Ye^{-bt}-Y_0, \quad (32)$$

and their statistical properties must be the same as those of

$$(2T\beta_1/m_1)^{1/2}\left(\int_0^t d\tau\, e^{-a\tau}\nu_1(\tau), \int_0^t d\tau\, e^{-b\tau}\nu_1(\tau)\right), \quad (33)$$

see Eqs. (14),(15). The random number $\nu_1(t)$ being Gaussian, x and y are also Gaussian random variables, with

$$\langle x^2(t)\rangle = \frac{T\beta_1}{am_1}(1-e^{-2at}), \quad \langle y^2(t)\rangle = \frac{T\beta_1}{bm_1}(1-e^{-2bt}),$$

$$\langle x(t)y(t)\rangle = \frac{2T\beta_1}{(a+b)m_1}[1-e^{-(a+b)t}], \quad (34)$$

see Eq. (16).

To evaluate the probability for passing over the barrier, one needs the following distribution function, necessarily a Gaussian in the present model:

$$W(q_1,t;q_{10},p_{10}) = \frac{1}{\sqrt{2\pi}\sigma_{q_1}(t)}\exp-\frac{[q_1-\langle q_1(t)\rangle]^2}{2\sigma_{q_1}^2(t)}. \quad (35)$$

According to the first row of θ, see Eq. (29), the valley coordinate is, in terms of the eigencoordinates,

$$q_1 = \frac{1}{\beta_1'}(xe^{at}-ye^{bt}) + \frac{1}{\beta_1'}(X_0e^{at}-Y_0e^{bt}). \quad (36)$$

The first part corresponds to the diffusion and the second one to the average trajectory. It is trivial to obtain X_0 and Y_0 from q_{10} and p_{10} according to Eq. (31), hence $\langle q_1\rangle$. It is also trivial to obtain $\langle q_1^2\rangle$ from Eq. (34). All told, elementary manipulations yield

$$\langle q_1(t)\rangle = q_{10}e^{-\beta_1t/2}\left[\cosh\left(\frac{1}{2}\beta_1't\right) + \frac{\beta_1}{\beta_1'}\sinh\left(\frac{1}{2}\beta_1't\right)\right]$$

$$+ 2\frac{p_{10}}{\beta_1'}e^{-\beta_1t/2}\sinh\left(\frac{1}{2}\beta_1't\right), \quad (37)$$

and

$$\sigma_{q_1}^2(t) = \langle q_1^2 \rangle - \langle q_1 \rangle^2$$

$$= -\frac{T}{m_1 \omega_1^2} \left\{ 1 - e^{-\beta_1 t} \left[2\frac{\beta_1^2}{\beta_1'^2} \sinh^2 \left(\frac{1}{2}\beta_1' t \right) \right. \right.$$

$$\left. \left. + \frac{\beta_1}{\beta_1'} \sinh(\beta_1' t) + 1 \right] \right\}. \tag{38}$$

These results are in agreement with the well-known calculation done for harmonically bound particles [3,4], where the sign of the spring force should be changed.

B. The critical initial kinetic energy

Defining the critical energy as the kinetic energy, $K = \frac{1}{2}m_1 p_{10}^2$, necessary to have half of the particles to pass over the barrier, it is obvious that it corresponds to $\lim_{t \to +\infty} \langle q_1(t) \rangle = 0$. From Eq. (37) it can be easily shown that

$$K_c = \left(\frac{\beta_1 + \beta_1'}{2\omega_1} \right)^2 B, \tag{39}$$

where $B = m_1 \omega_1^2 q_{10}^2/2$ is the barrier height. In the weak friction limit, $\beta_1 \simeq 0$, this condition becomes $K_c = B$ which is a trivial result. In the overdamped limit, $\beta_1 \gg 2\omega_1$, it becomes $K_c = (\beta_1/\omega_1)^2 B$.

In the case of nuclei, using typical values, $\hbar \omega_1 = 1 MeV$ and $\beta_1 = 5.10^{21} s^{-1}$, the overdamped limit is usually a good approximation and a big kinetic energy is necessary to overpass even a very small barrier. $K_c \simeq 10B$.

C. Diffusion time

As for many physical problems the diffusion process dynamically competes with some other processes, it is interesting to extract also the time necessary to reach the top of the potential barrier. When the previous condition, Eq. (39), is exactly fulfilled, then

$$\langle q_1(t) \rangle = q_{10} e^{-[(\beta_1 + \beta_1')/2]t}. \tag{40}$$

The average trajectory exponentially converges to the top of the barrier with a typical time equal to $2/(\beta_1 + \beta_1')$, which becomes $1/\omega_1$ in the weak damping limit and $1/\beta_1$ in the overdamped one.

When the initial kinetic energy is higher than the critical one, Eq. (39), the average trajectory reaches the top of the potential barrier at t_{top} such as

$$\coth\left(\frac{1}{2}\beta_1' t_{top} \right) = \frac{2\omega_1}{\beta_1'} \left(\sqrt{\frac{K}{B}} - \frac{\beta_1}{2\omega_1} \right). \tag{41}$$

The previous equation becomes

$$\coth(\omega_1 t_{top}) = \sqrt{\frac{K}{B}} \tag{42}$$

in the weak damping case,

$$\coth\left(\frac{1}{2}\beta_1 t_{top} \right) = \left(\frac{2\omega_1}{\beta_1} \sqrt{\frac{K}{B}} - 1 \right) \tag{43}$$

in the overdamped one.

D. Passing probability

In this model the probability at a given time that the particle has passed over the barrier is simply

$$P(t;q_{10},p_{10}) = \int_0^{+\infty} W(q_1,t;q_{10},p_{10}) dq_1 \tag{44}$$

$$= \frac{1}{2} \mathrm{erfc}\left(-\frac{\langle q_1(t) \rangle}{\sqrt{2}\sigma_{q_1}(t)} \right). \tag{45}$$

For large times $(t \gg 1/\beta_1')$,

$$-\frac{\langle q_1 \rangle}{\sqrt{2}\sigma_{q_1}} \to \frac{\beta_1 + \beta_1'}{\sqrt{2(\beta_1^2 + \beta_1 \beta_1')}} \left[\sqrt{\frac{B}{T}} - \frac{2\omega_1}{\beta_1 + \beta_1'} \sqrt{\frac{K}{T}} \right] \tag{46}$$

$$\to \sqrt{\frac{\omega_1}{T\beta_1}} (\sqrt{B} - \sqrt{K}) \tag{47}$$

in the underdamped limit,

$$\to \sqrt{\frac{B}{T}} - \frac{\omega_1}{\beta_1} \sqrt{\frac{K}{T}} \tag{48}$$

in the overdamped one. The passing probability is then known as a function of the initial kinetic energy and the temperature. It increases from 0 to 1 around the critical value K_c when increasing the initial kinetic energy. The higher the temperature, the smoother is this increase.

E. Heavy-ion fusion

When two nuclei are colliding, the kinetic energy of the projectile should be higher than the contact energy derived by Bass [10] to observe some fusion events. This so-called extra-push energy is generally interpreted as an additional barrier due to nuclear forces that has to be overcome by the viscous nuclear matter [11]. The critical energy derived above can then be seen as the extra-push energy here.

To calculate the fusion probability of two cold colliding nuclei, the difficulty is then to evaluate the temperature. For particles that can reach the barrier top, at a distance R_{12}, we will assume that all the remaining energy is totally dissipated. Therefore, with a level density a_{lev}, we assume that $a_{lev} T^2 = K - B$, neglecting the collective kinetic energy. Then the fusion probability is

$$P(q_{10},p_{10}) = \frac{1}{2}\mathrm{erfc}\left[\left(\frac{a_{lev}B^2}{K-B} \right)^{1/4} \right.$$

$$\left. \times \frac{\beta_1 + \beta_1'}{\sqrt{2(\beta_1^2 + \beta_1 \beta_1')}} \left(1 - \frac{2\omega_1}{\beta_1 + \beta_1'} \sqrt{\frac{K}{B}} \right) \right]. \tag{49}$$

In this formula, K is the available kinetic energy when the two nuclei are in contact, and B is the remaining barrier height:

$$K = E_{\text{c.m.}} - E_{\text{rot}} - B_{\text{Bass}}. \qquad (50)$$

In this equation, B_{Bass} is the Bass barrier [10] and E_{rot} is the rotational energy, $E_{\text{rot}} = E_{\text{c.m.}} b_{\text{imp}}^2 / R_{12}^2$, where b_{imp} is the impact parameter.

Therefore, the fusion probability reads

$$P(E_{\text{c.m.}}, b) = \frac{1}{2} \text{erfc} \left[\left(\frac{a_{\text{lev}} B^2}{E_{\text{c.m.}}(1 - b_{\text{imp}}^2/R_{12}^2) - B_{\text{Bass}} - B} \right)^{1/4} \right.$$

$$\times \frac{\beta_1 + \beta_1'}{\sqrt{2(\beta_1^2 + \beta_1 \beta_1')}} \left(1 - \frac{2\omega_1}{\beta_1 + \beta_1'} \right)$$

$$\times \left. \sqrt{\frac{E_{\text{c.m.}}(1 - b_{\text{imp}}^2/R_{12}^2) - B_{\text{Bass}}}{B}} \right]. \qquad (51)$$

To compare this probability with other theoretical calculations, we need to choose parameters specific to our problem and deduce the potential and dissipation terms. The present paper being rather dedicated to a good qualitative understanding of the Langevin model, numerics with realistic parameters will be kept for a future paper. However, numerical simulations already available seem to indicate that at least two dimensions are necessary to really have a good understanding of the diffusion phenomena in this problem [8].

IV. THE TWO-DIMENSIONAL MODEL

Passing probability

Choosing q_1 as the valley variable, the associated distribution function $W(q_1, t; q_{10}, q_{20}, p_{10}, p_{20})$ is a Gaussian and the probability at a given time to pass over the saddle reads

$$P(t; q_{10}, q_{20}, p_{10}, p_{20}) = \int_0^{+\infty} W(q_1, t; q_{10}, q_{20}, p_{10}, p_{20}) dq_1 \qquad (52)$$

$$= \frac{1}{2} \text{erfc} \left(-\frac{\langle q_1(t) \rangle}{\sqrt{2} \sigma_{q_1}(t)} \right). \qquad (53)$$

The difficulty is then to find $\langle q_1(t) \rangle$ and $\sigma_{q_1}(t)$, see Eqs. (25) and (27). When the two degrees of freedom are uncorrelated, namely, when $\beta_{12} = 0$, the eigenvalues of the DM are, obviously,

$$a_1 = (-\beta_1 + \sqrt{\beta_1^2 + 4\omega_1^2})/2,$$
$$a_2 = (-\beta_1 - \sqrt{\beta_1^2 + 4\omega_1^2})/2,$$
$$a_3 = (-\beta_2 + \sqrt{\beta_2^2 - 4\omega_2^2})/2,$$
$$a_4 = (-\beta_2 - \sqrt{\beta_2^2 - 4\omega_2^2})/2,$$

or   (54)

$$a_1 = (-\beta_1 + \sqrt{\beta_1^2 + 4\omega_1^2})/2,$$
$$a_2 = (-\beta_1 - \sqrt{\beta_1^2 + 4\omega_1^2})/2,$$
$$a_3 = (-\beta_2 + i\sqrt{-\beta_2^2 + 4\omega_2^2})/2,$$
$$a_4 = (-\beta_2 - i\sqrt{-\beta_2^2 + 4\omega_2^2})/2,$$

if $\omega_2 < \beta_2/2$ or $\omega_2 > \beta_2/2$, respectively. Note that only a_1 is positive, the other eigenvalues are negative or have a negative real part.

When $\beta_{12} \neq 0$, it is easy to show that there are always two real roots. The first one a_1 is positive and increasing as a function of β_{12}. The other one a_4 is negative and decreasing as a function of the same. When the other two roots are real, it is also trivial to show that they remain negative. For large values of β_{12}, which start reaching significant fractions of that maximum $(\beta_1 \beta_2)^{1/2}$, which is acceptable for a semipositivity of friction, the other two roots may become complex conjugate. But the statement $\text{Re}(a_i) < 0$ for $i > 1$, is still true. To illustrate the behavior of the eigenvalues, we consider the special case where $\beta_1 = \beta_2 = 1$ and $\omega_1 = \omega_2 = \omega$. The equal diagonal viscosities being taken as a unit, the polynomial equation whose roots are the eigenfrequencies of the problem reads

$$a^4 + 2a^3 + a^2 - \omega^4 = \beta_{12}^2 a^2. \qquad (55)$$

Figure 1 shows, when β_{12} increases from 0 to 1, the graphs of the four roots, or of their real parts when some of them become complex. Here $\omega = 0.35$, which corresponds to overdamping at the beginning, when $\beta_{12} = 0$. The merging of the two intermediate roots and their complexification are transparent. Once such roots have become complex conjugate, their common real part, however, remains negative. Then Fig. 2 shows the case $\omega = 0.6$, where the two intermediate roots are always complex, with a negative, common real part.

Hence, when $t \to \infty$, only the "a_1 mode" survives. The leading terms in Eqs. (25) and (27) for long times are

$$\langle q_1(t) \rangle = \theta_{11} X_{10} e^{a_1 t}, \quad \sigma_{q_1}^2(t) = \frac{\theta_{11}^2 e^{2a_1 t} (\alpha \alpha^T)_{11}}{2a_1}. \qquad (56)$$

The result for $t \to \infty$ reads

$$P(q_{10}, q_{20}, p_{10}, p_{20}) \to \frac{1}{2} \text{erfc} \left(-\frac{X_{10}}{\sqrt{2\bar{A}_{11}}} \right),$$

$$\bar{A}_{11} = (\alpha \alpha^T)_{11}/(2a_1). \qquad (57)$$

It is similar to the result obtained in 1D, provided we choose the proper coordinate

$$X_1 = \omega_1^2 q_1 + a_1 p_1 - \beta_{12} \frac{a_1}{\omega_2^2 + a_1^2 + \beta_2 a_1} (-\omega_2^2 q_2 + a_1 p_2). \qquad (58)$$

The condition to have half of the particles to overpass the barrier is then $X_{10} = 0$. When the two degrees of freedom are uncorrelated ($\beta_{12} = 0$), one gets the same condition as in one dimension, Eq. (39). But in general, it is not possible to
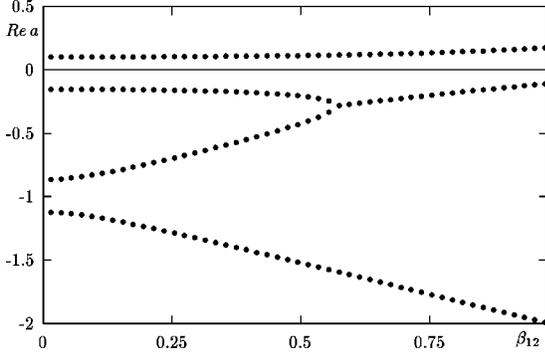
FIG. 1. Real part of eigenvalues as functions of nondiagonal friction. Overdamped regime, $\omega = 0.35 < \beta/2 = 0.5$. Notice how two real roots fuse, then become complex conjugate, to generate one branch instead of two.
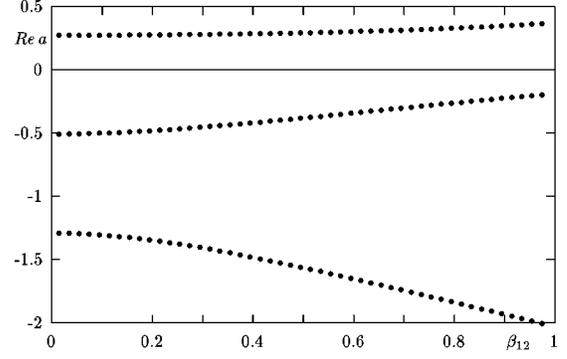

FIG. 2. Real parts of eigenvalues as functions of nondiagonal friction. Underdamped regime, $\omega = 0.6 > \beta/2 = 0.5$. Since two eigenvalues are complex conjugate, only three curves appear.

simply express it in terms of the initial kinetic energy because it also depends on the orientation of the initial velocity in the potential landscape. For the same reasons, the diffusion time is not easy to evaluate either.

Note that in the previous graphs (Figs. 1 and 2), a_1 is almost constant and could be approximated by the value given in Eqs. (54).

Then we can evaluate $\bar{A}_{11}$,

$$\bar{A}_{11} = \frac{T}{a_1} [\beta_1 (\theta^{-1})_{13}^2 + \beta_2 (\theta^{-1})_{14}^2 + 2\beta_{12} (\theta^{-1})_{13} (\theta^{-1})_{14}],$$
(59)

provided the diagonalization of the drift matrix can be done. Note that only $(\theta^{-1})_{13}$ and $(\theta^{-1})_{14}$ occurs, which are coupling X_1 with the velocity coordinates p_1 and p_2. From Eq. (58), one gets

$$\bar{A}_{11} = T a_1 \left(\beta_1 - \beta_{12}^2 a_1^2 \frac{2\omega_2^2 + 2a_1^2 + \beta_2 a_1}{(\omega_2^2 + a_1^2 + \beta_2 a_1)^2} \right).$$
(60)

Again, when the two degrees of freedom are uncorrelated ($\beta_{12} = 0$), one gets the same probability as in one dimension, Eqs. (45) and (46).

V. CONCLUSION

In this paper, we showed a general scheme to solve multidimensional Langevin equations near a saddle point. In one dimension, the solution is very simple and the diffusion condition, time, and probability can be easily expressed. This means that in the case of a simple one dimension model for heavy-ion fusion, one can analytically estimate the extra-push energy, the fusion time and its probability.

For higher dimensions, the stochastic dynamics is again easily solved, but a difficulty remains, namely, the explicit diagonalization of the drift matrix. In such conditions, a general analytic solution cannot be written, but the main features we found could be easily applied to very specific physical problems. In particular, we showed the difference between the dominant degree of freedom and the damped ones. The possible occurrence of complex eigenvalues corresponds to residual oscillations in subdominant degrees.

In every case, the Gaussian solution to the problem contradicts the naive, intuitive expectation of a distribution with two peaks moving apart from the fusion barrier. In fact, the way over the barrier simply results from a competition between the drift of the center of the Gaussian and its spreading.

For exotic noises leading to anomalous diffusion, such as Lévy flights, the Langevin equation can be analytically solved for a one-dimensional overdamped motion where the Langevin equation reduces to a Smoluchowski one. In that case, the solution is given in Ref. [5].

APPENDIX A

In order to avoid possible confusion brought by the three successive changes of representation expressed by the matrices $M^{-1/2}$, U, and θ, we prove again the well-known fluctuation-dissipation theorem. Our precise purpose is to parametrize the random force R, see Eq. (3), in terms of dimensionless, independent random numbers ν_i, normalized to unity, see Eq. (9). The starting point is a simplified form of Eq. (4), namely, a situation where just the friction and the random force are present,

$$M\ddot{Z} + \mathcal{G}\dot{Z} = \mathcal{F}(t).$$
(A1)

This leads at once to a simplified form of Eq. (5),

$$M^{1/2}\ddot{Z} + M^{-1/2}\mathcal{G}M^{-1/2}M^{1/2}\dot{Z} = M^{-1/2}\mathcal{F}(t).$$
(A2)

It is convenient at this stage to diagonalize the real, symmetric, positive definite matrix $\mathcal{B} \equiv M^{-1/2}\mathcal{G}M^{-1/2}$, and obtain its representation in terms of its eigenvectors $|i\rangle$ and eigenvalues λ_i,

$$\mathcal{B} = \sum_{i=1}^{n} |i\rangle \lambda_i \langle i|.$$
(A3)

This decouples Eq. (A2) into independent modes, relaxing separately towards thermal equilibrium for large times,

$$\langle i|M^{1/2}\ddot{Z}\rangle = -\lambda_i\langle i|M^{1/2}\dot{Z}\rangle + \langle i|M^{-1/2}\mathcal{F}(t)\rangle, \quad \text{(A4)}$$

namely,

$$\langle i|M^{1/2}\dot{Z}\rangle \rightarrow_{t\rightarrow+\infty} \int_0^t d\tau\, e^{-\lambda_i(t-\tau)}\langle i|M^{-1/2}\mathcal{F}(\tau)\rangle. \quad \text{(A5)}$$

The left-hand side of this limit, Eq. (A5), can now be squared as a kinetic energy and then ensemble averaged to be equated with the Boltzmann energy $T = (\langle i|M^{1/2}\dot{Z}\rangle)^2$. (We set the Boltzmann constant as a unit, $k = 1$, as usual.) The right-hand side of Eq. (A5), in turn, can be constrained by the following ansatz for ensemble averaging

$$\overline{\langle i|M^{-1/2}\mathcal{F}(\tau)\rangle\langle i|M^{-1/2}\mathcal{F}(\tau')\rangle} = \rho_i\delta(\tau-\tau'), \quad \text{(A6)}$$

where ρ_i is an unknown normalization. The square of the right-hand side of Eq. (A5) thus becomes

$$\rho_i\int_0^{t\rightarrow\infty} d\tau\, e^{-2\lambda_i(t-\tau)} = \frac{\rho_i}{2\lambda_i}, \quad \text{(A7)}$$

hence the normalization result, $\rho_i = 2T\lambda_i$. Let Λ be the diagonal matrix defined by the square roots $(2T\lambda_i)^{1/2}$ of such normalizations ρ_i. Let $\mathcal{U}$ be that orthogonal matrix which lists the eigenvectors $|i\rangle$ as columns. Let $\nu \equiv \{\nu_1, \ldots, \nu_n\}$ be a column vector of normalized, Gaussian, independent random numbers. Since our fluctuation-dissipation theorem states that $M^{-1/2}\mathcal{F} = \sum_{i=1}^n |i\rangle(T\lambda_i)^{1/2}\nu_i = \mathcal{U}\Lambda\nu$, the stochastic force R present in Eq. (3) reads $R = \Gamma\nu$, with $\Gamma = U^{-1}\mathcal{U}\Lambda$. This explains why Γ is not expected to be symmetric. Eventually, the fluctuation-dissipation can be written in a more classical way,

$$\Gamma\Gamma^T = 2T\beta, \quad \text{(A8)}$$

where $\beta = U^{-1}M^{-1/2}\mathcal{G}M^{-1/2}U$ is the reduced friction matrix.

APPENDIX B

The solution of multidimensional Langevin equations is shown here for Markovian noises. Using the fact that the Euler type variables $(x_1, \ldots, x_{2n})$ have the same statistical properties as those of Eq. (15), we find

$$W(x_1, \ldots, x_{2n}, t; X_{10}, \ldots, X_{2n0})$$

$$= \langle \delta[x_1 - x_1(t)] \cdots \delta[x_{2n} - x_{2n}(t)]\rangle, \quad \text{(B1)}$$

$$= \int \frac{dk_1}{2\pi} \cdots \frac{dk_{2n}}{2\pi}$$

$$\times \left\langle \exp\left(i[k_1, \ldots, k_{2n}] \begin{bmatrix} x_1 - x_1(t) \\ \vdots \\ x_{2n} - x_{2n}(t) \end{bmatrix} \right) \right\rangle, \quad \text{(B2)}$$

where the $x_i(t)$'s are shown in Eq. (14). The time integral will be discretized, with $\delta\tau = t/L$,

$$\begin{bmatrix} x_1(t) \\ \vdots \\ x_{2n}(t) \end{bmatrix} = \int_0^t d\tau\, e^{-\tau D}\alpha \begin{bmatrix} \nu_1(\tau) \\ \vdots \\ \nu_n(\tau) \end{bmatrix}$$

$$= \lim_{L\rightarrow\infty} \sum_{\ell=1}^L e^{-(\ell-1/2)\delta\tau D}\alpha \begin{bmatrix} \nu_1(\delta\tau) \\ \vdots \\ \nu_n(\delta\tau) \end{bmatrix}. \quad \text{(B3)}$$

Here, D is the diagonal drift matrix, see Eq. (12) and $\nu_j(\delta\tau) = \int_{(\ell-1)\delta\tau}^{\ell\delta\tau} d\tau\,\nu_j(\tau)$ are the results of random walks in the force space during the time interval $\delta\tau$. Then the distribution function can be evaluated in its Fourier space, using the statistical properties of such random walks,

$$W(x_1, \ldots, x_{2n}, t; X_{10}, \ldots, X_{(2n)0})$$

$$= \int \frac{dk_1}{2\pi} \cdots \frac{dk_{2n}}{2\pi} \exp\left(i[k_1, \ldots, k_{2n}] \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \right)$$

$$\times p(k_1, \ldots, k_{2n}, t), \quad \text{(B4)}$$

with

$$p(k_1, \ldots, k_{2n}, t) = \lim_{L\rightarrow\infty} \prod_{\ell=1}^L \left\langle \exp\left(-i[k_1, \ldots, k_{2n}] \right. \right.$$

$$\left. \left. \times e^{-(\ell-1/2)\delta\tau D}\alpha \begin{bmatrix} \nu_1(\delta\tau) \\ \vdots \\ \nu_n(\delta\tau) \end{bmatrix} \right) \right\rangle. \quad \text{(B5)}$$

We have used the fact that the random numbers are Markovian to say that the average of a product is the product of the averages of its factors.

In the case of a Gaussian noise, the distribution function of the random numbers reads

$$p(\nu_1, \ldots, \nu_n) = \frac{1}{\sqrt{(2\pi)^n}} \exp\left(-\frac{1}{2}[\nu_1, \ldots, \nu_n] \begin{bmatrix} \nu_1 \\ \vdots \\ \nu_n \end{bmatrix} \right) \quad \text{(B6)}$$

and, due to their Markovian properties, their integration over a time step $\delta\tau$ leads to

$$p[\nu_1(\delta\tau), \ldots, \nu_n(\delta\tau)]$$

$$= \frac{1}{\sqrt{(2\pi\delta\tau)^n}}$$

$$\times \exp\left(-\frac{1}{2\delta_\tau}[\nu_1(\delta\tau), \ldots, \nu_n(\delta\tau)] \right.$$

$$\left. \times \begin{bmatrix} \nu_1(\delta\tau) \\ \vdots \\ \nu_n(\delta\tau) \end{bmatrix} \right). \quad \text{(B7)}$$

Therefore,

$$p(k_1, \ldots, k_{2n}, t)$$

$$= \lim_{L \to \infty} \prod_{\ell=1}^{L} \exp\left(-\frac{\delta\tau}{2}[k_1, \ldots, k_{2n}] \right.$$

$$\left. \times e^{-(\ell-1/2)\delta\tau D}\alpha\alpha^T e^{-(\ell-1/2)\delta\tau D} \begin{bmatrix} k_1 \\ \vdots \\ k_{2n} \end{bmatrix} \right).$$

(B8)

Reintroducing the time integral, one obtains

$$p(k_1, \ldots, k_{2n}, t)$$

$$= \exp\left(-\frac{1}{2}[k_1, \ldots, k_{2n}]A \begin{bmatrix} k_1 \\ \vdots \\ k_{2n} \end{bmatrix} \right), \quad (B9)$$

where the matrix A is defined by Eq. (17). Inverting the Fourier transform, upon $p(k_1, \ldots, k_{2n}, t)$, one eventually gets

$$W(x_1, \ldots, x_{2n}, t; X_{10}, \ldots, X_{(2n)0})$$

$$= \frac{1}{(2\pi)^n} \frac{1}{\sqrt{\det A}} \exp\left(-\frac{1}{2}[x_1, \ldots, x_{2n}]A^{-1} \begin{bmatrix} x_1 \\ \vdots \\ x_{2n} \end{bmatrix} \right).$$

(B10)

For Lévy flights, we will restrict ourselves to a one dimension problem. The noise is defined by its characteristic function $p(k)$ in the Fourier space

$$p(k) = \int d\nu \, e^{-ik\nu} p(\nu) = \exp[-\Delta|k|^\mu], \quad (B11)$$

and is the source of an anomalous behavior characterized by a mean square displacement of the form $\langle\sigma_q(t)\rangle \propto 2\Delta t^\gamma$ [12]. As the fluctuation-dissipation theorem is not satisfied any more, we keep a generalized diffusion coefficient, Δ. For the special case $\mu = 2$, the noise is Gaussian. Similarly to the Gaussian case, the integration over a time step $\delta\tau$ leads to

$$p'(k) = \int d\nu(\delta\tau) e^{-ik\nu(\delta\tau)} p[\nu(\delta\tau)]$$

$$= \exp[-\Delta(\delta\tau)^{1-\mu}|k|^\mu], \quad (B12)$$

after renormalization [13]. Therefore, the average value in the right-hand side of Eq. (B5) can be calculated as

$$\langle \exp[-i\delta\tau\nu_i(\delta\tau)(k_1 e^{-a(\ell-1/2)\delta\tau} + k_2 e^{-b(\ell-1/2)\delta\tau})]\rangle$$

$$= \exp[-\Delta\delta\tau(k_1 e^{-a(\ell-1/2)\delta\tau} + k_2 e^{-b(\ell-1/2)\delta\tau})^\mu].$$

(B13)

Reintroducing the time integral, one finally gets

$$p(k_1, k_2, t) = \exp\left[-\Delta \int_0^t (k_1 e^{-a\tau} + k_2 e^{-b\tau})^\mu d\tau \right].$$

(B14)

For $\mu = 2$, i.e., in the Gaussian case, the time integral can be evaluated analytically, but such is not the case for any value of μ. The only favorable situation occurs for a one-dimensional Smoluchowski equation where

$$p(k_1, t) = \exp\left(-\Delta \int_0^t k_1^\mu e^{-a\mu\tau} d\tau \right), \quad (B15)$$

see Ref. [5]. This is why we restrict our study to classical Gaussian noises.

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