Normalized Gaussian path integrals

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Path integrals play a crucial role in describing the dynamics of physical systems subject to classical or quantum noise. In fact, when correctly normalized, they express the probability of transition between two states of the system. In this work, we show a consistent approach to solve conditional and unconditional Euclidean (Wiener) Gaussian path integrals that allow us to compute transition probabilities in the semiclassical approximation from the solutions of a system of linear differential equations. Our method is particularly useful for investigating Fokker-Planck dynamics and the physics of stringlike objects such as polymers. To give some examples, we derive the time evolution of the d-dimensional Ornstein-Uhlenbeck process and of the Van der Pol oscillator driven by white noise. Moreover, we compute the end-to-end transition probability for a charged string at thermal equilibrium, when an external field is applied.

I. INTRODUCTION

Path integrals are an essential tool in many branches of physics and mathematics [1–5]. Originally introduced by Wiener as a method to study Brownian motion [6,7], their formalism was significantly developed by Feynman in the context of quantum mechanics [8,9]. Since then, path integrals have revealed themselves to be a powerful method for the investigation of systems subject to classical or quantum fluctuations and therefore have a plethora of different applications.

In many relevant situations one is interested in evaluating transition (i.e., conditional) probabilities, namely, the probability for a system to be in a specific final state, given its initial state. Path integrals are precisely tailored to answer such questions by expressing transition probabilities as an infinite weighted sum over all possible trajectories passing through both states. Typical examples where this formulation arises naturally include the stochastic motion of particles in diffusion processes and the dynamics of quantum particles and fields.

It is worth emphasizing that the "paths" entering a path integral do not need to be the trajectories of a moving particle, but they can also be the stationary configurations of stringlike objects [10–13]. In this context, transition probabilities represent the probability of finding the string's endpoints in specific positions. This observation turns out to be extremely useful for the study of organic and inorganic polymers at thermal equilibrium, such as chains of molecules (e.g., DNA, actin filaments) and flexible rods [14–17].

Despite their intuitive interpretation, path integrals are in general difficult to compute. Among several different strate-

gies to circumvent this issue, the semiclassical (quadratic) approximation is one of the most adopted [18–20]. In brief, the idea consists of approximating the weights for the paths so that a Gaussian integral is obtained. The solution is then straightforward for conditional path integrals (where both extremal points are fixed), while it often remains nontrivial for the unconditional case (where only the starting point is fixed). Addressing this remaining problem is of special interest for expressing transition probability distributions that are properly normalized.

Here we focus on Euclidean (Wiener) path integrals and propose a consistent method to compute from them transition probabilities in the semiclassical approximation. Our approach is based on the generalization of a result by Papadopoulos [21], which allows us to evaluate both conditional and unconditional path integrals for general quadratic Lagrangians, from the solutions of the Euler-Lagrange equations and of a system of second-order nonlinear differential equations. Furthermore, we then show that the latter can be related to a simpler system of linear differential equations by exploiting a link with the Jacobi equation. Interestingly, our study also sheds light on the relation between the choice for the discretization of continuous paths and the path integral measure.

Our results are of interest for studying the dynamics of stochastic processes, such as the one described by the Fokker-Planck equation, and for investigating equilibrium configurations of stringlike objects. This is illustrated here with three concrete examples. First, we show how to recover the transition probability for a d-dimensional Ornstein-Uhlenbeck process [22–24]. Second, we investigate the nonlinear Van der Pol oscillator driven by white noise, for which transition probabilities are not known analytically due to its chaotic dynamics [25]. Third, we compute in one spatial dimension the end-to-end transition probability for an elastic and

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electrically charged string at thermal equilibrium, when an external electric field is applied.

II. STATEMENT OF THE PROBLEM AND MAIN RESULTS

Consider a system in configuration $q(\tau) \in \mathbb{R}^d$, whose dynamics is described by the Lagrangian $\mathcal{L}(q, \dot{q}, \tau)$. Our goal is to calculate the transition probability for the system of being in the final state $q(t) = q$, given its initial state $q(t_0) = q_0$, namely, the conditional probability $\rho(q, t|q_0, t_0)$ satisfying $\rho(q, t_0|q_0, t_0) = \delta(q - q_0)$. A prescription for this calculation is given by the path integral formalism, which allows us to write

$$\rho(q, t|q_0, t_0) := \frac{\mathcal{K}}{\mathcal{N}} = \frac{1}{\mathcal{N}} \int_{q(t_0)=q_0}^{q(t)=q} \mathcal{D}q \, e^{-S(q,\dot{q})}, \quad (1)$$

where the (conditional) integration is taken over all paths with fixed extremal points, weighted depending on the action $S(q, \dot{q}) := \int_{t_0}^{t} d\tau \, \mathcal{L}(q, \dot{q}, \tau)$, and normalized by $\mathcal{N}$ to ensure

$$\int_{\mathbb{R}^d} \rho(q, t|q_0, t_0) dq = 1, \quad \forall t \geqslant t_0. \quad (2)$$

From Eqs. (1) and (2), we see that the normalization can be formally written as the (unconditional) path integral

$$\mathcal{N} = \int_{q(t_0)=q_0} \mathcal{D}q \, e^{-S(q,\dot{q})}, \quad (3)$$

where now the integral is over all paths satisfying only the initial condition $q(t_0) = q_0$.

For typical cases of interest, we are often in the situation where $\mathcal{L}$ is complicated enough that closed-form solutions for $\mathcal{K}$ and $\mathcal{N}$ do not exist. A standard technique to simplify part of the problem consists of taking the semiclassical approximation, where the action is expanded to second order around an isolated minimum. This allows us to approximate $\mathcal{K}$ by a solvable Gaussian integral, but the evaluation of $\mathcal{N}$ remains nontrivial because of the free boundary condition $q(t)$. The latter difficulty is often circumvented through demanding Monte Carlo integrations or by setting $\mathcal{N} = 1$ and considering in $\mathcal{K}$ an effective (Onsager-Machlup) Lagrangian containing additional terms that ensure normalization [23,26,27]. Our main result consists of solving this problem in a more general situation. In brief, we formulate a consistent approach to solve in the semiclassical approximations both path integrals appearing in Eq. (1), by relating their solutions to the solutions of a system of linear differential equations. The procedure we propose is the following.

As a starting point, in order to ensure the accuracy of the semiclassical approximation, let us restrict to Lagrangian functions where the leading-order term for the second variation of the action, $G(\tau) := \frac{\partial^2 \mathcal{L}}{\partial \dot{q}^2}$, is independent of q and $\dot{q}$. This assumption is still general enough to include most cases of interest. On the other hand, we consider in the second variation arbitrary $V := \frac{\partial^2 \mathcal{L}}{\partial q^2}$, and cross term matrix $A := \frac{\partial^2 \mathcal{L}}{\partial \dot{q} \partial q}$ to not necessarily be symmetric.

Following the idea behind the semiclassical approximation, the first step of our method consists of deriving two solutions from the Euler-Lagrange equations for $\mathcal{L}$:

(i) an isolated minimizer of the action $q^D(\tau)$, satisfying the Dirichlet boundary conditions $q^D(t_0) = q_0$ and $q^D(t) = q$,

(ii) an isolated minimizer $q^N(\tau)$, satisfying $q^N(t_0) = q_0$ and the Neumann natural boundary condition $\frac{\partial \mathcal{L}}{\partial \dot{q}}(t) = 0$.

Then, the second step of our method consists of deriving a set of solutions $W^{D(N)}(\tau)$ of the Jacobi equation for the second variation of the action on the Dirichlet (Neumann) minimum. These can be obtained from the Hamiltonian formulation of the Jacobi equation, together with the appropriate boundary conditions, as solutions of

$$\begin{cases} \dfrac{d}{d\tau}\begin{pmatrix} W^D \\ M^D \end{pmatrix} = JE^D \begin{pmatrix} W^D \\ M^D \end{pmatrix}, \\ \begin{pmatrix} W^D \\ M^D \end{pmatrix}(t) = J \begin{pmatrix} \mathbb{1} \\ \mathbb{0} \end{pmatrix}, \end{cases} \begin{cases} \dfrac{d}{d\tau}\begin{pmatrix} W^N \\ M^N \end{pmatrix} = JE^N \begin{pmatrix} W^N \\ M^N \end{pmatrix}, \\ \begin{pmatrix} W^N \\ M^N \end{pmatrix}(t) = J \begin{pmatrix} \mathbb{0} \\ \mathbb{1} \end{pmatrix}, \end{cases}$$

$$(4)$$

where $M^{D(N)}$ is the conjugate variable under the Legendre transform, $J = \begin{pmatrix} \mathbb{0} & \mathbb{1} \\ -\mathbb{1} & \mathbb{0} \end{pmatrix}$ is the symplectic matrix, and $E^{D(N)}$ is the symmetric matrix driving the system, which reads

$$E^i = \begin{pmatrix} A^T G^{-1} A - V & -A^T G^{-1} \\ -G^{-1} A & G^{-1} \end{pmatrix}\bigg|_{q^i}, \quad i = D, N. \quad (5)$$

Finally, our first main result consists of showing that we can write the semiclassical approximation of the transition probability Eq. (1) as

$$\rho^{\text{sc}}(q, t|q_0, t_0) = e^{S(q^N)-S(q^D)} \sqrt{\det\left[\frac{1}{2\pi}\frac{W^N}{W^D}(t_0)\right]}, \quad (6)$$

where $S(q^{D(N)})$ is the action evaluated on the Dirichlet (Neumann) minimum, and $W^{D(N)}$ are the solutions of Eq. (4).

In general, due to the semiclassical approximation, we have $\rho(q, t|q_0, t_0) \approx \rho^{\text{sc}}(q, t|q_0, t_0)$. However, let us mention that, in the particular case where the Lagrangian is a quadratic function of q and $\dot{q}$, no error is introduced by the semiclassical approximation, and $\rho(q, t|q_0, t_0) = \rho^{\text{sc}}(q, t|q_0, t_0)$. In the latter case the matrix E is now independent of the particular minimum, and Eq. (4) simplifies further to

$$\begin{cases} \dfrac{d}{d\tau}\begin{pmatrix} W^D & W^N \\ M^D & M^N \end{pmatrix} = JE \begin{pmatrix} W^D & W^N \\ M^D & M^N \end{pmatrix}, \\ \begin{pmatrix} W^D & W^N \\ M^D & M^N \end{pmatrix}(t) = J. \end{cases}$$

$$(7)$$

In addition, as a second main result, we present a generalization of Eq. (6) that allows us to compute marginal transition probabilities defined as follows. We reorder the configuration variables as $q(\tau) = (q_v(\tau), q_F(\tau)) \in \mathbb{R}^d$, where $q_v(\tau) := (q_1, \ldots, q_l)(\tau) \in \mathbb{R}^l$ and $q_F(\tau) := (q_{l+1}, \ldots, q_d)(\tau) \in \mathbb{R}^{d-l}$, and consider the marginals $\rho_{\mathcal{M}}(q_F, t|q_0, t_0) := \int dq_v \rho(q, t|q_0, t_0)$. The latter can be expressed as the path integral

$$\rho_{\mathcal{M}}(q_F, t|q_0, t_0) := \frac{\mathcal{K}_{\mathcal{M}}}{\mathcal{N}} = \frac{1}{\mathcal{N}} \int_{q(t_0)=q_0}^{q_F(t)=q_F} \mathcal{D}q \, e^{-S(q,\dot{q})}, \quad (8)$$

where the integration for $K_{\mathcal{M}}$ is taken over all paths starting at $q(t_0) = q_0$ and with the mixed endpoint conditions $q_F(t) = q_F$ fixed and $q_v(t)$ variable. Note that the normalization term $\mathcal{N}$ remains the same as that in Eq. (3).

To derive a generalization of Eq. (6) for Eq. (8), we follow the same strategy as before and start by computing an isolated minimizer $q^{DN}(\tau)$ that satisfies the Euler-Lagrange equations with $q^{DN}(t_0) = q_0$, $q_F^{DN}(t) = q_F$ and with the Neumann natural boundary condition for the remaining variables $\frac{\partial \mathcal{L}}{\partial \dot{q}_V}(t) = 0$. Then, the semiclassical approximation of the transition probability Eq. (8) is

$$\rho_{\mathcal{M}}^{\mathrm{sc}}(q_F, t | q_0, t_0) = e^{S(q^N) - S(q^{DN})} \sqrt{(2\pi)^{l-d} \det\left[\frac{W^N}{W^{DN}}(t_0)\right]}, \tag{9}$$

with W^{DN} obtained from

$$\begin{cases} \dfrac{d}{d\tau}\begin{pmatrix} W^{DN} \\ M^{DN} \end{pmatrix} = JE^{DN}\begin{pmatrix} W^{DN} \\ M^{DN} \end{pmatrix}, \\ \begin{pmatrix} W^{DN} \\ M^{DN} \end{pmatrix}(t) = \begin{pmatrix} \mathbb{1}_{l \times l} & \mathbb{0}_{d+l \times d-l} \\ \mathbb{0}_{2d-l \times l} & -\mathbb{1}_{d-l \times d-l} \end{pmatrix}, \end{cases} \tag{10}$$

where M^{DN} is the conjugate variable under the Legendre transform for the Jacobi equation in Hamiltonian form, and E^{DN} is the symmetric matrix Eq. (5) here computed on the mixed minimum $q^{DN}(\tau)$. Note that for $l = 0$ we have that Eq. (9) reduces to Eq. (6), since $q^{DN}(\tau)$ becomes $q^D(\tau)$ for the boundary conditions of the Euler-Lagrange equations, and Eq. (10) reduces to the the first system for W^D in Eq. (4). On the other hand, for $l = d$ we have that $\mathcal{K}_{\mathcal{M}}$ coincides with the normalization factor $\mathcal{N}$.

To summarize, our approach for computing the transition probabilities Eqs. (1) and (8) consists of taking the ratio of the conditional and unconditional Wiener path integrals in the semiclassical approximation and then expressing their solutions in terms of the solutions of a set of ordinary differential equations. In the following we present the derivation of our results, and we apply them to three relevant examples.

III. DESCRIPTION OF THE METHOD

The evaluation of $\mathcal{K}$ in the semiclassical approximation is a standard textbook technique, and for our Euclidean path integrals it is also known as the Laplace asymptotic method [28]. The idea is to first Taylor expand the action $S(q(\tau))$ to second order around the Dirichlet minimum $q^D(\tau)$, exploiting the fact that the first-order variation on a minimum is zero. Here, the existence and stability of $q^D(\tau)$ are assumed. In particular, the second property involves, e.g., the conjugate point theory, as discussed in Ref. [29]. Then, from the second variation of the action computed in $q^D(\tau)$, namely,

$$\delta^2 S(q^D, y) = \int_{t_0}^t d\tau (\dot{y}^T G\dot{y} + 2\dot{y}^T A^D y + y^T V^D y), \tag{11}$$

and from the discretization of $\tau \in [t_0, t]$ into n intervals of length $\varepsilon = (t - t_0)/n$, the semiclassical approximation for $\mathcal{K}$ reads

$$\mathcal{K}^{\mathrm{sc}} = e^{-S(q^D)} \lim_{n \to \infty} I_n^D, \tag{12}$$

$$I_n^D = \int_{y(t_0)=0}^{y(t)=0} \prod_{j=1}^n \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d}\right]^{\frac{1}{2}} \prod_{j=1}^{n-1} dy_j \ e^{-\frac{\varepsilon}{2}\sum_{j=0}^n \delta^2 S(q^D, y)_j}. \tag{13}$$

The subscript j indicates that the associated term is evaluated in $\tau_j = t_0 + j\varepsilon$, e.g., $y_j = y(\tau_j)$. Moreover, the integration boundaries come from the fact that $y(\tau)$ represents a perturbation around the minimum $q^D(\tau)$, and as such it must satisfy null Dirichlet boundary conditions. Let us mention that the products in Eq. (13) give the integration measure for the integral, which is here a conditional Wiener measure [3].

At this point, it is straightforward to solve Eq. (12) using the method presented by Papadopoulos in Ref. [21]. This results in the following Gelfand-Yaglom-type expression:

$$\mathcal{K}^{\mathrm{sc}} = e^{-S(q^D)} \det[2\pi D^D(t)]^{-\frac{1}{2}}, \tag{14}$$

where $D^D(\tau)$ solves the second-order nonlinear differential equation (omitting superscripts 'D' for A, V, and D)

$$\frac{d}{d\tau}[\dot{D}G] + D\dot{A}^{(s)} - D[V + A^{(a)}G^{-1}A^{(a)}] = \dot{D}A^{(a)} - DA^{(a)}G^{-1}D^{-1}\dot{D}G, \tag{15}$$

with $A^{(s)}$ ($A^{(a)}$) being the (anti-)symmetric part of A^D, and with initial conditions $D^D(t_0) = \mathbb{0}$, $\dot{D}^D(t_0) = G(t_0)^{-1}$.

We point out that the result described by Eq. (14) is specific to the (Stratonovich-type) discretization prescription adopted in Ref. [21] for the cross terms $2\dot{y}(\tau)^T A(\tau)y(\tau)$, which gives $\frac{1}{\varepsilon}(y_{j+1} - y_j)^T (A_j y_j + A_{j+1}y_{j+1})$. In fact, there is in general a one-parameter family of discretizations,

$$\frac{2}{\varepsilon}(y_{j+1} - y_j)^T [(1 - \gamma)A_j y_j + \gamma A_{j+1}y_{j+1}], \quad \gamma \in [0, 1], \tag{16}$$

leading to different results for Eq. (14) [30,31]. Interestingly, we notice that the midpoint rule ($\gamma = 1/2$) is the only one giving a finite result for Eq. (13) when $A(\tau)$ is not symmetric. For more details see Appendix B.

It is now easy to show that, even for simple quadratic Lagrangians, Eq. (14) alone does not represent a transition probability satisfying the normalization condition Eq. (2). This can happen even if there are no cross terms (i.e., $A = \mathbb{0}$), as we will see in the string example. To fix this issue, the condition Eq. (2) is enforced by introducing the normalization factor $\mathcal{N}$ [see Eq. (1)]. Unfortunately, computing $\mathcal{N}$ can be a nontrivial task, which we are now going to tackle.

Following the same approach as for $\mathcal{K}$, we compute the semiclassical approximation for $\mathcal{N}$ as defined in Eq. (3). This time we Taylor expand the action $S(q(\tau))$ to second order around the Neumann minimum $q^N(\tau)$, since the point $q(t)$ is unconstrained. Then, from the second variation of the action computed in $q^N(\tau)$, namely,

$$\delta^2 S(q^N, h) = \int_{t_0}^t d\tau (\dot{h}^T G\dot{h} + 2\dot{h}^T A^N h + h^T V^N h), \tag{17}$$

and the same discretization as before, the semiclassical approximation for $\mathcal{N}$ reads

$$\mathcal{N}^{\mathrm{sc}} = e^{-S(q^N)} \lim_{n \to \infty} I_n^N, \tag{18}$$

$$I_n^N = \int_{h(t_0)=0} \prod_{j=1}^n \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d}\right]^{\frac{1}{2}} \prod_{j=1}^n dh_j e^{-\frac{\varepsilon}{2}\sum_{j=0}^n \delta^2 S(q^N, h)_j}. \tag{19}$$

Here, similarly to Eq. (13), the subscript j indicates that the associated term is evaluated in τ_j, and the integration

boundaries come from the fact that $h(\tau)$ represents a perturbation around the minimum $q^N(\tau)$, and as such it must satisfy only the initial null Dirichlet boundary condition. The products in Eq. (19) give the integration measure for the integral, which is here an unconditional Wiener measure [3]. In fact, note that contrary to Eq. (13) the product of dh_j runs here until n, which is what makes the integration of Eq. (19) in general nontrivial.

One of our main results is now to show how to compute Eq. (19) from a modification of the method used by Papadopoulos in Ref. [21] to derive Eq. (14). The idea consists of performing a backward integration of Eq. (19), meaning that the standard direction of discretization $(q_0, t_0) \to (q, t)$ is now replaced by $(q, t) \to (q_0, t_0)$. In summary, we are able to find a set of symmetric and positive-definite matrices F_j^N, depending on G, A^N, and V^N, such that (see Appendix A 1)

$$I_n^N = \det \left[\prod_{j=1}^n F_j^N \right]^{-\frac{1}{2}}. \tag{20}$$

Using then the recursion relations for I_n^N and F_j^N, we show that the limit in Eq. (20) gives

$$\mathcal{N}^{\text{sc}} = e^{-S(q^N)} \det[D^N(t_0)]^{-\frac{1}{2}}, \tag{21}$$

where $D^N(\tau)$ solves Eq. (15), but this time with $A^N(\tau)$ and $V^N(\tau)$. As a consequence of the backward integration necessary for deriving the matrices F_j^N, also Eq. (15) is now solved in the backward direction with boundary conditions $D^N(t) = \mathbb{1}$ and $\dot{D}^N(t) = -A^{N(s)}(t)G(t)^{-1}$. Detailed calculations to derive this result are given in Appendix A 2.

Inspired by this strategy we compute again Eq. (12), but this time using the backward integration procedure. We find that the result coincides with Eq. (14), where now $D^D(\tau)$ solves Eq. (15) in the backward direction, with boundary conditions $D^D(t) = \mathbb{0}$ and $\dot{D}^D(t) = -G(t)^{-1}$.

In conclusion, the results obtained so far allow us to express the transition probability Eq. (1) in the semiclassical approximation as

$$\rho^{\text{sc}}(q, t | q_0, t_0) := \frac{\mathcal{K}^{\text{sc}}}{\mathcal{N}^{\text{sc}}} = e^{S(q^N) - S(q^D)} \sqrt{\det \left[\frac{1}{2\pi} \frac{D^N}{D^D}(t_0) \right]}. \tag{22}$$

Despite the simplicity of Eq. (22), let us remember that the D's have to be found by solving two second-order nonlinear differential equations of the form of Eq. (15), which can be a demanding task. Remarkably, we are able to simplify this problem significantly by relating Eq. (15) to a system of linear differential equations.

As noted in Ref. [17], it turns out that there is a relation between the matrix Eq. (15) and the linear Jacobi equation for a vector field $w \in \mathbb{R}^d$:

$$\frac{d}{d\tau}[G\dot{w} + Aw] - A^T \dot{w} - Vw = 0. \tag{23}$$

In fact, if $W = L^T$ is a matrix whose columns w are solutions of the Jacobi equation, (23), then the solutions of Eq. (15) and the ones of

$$\frac{d}{d\tau}[\dot{L}G + LA^T] - \dot{L}A - LV = \mathbb{0} \tag{24}$$

are related by the nonlinear transformation

$$L^{-1}\dot{L} = D^{-1}\dot{D} + A^{(a)}G^{-1}. \tag{25}$$

Then, it is possible to impose the condition $\det(L) = \det(D)$, which is also equal to $\det(W)$, to ensure the uniqueness of the change of variables and to find the associated boundary conditions for the Jacobi equation. These read as $W^D(t) = \mathbb{0}$, $\dot{W}^D(t) = -G(t)^{-1}$ for $\mathcal{K}^{\text{sc}}$, and $W^N(t) = \mathbb{1}$, $\dot{W}^N(t) = -G(t)^{-1}A(t)$ for $\mathcal{N}^{\text{sc}}$. More details on this transformation are given in Appendix C.

As a final step, since the Jacobi equation is the Euler-Lagrange equation for the second variation of the action, we can easily provide the more elegant Hamiltonian formulation given in Eq. (4). Namely, if $m = G\dot{w} + Aw$ is the conjugate variable under the Legendre transform of the second variation with respect to $\dot{w}$, and if we define $M = G\dot{W} + AW$, we can express Eq. (22) in terms of the solutions W^D and W^N of the Jacobi equation in Hamiltonian form subjected to the transformed final boundary conditions, i.e., Eq. (4). This results then in Eq. (6).

To extend this result to marginal distributions Eq. (8), we first explain how to combine the techniques involved in the computation of $\mathcal{K}$ and $\mathcal{N}$ in order to evaluate the path integral defining $\mathcal{K}_{\mathcal{M}}$. The semiclassical approximation for $\mathcal{K}_{\mathcal{M}}$ reads

$$\mathcal{K}_{\mathcal{M}}^{\text{sc}} = e^{-S(q^{DN})} \lim_{n \to \infty} I_n^{DN}, \tag{26}$$

$$I_n^{DN} = \int_{v(t_0)=0}^{v_F(t)=0} \prod_{j=1}^n \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d} \right]^{\frac{1}{2}}$$

$$\times \prod_{j=1}^{n-1} dv_j dv_{vn} e^{-\frac{\varepsilon}{2} \sum_{j=0}^n \delta^2 S(q^{DN}, v)_j}, \tag{27}$$

where $v(\tau) := (v_v(\tau), v_F(\tau))$ represents a perturbation around the minimum $q^{DN}(\tau)$, and as such it must satisfy null Dirichlet boundary conditions corresponding to the fixed variables. Note that the integration involves only the variable part of the variation at $\tau = t$, namely, $v_{vn} := v_v(\tau_n) = v_v(t)$.

Analogously to what was done previously for $\mathcal{K}$ and $\mathcal{N}$, we perform a backward integration of Eq. (27) by finding a set of positive-definite matrices F_j^{DN}, which depend on the coefficients of the second variation on $q^{DN}(\tau)$, i.e., G, A^{DN}, and V^{DN}, such that (see Appendix D 1)

$$I_n^{DN} = (2\pi)^{\frac{l-d}{2}} \det \left[\prod_{j=1}^n F_j^{DN} \right]^{-\frac{1}{2}}. \tag{28}$$

Using the recursion relations for I_n^{DN} and F_j^{DN}, we show that the limit in Eq. (28) gives

$$\mathcal{K}_{\mathcal{M}}^{\text{sc}} = e^{-S(q^{DN})}(2\pi)^{\frac{l-d}{2}} \det[D^{DN}(t_0)]^{-\frac{1}{2}}, \tag{29}$$

where $D^{DN}(\tau)$ solves Eq. (15) with $A = A^{DN}(\tau)$ and $V = V^{DN}(\tau)$. In addition, as a consequence of the backward integration necessary for deriving the matrices F_j^{DN}, Eq. (15) is solved in the backward direction and the boundary conditions (which are reported in Appendix D 2) are given in $\tau = t$. Exploiting the link with the Jacobi equation through the nonlinear transformation Eq. (25), we derive the new boundary

conditions given in Eq. (10) and recover the general expression for marginal transition distributions Eq. (9). Detailed calculations for this last part can be found in Appendix D 3.

Let us emphasize that when the Lagrangian is quadratic in its variables we have $\rho_{(\mathcal{M})}(q_{(F)}, t|q_0, t_0) = \rho^{sc}_{(\mathcal{M})}(q_{(F)}, t|q_0, t_0)$, since the second-order expansion used in the semiclassical approximation does not neglect any term of higher order.

In conclusion, we have shown how to compute the path integrals appearing in Eqs. (1) and (8) in the semiclassical approximation from the solutions of the Euler-Lagrange equations and of the systems of linear differential equations, Eqs. (4) and (10).

IV. EXAMPLES

To show how our approach applies to a number of relevant problems, we present here three illustrative examples.

To begin, let us summarize briefly the relations between the Langevin and the Fokker-Planck equations, with the associated path integral formulation [23,26,27].

We consider the Langevin equation

$$dQ(t) = \mu(Q(t), t)dt + \sigma(t)dB(t), \qquad (30)$$

with $Q(t)$, $\mu(Q(t), t) \in \mathbb{R}^d$, $\sigma(t) \in \mathbb{R}^{d \times l}$, and $B(t)$ being an l-dimensional standard Wiener process. It is known that the transition probability $\rho(q, t|q_0, t_0)$ for the continuous Markovian process $Q(t)$ is the fundamental solution of the Fokker-Planck equation

$$\frac{\partial}{\partial t}\rho = -\frac{\partial}{\partial q_i}[\mu_i(q, t)\rho] + \frac{1}{2}\Sigma_{ij}(t)\frac{\partial^2}{\partial q_i \partial q_j}\rho, \qquad (31)$$

with $\rho(q, t_0|q_0, t_0) = \delta(q - q_0)$, and where $\Sigma(t) = \sigma(t)\sigma(t)^T \in \mathbb{R}^{d \times d}$ is the diffusion matrix, $\mu(q, t)$ is the drift vector, and the Einstein summation convention is adopted for $i, j = 1, \ldots, d$. In particular, if Σ is constant and $\mu(q)$ is a function of the configuration, $\rho(q, t|q_0, t_0)$ has the path integral representation (1), where the Lagrangian is given by the Onsager-Machlup function [32]

$$\mathcal{L}(q(\tau), \dot{q}(\tau)) = \frac{1}{2}[(\dot{q} - \mu(q))^T \Sigma^{-1}(\dot{q} - \mu(q))]. \qquad (32)$$

In the literature, however, an additional factor $+\frac{1}{2}\text{div}(\mu(q))$ usually appears in Eq. (32). As mentioned before, we observe that this correction is necessary for providing a normalized result when the path integral expression for the transition probability is only defined by $\mathcal{K}$. Our method offers an alternative approach, where we avoid the problem of finding an effective Lagrangian for every application by introducing explicitly the normalization constant $\mathcal{N}$ [see Eq. (1)].

In the situation where Σ is not strictly positive definite, even if the Onsager-Machlup Lagrangian Eq. (32) is ill defined, its Hamiltonian form is well defined by $\mathcal{L}(p(\tau)) = \frac{1}{2}p^T \Sigma p$, where $\dot{q} = \Sigma p + \mu(q)$, and p is the conjugate variable of $\dot{q}$ under the Legendre transform. This procedure is justified by taking the limit for a sequence of strictly positive-definite matrices converging to Σ. At the same time the Hamilton and Jacobi equations for the minima and the fluctuations are also well defined. In particular, the Hamilton

equations

$$\frac{d}{d\tau}\begin{pmatrix} q \\ p \end{pmatrix} = J\begin{pmatrix} d[\mu(q)]^T p \\ \Sigma p + \mu(q) \end{pmatrix} \qquad (33)$$

are subject to the boundary conditions $q^D(t_0) = q_0$, $q^D(t) = q$ for the Dirichlet minimum $q^D(\tau)$, $q^N(t_0) = q_0$, $p^N(t) = 0$ for the Neumann minimum $q^N(\tau)$, and $q^{DN}(t_0) = q_0$, $q^{DN}_F(t) = q_F$, $p^{DN}_V(t) = 0$ for the "mixed" minimizer $q^{DN}(\tau)$. On the other hand, the Jacobi equation in the Hamiltonian form presented in Eqs. (4) and (10) is driven by the matrix

$$E^i = \begin{pmatrix} d^2[\mu(q)]^T p & d[\mu(q)]^T \\ d[\mu(q)] & \Sigma \end{pmatrix}\bigg|_{q^i, p^i}, \quad i = D, N, DN.$$

Here and in Eq. (33), $d[\mu(q)]$ and $d^2[\mu(q)]$ denote respectively the rank-2 and rank-3 tensors of the first and second derivatives in q of the vector field $\mu(q)$.

A. Ornstein-Uhlenbeck process

As a first application of our method, we consider the d-dimensional Ornstein-Uhlenbeck process [22–24], which is described by the Fokker-Planck Eq. (31) where $\Sigma \in \mathbb{R}^{d \times d}$ is a constant symmetric diffusion matrix and $\mu(q) = -\Theta q$, with $\Theta \in \mathbb{R}^{d \times d}$ defining the drift. It is easy to see that the system is exactly characterized by the same linear Hamilton and Jacobi equation:

$$\frac{d}{d\tau}\begin{pmatrix} w \\ m \end{pmatrix} = \begin{pmatrix} -\Theta & \Sigma \\ \mathbb{0} & \Theta^T \end{pmatrix}\begin{pmatrix} w \\ m \end{pmatrix}. \qquad (34)$$

The analytical solution is given by

$$w(\tau) = e^{-\Theta\tau}\left[\int_0^\tau e^{\Theta s} \Sigma e^{\Theta^T s}C_1 ds + C_2\right], \qquad (35)$$

$$m(\tau) = e^{\Theta^T \tau}C_1, \qquad (36)$$

where C_1 and C_2 are determined from the appropriate boundary conditions. In particular, setting $t_0 = 0$, we find that $S(q^N) = 0$ and that

$$S(q^D) = \frac{1}{2}\hat{q}^T\left[\int_0^t e^{\Theta(s-t)} \Sigma e^{\Theta^T(s-t)}ds\right]^{-1}\hat{q}, \qquad (37)$$

where $\hat{q} = q - e^{-\Theta t}q_0$. The Jacobi fields lead to the factors

$$W^N(0) = e^{\Theta t}, \quad W^D(0) = \int_0^t e^{\Theta s} \Sigma e^{\Theta^T(s-t)}ds. \qquad (38)$$

Finally, inserting these quantities in Eq. (6), we recover the Gaussian transition probability

$$\rho(q, t|q_0, 0) = \frac{\exp\left[-\frac{1}{2}\hat{q}^T \text{Co}^{-1}(t)\hat{q}\right]}{\sqrt{\det[2\pi \, \text{Co}(t)]}}, \qquad (39)$$

with the mean $\text{Av}(q_0, t) := e^{-\Theta t}q_0$ and the covariance matrix

$$\text{Co}(t) := \int_0^t e^{\Theta(s-t)}\Sigma e^{\Theta^T(s-t)}ds. \qquad (40)$$

In addition, notice that the marginal probability density Eq. (8) for the Ornstein-Uhlenbeck process can be derived

analytically by means of Eq. (9). In fact, simple algebra gives us

$$S(q^{DN}) = \frac{1}{2}[q_F - \text{Av}_{\mathcal{M}}(q_0, t)]^T \text{Co}_{\mathcal{M}}^{-1}(t)[q_F - \text{Av}_{\mathcal{M}}(q_0, t)],$$
(41)

$$(W^N)^{-1} W^{DN}(0) = \begin{pmatrix} \mathbb{1}_{l \times l} & * \\ \mathbb{0}_{d-l \times l} & \text{Co}_{\mathcal{M}}(t) \end{pmatrix},$$
(42)

with $\text{Av}_{\mathcal{M}}(q_0, t) = (\mathbb{0}_{d-l \times l}, \mathbb{1}_{d-l \times d-l})\text{Av}(q_0, t)$ and

$$\text{Co}_{\mathcal{M}}(t) = (\mathbb{0}_{d-l \times l} \quad \mathbb{1}_{d-l \times d-l})\text{Co}(t)\begin{pmatrix} \mathbb{0}_{l \times d-l} \\ \mathbb{1}_{d-l \times d-l} \end{pmatrix}.$$
(43)

Since in Eq. (42) the entry denoted by "$*$" is not relevant, Eq. (9) automatically implies that

$$\rho_{\mathcal{M}}(q_F, t|q_0, 0) = \frac{\exp\left[-\frac{1}{2}\hat{q}_F^T \text{Co}_{\mathcal{M}}^{-1}(t)\hat{q}_F\right]}{\sqrt{\det[2\pi \, \text{Co}_{\mathcal{M}}(t)]}},$$
(44)

with $\hat{q}_F = q_F - \text{Av}_{\mathcal{M}}(q_0, t)$, which is indeed the (Gaussian) marginal of the full transition probability distribution Eq. (39).

B. Van der Pol oscillator

As a second application, we consider the Van der Pol oscillator driven by white noise [25], which is described by the Langevin equation of motion for the coordinate z as

$$\ddot{z}(t) + 2\xi[z(t)^2 - 1]\dot{z}(t) + z(t) = \sqrt{2\lambda}f(t),$$
(45)

where $f(t)$ denotes a standard stationary Gaussian white noise, $\lambda > 0$ represents the diffusion coefficient, and $\xi > 0$ represents the strength of the nonlinearity. By defining the terms

$$\Omega := \begin{pmatrix} 0 & -1 \\ 1 & -2\xi \end{pmatrix} \quad \text{and} \quad \nu(q) := \begin{pmatrix} 0 \\ q_1^2 q_2 \end{pmatrix},$$

it is possible to write the stochastic equation of motion in phase space as a two-dimensional Langevin equation in the form of Eq. (30), with $\sigma = (0, \sqrt{2\lambda})^T$. The associated Fokker-Planck equation has then the coefficients

$$\Sigma = \begin{pmatrix} 0 & 0 \\ 0 & 2\lambda \end{pmatrix} \quad \text{and} \quad \mu(q) = -\Omega q - 2\xi \nu(q).$$

Note that, in this example, the corresponding Onsager-Machlup function, Eq. (32), is no longer a quadratic function of q and $\dot{q}$. Therefore, the semiclassical approximation will lead to a result that is *a priori* not exact. From the second-order expansion we nevertheless expect the result to be accurate for small values of diffusion λ and final time t. Applying the method we presented, we obtain that the Hamilton and Jacobi equations for the system are respectively of the forms

$$\frac{d}{d\tau}\begin{pmatrix} q \\ p \end{pmatrix} = \begin{pmatrix} -\Omega & \Sigma \\ \mathbb{0} & \Omega^T \end{pmatrix}\begin{pmatrix} q \\ p \end{pmatrix} - 2\xi \psi(q, p),$$
(46)

$$\frac{d}{d\tau}\begin{pmatrix} W^i \\ M^i \end{pmatrix} = \begin{pmatrix} -\Omega & \Sigma \\ \mathbb{0} & \Omega^T \end{pmatrix}\begin{pmatrix} W^i \\ M^i \end{pmatrix} - 2\xi \Psi^i\begin{pmatrix} W^i \\ M^i \end{pmatrix},$$
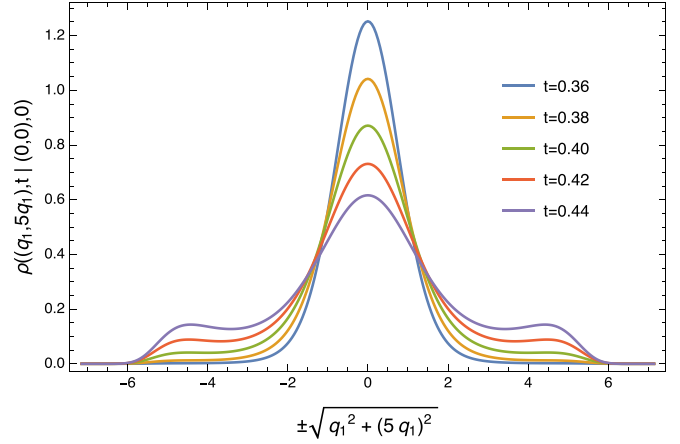(47)

FIG. 1. Slices along the direction $(q_1, q_2) = (q_1, 5q_1)$ of the transition probability $\rho((q_1, q_2), t|(0, 0), 0)$ for the Van der Pol oscillator Eq. (45) with $\xi = 3$ and $\lambda = 0.5$. Note that, despite the semiclassical approximation, the resulting probability density is not necessarily Gaussian. The peak of the transition probability in zero is decreasing when the time is increasing; the opposite behaviour occurs in the formation of the two symmetric lateral peaks.

with $i = D, N$, $\psi(q, p) = (0, q_1^2 q_2, -2q_1 q_2 p_2, -q_1^2 p_2)^T$, and

$$\Psi^i = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 2q_1^i q_2^i & (q_1^i)^2 & 0 & 0 \\ -2q_2^i p_2^i & -2q_1^i p_2^i & 0 & -2q_1^i q_2^i \\ -2q_1^i p_2^i & 0 & 0 & -(q_1^i)^2 \end{pmatrix}.$$

Solving numerically Eqs. (46) and (47), subject to the associated boundary conditions, we are able to obtain through Eq. (6) the semiclassical approximation of the (non-Gaussian) transition probability solving the Fokker-Planck equation for the stochastic Van der Pol oscillator (see Fig. 1).

C. String at thermal equilibrium

As a final example, let us investigate in one dimension the stationary configuration of a charged extensible string at thermal equilibrium, when an external field is applied. We consider the action [33]

$$S = \beta \int_0^L \left[\frac{1}{2}\alpha \dot{q}(\tau)^2 - \sigma \phi(q(\tau))\right] d\tau,$$
(48)

where β is the inverse temperature, α the elastic constant, σ the charge density per unit length, and $\phi(q(\tau))$ the electric potential. Note that here $\tau \in [0, L]$ is a parametrization of the string, and not a time, so that $\dot{q}(\tau)$ represents the elongation. To be concrete, let us assume a potential of the form $\phi(q) = aq^2 + bq$, which could be the second-order approximation of a more general potential. Let us define $\kappa := \sqrt{2\sigma a/\alpha}$. From the Euler-Lagrange equations with the appropriate boundary conditions we obtain $q^D(\tau)$ and $q^N(\tau)$, while from the Jacobi equation we obtain $W^D(\tau) = (\beta\alpha\kappa)^{-1}\sin(\kappa(L - \tau))$ and $W^N(\tau) = \cos(\kappa(L - \tau))$. These results allow us to express the probability that $q(L) = q_L$, given that $q(0) = 0$, as $p(q_L, L|0, 0) = e^{-\frac{1}{2}\frac{(q_L - \text{Av})^2}{\text{Var}}}/\sqrt{2\pi \text{Var}}$, which is a Gaussian

probability distribution with the mean $\text{Av} := \frac{b}{2a}\left(\frac{1-\cos(\kappa L)}{\cos(\kappa L)}\right)$ and the variance $\text{Var} := \frac{1}{\beta\alpha\kappa}\tan(\kappa L)$. Interestingly, this example illustrates how $\mathcal{N} \neq 1$ in general, even if $A = 0$. Furthermore, let us emphasize that the dynamics of elastic chains is properly described by complex models which allow for the motion in the three-dimensional space. In particular, these models typically exploit the concept of framed curve, which takes into account both translational and rotational degrees of freedom.

V. CONCLUSIONS

In this work we presented a consistent approach to compute transition probabilities in the semiclassical approximation, from a path integral formulation. Our method is based on the generalization of a work by Papadopoulos [21], which allows us to express the solutions of both conditional and unconditional Gaussian path integrals from the solutions of the Euler-Lagrange equations and a system of linear differential equations. Remarkably, the accuracy of our method is only dependent on the accuracy of the semiclassical approximation. In particular, when the Lagrangian of the system is quadratic in position and velocity there is no approximation, and the results are exact. As a side note, we discussed what is the effect of choosing different discretization prescriptions for continuous paths, and we mentioned under which circumstances this can be arbitrary. To conclude, we applied our method to three examples of general interest. These illustrate how our results can be applied to a variety of problems in physics and mathematics, such as the study of stochastic processes or the analysis of equilibrium configurations of polymers.

APPENDIX A: EVALUATION OF $\mathcal{N}^{\text{sc}}$

1. Derivation of Eq. (20)

In order to derive Eq. (20), we first express the second variation, Eq. (17), using the method of finite differences. Recalling that we discretised $\tau \in [t_0, t]$ into n intervals of the length $\varepsilon = (t - t_0)/n$, we obtain

$$\delta^2 S(q^N, h) \approx \varepsilon \sum_{j=0}^{n} \delta^2 S(q^N, h)_j := \frac{1}{\varepsilon} \sum_{j=1}^{n} \left[\Delta h_j^T G_j \Delta h_j + \varepsilon \Delta h_j^T \left(A_j^N h_j + A_{j-1}^N h_{j-1} \right) + \varepsilon^2 h_j^T V_j^N h_j \right]$$

$$= \frac{1}{\varepsilon} \sum_{j=1}^{n} \left[h_j^T \left(G_j + \varepsilon A_j^N + \varepsilon^2 V_j^N \right) h_j + h_{j-1}^T \left(G_j - \varepsilon A_{j-1}^N \right) h_{j-1} \right.$$

$$\left. - h_j^T \left(G_j - \varepsilon A_{j-1}^N \right) h_{j-1} - h_{j-1}^T \left(G_j + \varepsilon A_j^N \right) h_j \right], \tag{A1}$$

where we defined $\Delta h_j := h_j - h_{j-1}$ for $j = 1, \ldots, n$, and the subscript j indicates that the associated term is evaluated in $\tau_j = t_0 + j\varepsilon$ for $j = 0, 1, \ldots, n$.

Since $h(\tau)$ is a perturbation around the Neumann minimum, then $h_0 = 0$, and we can rearrange the terms in the sum in order to isolate the slice for $j = n$:

$$\varepsilon \sum_{j=0}^{n} \delta^2 S(q^N, h)_j = \frac{1}{\varepsilon} \sum_{j=1}^{n-1} \left[h_j^T \left(G_j + G_{j+1} + \varepsilon^2 V_j^N \right) h_j - h_j^T \left(G_j - \varepsilon A_{j-1}^N \right) h_{j-1} - h_{j-1}^T \left(G_j + \varepsilon A_j^N \right) h_j \right]$$

$$+ \frac{1}{\varepsilon} \left[h_n^T \left(G_n + \varepsilon A_n^N + \varepsilon^2 V_n^N \right) h_n - h_n^T \left(G_n - \varepsilon A_{n-1}^N \right) h_{n-1} - h_{n-1}^T \left(G_n + \varepsilon A_n^N \right) h_n \right]. \tag{A2}$$

Introducing now the matrices $U_j^N := G_j + \frac{\varepsilon}{2}[(A_j^N)^T - A_{j-1}^N]$ for $j = 1, \ldots, n$, we have that Eq. (A2) can be written as

$$\frac{1}{\varepsilon} \sum_{j=1}^{n-1} \left[h_j^T \left(G_j + G_{j+1} + \varepsilon^2 V_j^N \right) h_j - h_j^T U_j^N h_{j-1} - h_{j-1}^T \left(U_j^N \right)^T h_j \right] + \frac{1}{\varepsilon} \left[h_n^T \left(G_n + \varepsilon A_n^N + \varepsilon^2 V_n^N \right) h_n - h_n^T U_n^N h_{n-1} - h_{n-1}^T \left(U_n^N \right)^T h_n \right]. \tag{A3}$$

At this point, we perform a change of variables. We define the transformation (with unit Jacobian) $\phi_j := h_j - \beta_j^N h_{j-1}$ for $j = 1, \ldots, n$, where the matrices β_j^N are given recursively by the following construction:

$$\alpha_n^N := G_n + \varepsilon \frac{A_n^N + \left(A_n^N \right)^T}{2} + \varepsilon^2 V_n^N, \tag{A4a}$$

$$\alpha_j^N := G_j + G_{j+1} + \varepsilon^2 V_j^N - \left(\beta_{j+1}^N \right)^T \alpha_{j+1}^N \beta_{j+1}^N \quad \text{for } j = n-1, \ldots, 1, \tag{A4b}$$

$$U_j^N = \alpha_j^N \beta_j^N \quad \text{for } j = 1, \ldots, n. \tag{A4c}$$

These expressions are motivated by the fact that they allow one to express Eq. (A1) as a sum of quadratic forms, which is desired in view of a Gaussian integration. In fact, $\phi_j^T \alpha_j^N \phi_j = h_j^T \alpha_j^N h_j - h_j^T U_j^N h_{j-1} - h_{j-1}^T (U_j^N)^T h_j + h_{j-1}^T (\beta_j^N)^T \alpha_j^N \beta_j^N h_{j-1}$, which gives

$$\varepsilon \sum_{j=0}^n \delta^2 S(q^N, h)_j = \frac{1}{\varepsilon} \sum_{j=1}^n \phi_j^T \alpha_j^N \phi_j. \tag{A5}$$

Finally, we define $F_j^N := \alpha_j^N G_j^{-1}$ for $j = 1, \ldots, n$ to recover Eq. (20) by computing the Gaussian integrals as

$$I_n^N = \int_{h(t_0)=0} \prod_{j=1}^n \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d} \right]^{\frac{1}{2}} dh_j e^{-\frac{\varepsilon}{2} \sum_{j=0}^n \delta^2 S(q^N, h)_j} = \int \prod_{j=1}^n \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d} \right]^{\frac{1}{2}} d\phi_j e^{-\frac{1}{2\varepsilon} \sum_{j=1}^n \phi_j^T \alpha_j^N \phi_j} = \det \left[\prod_{j=1}^n F_j^N \right]^{-\frac{1}{2}}. \tag{A6}$$

2. Derivation of Eq. (21)

In order to derive Eq. (21) we need to compute the limit in Eq. (18). To this end, we look for recurrence relations in order to express Eq. (D5) through a difference equation. On the basis of the construction given in the previous section, we define $D_{n-k}^N := \prod_{j=0}^k F_{n-j}^N$ for $k = 0, 1, \ldots, n-1$ and provide the following iterative method for D^N and α^N: initial condition, $D_n^N = \alpha_n^N G_n^{-1}$; iteration scheme, $D_{n-(k+1)}^N = D_{n-k}^N \alpha_{n-(k+1)}^N G_{n-(k+1)}^{-1}$ for $k = 0, 1, \ldots, n-2$; and initial condition, $\alpha_n^N = G_n + \varepsilon \frac{A_n^N + (A_n^N)^T}{2} + \varepsilon^2 V_n^N$; iteration scheme, $\alpha_{n-(k+1)}^N = G_{n-(k+1)} + G_{n-k} + \varepsilon^2 V_{n-(k+1)}^N - (\beta_{n-k}^N)^T \alpha_{n-k}^N \beta_{n-k}^N$ for $k = 0, 1, \ldots, n-2$.

Reminding that $\beta_{n-k}^N = (\alpha_{n-k}^N)^{-1} U_{n-k}^N$ and that $U_{n-k}^N = G_{n-k} + \frac{\varepsilon}{2}[(A_{n-k}^N)^T - A_{n-(k+1)}^N]$, it is possible to give the explicit recurrence relation for $\alpha_{n-(k+1)}^N$, $k = 0, 1, \ldots, n-2$, as

$$\alpha_{n-(k+1)}^N = G_{n-(k+1)} + G_{n-k} + \varepsilon^2 V_{n-(k+1)}^N - G_{n-k} (\alpha_{n-k}^N)^{-1} G_{n-k}$$
$$- \varepsilon \left[\frac{A_{n-k}^N - (A_{n-(k+1)}^N)^T}{2} \right] (\alpha_{n-k}^N)^{-1} G_{n-k} - \varepsilon G_{n-k} (\alpha_{n-k}^N)^{-1} \left[\frac{(A_{n-k}^N)^T - A_{n-(k+1)}^N}{2} \right]$$
$$- \varepsilon^2 \left[\frac{A_{n-k}^N - (A_{n-(k+1)}^N)^T}{2} \right] (\alpha_{n-k}^N)^{-1} \left[\frac{(A_{n-k}^N)^T - A_{n-(k+1)}^N}{2} \right]. \tag{A7}$$

Moreover, the recurrence formula for D^N provides the additional useful relations:

$$\alpha_{n-(k+1)}^N = (D_{n-k}^N)^{-1} D_{n-(k+1)}^N G_{n-(k+1)}, \tag{A8a}$$

$$(\alpha_{n-k}^N)^{-1} = G_{n-k}^{-1} (D_{n-k}^N)^{-1} D_{n-(k-1)}^N. \tag{A8b}$$

Finally, substituting Eqs. (A8) in Eq. (A7) and multiplying to the left both sides by D_{n-k}^N, we get the full difference equation for the matrix D^N, in terms of G, A^N, and V^N, for $k = 1, 2, \ldots, n-2$:

$$D_{n-(k+1)}^N G_{n-(k+1)} = D_{n-k}^N G_{n-(k+1)} + D_{n-k}^N G_{n-k} - D_{n-(k-1)}^N G_{n-k} + \varepsilon^2 D_{n-k}^N V_{n-(k+1)}^N$$
$$- \varepsilon D_{n-k}^N \left[\frac{A_{n-k}^N - (A_{n-(k+1)}^N)^T}{2} \right] G_{n-k}^{-1} (D_{n-k}^N)^{-1} D_{n-(k-1)}^N G_{n-k} - \varepsilon D_{n-(k-1)}^N \left[\frac{(A_{n-k}^N)^T - A_{n-(k+1)}^N}{2} \right]$$
$$- \varepsilon^2 D_{n-k}^N \left[\frac{A_{n-k}^N - (A_{n-(k+1)}^N)^T}{2} \right] G_{n-k}^{-1} (D_{n-k}^N)^{-1} D_{n-(k-1)}^N \left[\frac{(A_{n-k}^N)^T - A_{n-(k+1)}^N}{2} \right]. \tag{A9}$$

Our goal is now to take the continuous limit ($n \to \infty$, $\epsilon \to 0$) for this expression in order to obtain a differential equation for the unknown D^N. To this end, remember that, e.g., $D_{n-(k+1)}^N$ stands for $D^N(t - s_{k+1})$ with $s_{k+1} = (k+1)\varepsilon = s_k + \varepsilon$ and that similar expressions hold for all other terms. We can therefore Taylor expand each D^N around s_k to second order in ε and each other coefficient to first order. Then, dividing everything by ε^2 we obtain

$$\frac{d}{ds}\left[\frac{d}{ds}[D^N(t-s)]G(t-s) \right] - D^N(t-s)\frac{d}{ds}[(A^N)^{(s)}(t-s)] - D^N(t-s)[V^N(t-s) + (A^N)^{(a)}(t-s)G^{-1}(t-s)(A^N)^{(a)}(t-s)]$$
$$= -\frac{d}{ds}[D^N(t-s)](A^N)^{(a)}(t-s) + D^N(t-s)(A^N)^{(a)}(t-s)G^{-1}(t-s)(D^N)^{-1}(t-s)\frac{d}{ds}[D^N(t-s)]G(t-s), \tag{A10}$$

subject to the boundary conditions $D^N(t - s)|_{s=0} = \mathbb{1}$ and $\frac{d}{ds}[D^N(t - s)]|_{s=0} = (A^N)^{(s)}(t)G(t)^{-1}$. These are a consequence of the recurrence relations for D^N and α^N, and they are derived as follows. For the former we have

$$\alpha_n^N = G_n + \varepsilon \frac{A_n^N + (A_n^N)^T}{2} + \varepsilon^2 V_n^N \sim G_n \text{ as } \varepsilon \to 0 \Rightarrow D_n^N = \alpha_n^N G_n^{-1} \sim \mathbb{1} \text{ as } \varepsilon \to 0. \tag{A11}$$

For the latter, note that

$$\frac{D_{n-1}^N - D_n^N}{\varepsilon} = \frac{D_n^N(\alpha_{n-1}^N G_{n-1}^{-1} - \mathbb{1})}{\varepsilon} \sim \frac{(\alpha_{n-1}^N G_{n-1}^{-1} - \mathbb{1})}{\varepsilon} \quad \text{as } \varepsilon \to 0, \tag{A12}$$

and, because $[\frac{A_n^N - (A_{n-1}^N)^T + (A_n^N)^T - A_{n-1}^N}{2}]G_{n-1}^{-1} \to 0$ as $\varepsilon \to 0$, this can also be written as

$$\begin{aligned}
\frac{\alpha_{n-1}^N G_{n-1}^{-1} - \mathbb{1}}{\varepsilon} &= \frac{1}{\varepsilon}\left\{ G_n G_{n-1}^{-1} + \varepsilon^2 V_{n-1}^N G_{n-1}^{-1} - G_n(\alpha_n^N)^{-1}G_n G_{n-1}^{-1} - \varepsilon\left[\frac{A_n^N - (A_{n-1}^N)^T}{2}\right](\alpha_n^N)^{-1}G_n G_{n-1}^{-1} \right. \\
&\quad \left. - \varepsilon G_n(\alpha_n^N)^{-1}\left[\frac{(A_n^N)^T - A_{n-1}^N}{2}\right]G_{n-1}^{-1} - \varepsilon^2\left[\frac{A_n^N - (A_{n-1}^N)^T}{2}\right](\alpha_n^N)^{-1}\left[\frac{(A_n^N)^T - A_{n-1}^N}{2}\right]G_{n-1}^{-1} \right\} \\
&\sim \frac{1}{\varepsilon}\left[\mathbb{1} - G_n(\alpha_n^N)^{-1}\right] \quad \text{as } \varepsilon \to 0.
\end{aligned} \tag{A13}$$

Inserting now the definition for α_n^N we have

$$\frac{1}{\varepsilon}\left[\mathbb{1} - G_n(\alpha_n^N)^{-1}\right] = \frac{1}{\varepsilon}\left[\mathbb{1} - \left(\mathbb{1} + \varepsilon\frac{A_n^N + (A_n^N)^T}{2}G_n^{-1} + \varepsilon^2 V_n^N G_n^{-1}\right)^{-1}\right], \tag{A14}$$

which, exploiting the Neumann series $(\mathbb{1} + \Lambda)^{-1} = \mathbb{1} - \Lambda + \Lambda^2 - \Lambda^3 + \cdots$, with $\Lambda = \varepsilon\frac{A_n^N + (A_n^N)^T}{2}G_n^{-1} + \varepsilon^2 V_n^N G_n^{-1}$, gives

$$\frac{D_{n-1}^N - D_n^N}{\varepsilon} \sim (A_n^N)^{(s)}G_n^{-1} \text{ as } \quad \varepsilon \to 0. \tag{A15}$$

To summarize, setting $\tau = t - s$ in Eq. (A10), this leads to the second-order nonlinear differential equation, Eq. (15), subject to the boundary conditions $D^N(t) = \mathbb{1}$ and $\dot{D}^N(t) = -(A^N)^{(s)}(t)G(t)^{-1}$.

APPENDIX B: DIFFERENT DISCRETIZATION CHOICES

According to Eq. (16), the most general discretization prescription for Eq. (A1) is given as a function of $\gamma \in [0, 1]$ as

$$\delta^2 S(q^N, h) \approx \varepsilon \sum_{j=0}^n \delta^2 S(q^N, h)_{\gamma_j} := \frac{1}{\varepsilon}\sum_{j=1}^n \left\{ \Delta h_j^T G_j \Delta h_j + 2\varepsilon \Delta h_j^T\left[\gamma A_j^N h_j + (1 - \gamma)A_{j-1}^N h_{j-1}\right] + \varepsilon^2 h_j^T V_j^N h_j\right\}. \tag{B1}$$

From this expression, we can repeat all the steps followed in Appendices A 1 and A 2 to see that the difference Eq. (A9) now becomes

$$\begin{aligned}
D_{n-(k+1)}^N G_{n-(k+1)} &= D_{n-k}^N G_{n-(k+1)} + D_{n-k}^N G_{n-k} - D_{n-(k-1)}^N G_{n-k} + \varepsilon^2 D_{n-k}^N V_{n-(k+1)}^N + 2\varepsilon(2\gamma - 1)D_{n-k}^N A_{n-(k+1)}^N \\
&\quad - \varepsilon D_{n-k}^N\left[\gamma A_{n-k}^N - (1 - \gamma)(A_{n-(k+1)}^N)^T\right]G_{n-k}^{-1}(D_{n-k}^N)^{-1}D_{n-(k-1)}^N G_{n-k} \\
&\quad - \varepsilon D_{n-(k-1)}^N\left[\gamma(A_{n-k}^N)^T - (1 - \gamma)A_{n-(k+1)}^N\right] \\
&\quad - \varepsilon^2 D_{n-k}^N\left[\gamma A_{n-k}^N - (1 - \gamma)(A_{n-(k+1)}^N)^T\right]G_{n-k}^{-1}(D_{n-k}^N)^{-1}D_{n-(k-1)}^N\left[\gamma(A_{n-k}^N)^T - (1 - \gamma)A_{n-(k+1)}^N\right]. \tag{B2}
\end{aligned}$$

If A^N is not symmetric, it is possible to derive a differential equation from Eq. (B2) through Taylor expansion only if $\gamma = \frac{1}{2}$, which gives Eq. (15). This is easy to check by performing the calculation. The same is also true for $\mathcal{K}$, for which the expansion is now taken around the isolated minimum q^D.

If A^D and A^N are symmetric, and if we adopt the same discretization prescription for both $\mathcal{K}$ and $\mathcal{N}$, then there is a one parameter family of different equations providing the same normalized result for the transition probability density, namely,

$$\frac{d}{d\tau}[\dot{D}G] + 2\gamma D\dot{A} - D[V - (1 - 2\gamma)^2 AG^{-1}A] = (1 - 2\gamma)\dot{D}A + (1 - 2\gamma)DAG^{-1}D^{-1}\dot{D}G, \tag{B3}$$

subject to the boundary conditions $D^D(t) = \mathbb{0}$, $\dot{D}^D(t) = -G(t)^{-1}$ and $D^N(t) = \mathbb{1}$, $\dot{D}^N(t) = -2\gamma A^N(t)G(t)^{-1}$.

APPENDIX C: THE NONLINEAR TRANSFORMATION EQ. (25)

As mentioned in the main text, the solutions D of Eq. (15) and L of Eq. (24) are related by the nonlinear transformation Eq. (25) presented in Ref. [17]. Here we present in detail how the boundary conditions for D translate into boundary conditions for L, in the context of the backward integration procedure.

First, let us consider the case for q^D. Equation (25) gives us a mapping between L^D and D^D, as far as they are invertible. If we assume L^D and D^D to be invertible for all $\tau \neq t$ (no conjugate points) the transformation is valid except for $\tau = t$, where $D^D(t) = \mathbb{0}$ because of the boundary conditions in the backward direction [see paragraph after Eq. (21)].

To derive the boundary conditions for L^D in $\tau = t$ from the boundary conditions for D^D in $\tau = t$, we consider the following reasoning. For $\tau \neq t$ we can write $L^D = L^D(D^D)^{-1}\dot{D}^D + L^D(A^D)^{(a)}G^{-1}$, and we know that $D^D \to \mathbb{0}$ and $\dot{D}^D \to -G(t)^{-1}$ as $\tau \to t$, for continuity of D^D and $\dot{D}^D$. As a consequence, in order to obtain a finite boundary condition for $\dot{L}^D$, we necessarily want $L^D(D^D)^{-1} \to X$ as $\tau \to t$, where X is a finite-valued matrix. This implies that $L^D(t) = \lim_{\tau \to t} L^D = \mathbb{0}$, for continuity of L^D. Furthermore, having L^D be invertible for $\tau \neq t$ implies $\dot{L}^D(t)$ is not singular, meaning that the matrix X is not singular as well, since $L^D(t) = \mathbb{0}$. To summarize, we have that

$$\frac{d}{d\tau}[\dot{L}^D G + L^D (A^D)^T] - \dot{L}^D A^D - L^D V^D = \mathbb{0} \tag{C1}$$

is subject to the boundary conditions $L^D(t) = \mathbb{0}$ and $\dot{L}^D(t) = -XG(t)^{-1}$.

In the same way, we now consider the case for q^N. Assuming L^N and D^N to be nonsingular also for $\tau = t$ (note $D^N(t) = \mathbb{1}$), we have

$$L^N(t)^{-1}\dot{L}^N(t) = -(A^N)^{(s)}(t)G(t)^{-1} + (A^N)^{(a)}(t)G(t)^{-1} = -(A^N)^T(t)G(t)^{-1}. \tag{C2}$$

In addition, as we want L^N to be invertible in $\tau = t$, then $Y := L^N(t)$ must be a nonsingular matrix. To summarize, we have that

$$\frac{d}{d\tau}[\dot{L}^N G + L^N (A^N)^T] - \dot{L}^N A^N - L^N V^N = \mathbb{0} \tag{C3}$$

is subject to the boundary conditions $L^N(t) = Y$ and $\dot{L}^N(t) = -Y(A^N)^T(t)G(t)^{-1}$.

At this point, we use the observation that $\det L = c \det D$ for all τ, where c is a constant [17]. In order to make the transformation unique (up to invertible matrices sharing the same determinant), we impose $c = 1$ for both L^D, D^D and L^N, D^N, which allows us to fix the matrices X and Y. Namely,

$$\lim_{\tau \to t} \det(L^D(\tau)(D^D)^{-1}(\tau)) = \det(X), \tag{C4}$$

$$\lim_{\tau \to t} \det(L^N(\tau)(D^N)^{-1}(\tau)) = \det(Y), \tag{C5}$$

so that we can set $X = Y = \mathbb{1}$.

APPENDIX D: THE GENERAL FORMULATION FOR MARGINALS

1. Derivation of Eq. (28)

In order to derive Eq. (28), we first express the second variation of the energy in $q^{DN}(\tau)$ using the method of finite differences. Recalling that we discretized $\tau \in [t_0, t]$ into n intervals of length $\varepsilon = (t - t_0)/n$ and that $v(\tau) := (v_v(\tau), v_F(\tau))$ represents a perturbation around the latter minimum, we can start our calculation from expression (A3), since the previous steps are identical, obtaining now

$$\varepsilon \sum_{j=0}^{n} \delta^2 S(q^{DN}, v)_j = \frac{1}{\varepsilon} \sum_{j=1}^{n-1} \left[v_j^T \left(G_j + G_{j+1} + \varepsilon^2 V_j^{DN} \right) v_j - v_j^T U_j^{DN} v_{j-1} - v_{j-1}^T \left(U_j^{DN} \right)^T v_j \right]$$
$$+ \frac{1}{\varepsilon} \left[v_n^T \left(G_n + \varepsilon A_n^{DN} + \varepsilon^2 V_n^{DN} \right) v_n - v_n^T U_n^{DN} v_{n-1} - v_{n-1}^T \left(U_n^{DN} \right)^T v_n \right], \tag{D1}$$

with $U_j^{DN} := G_j + \frac{\varepsilon}{2}[(A_j^{DN})^T - A_{j-1}^{DN}]$ for $j = 1, \ldots, n$.

To proceed further, let us introduce the following notation. For a given matrix $M \in \mathbb{R}^{d \times d}$, we label the submatrices $\check{M} \in \mathbb{R}^{l \times l}$, $\hat{M} \in \mathbb{R}^{l \times d-l}$, $\grave{M} \in \mathbb{R}^{d-l \times l}$, $\tilde{M} \in \mathbb{R}^{d-l \times d-l}$, and $\bar{M} \in \mathbb{R}^{l \times d}$, such that $M = \left(\begin{smallmatrix} \check{M} & \hat{M} \\ \grave{M} & \tilde{M} \end{smallmatrix} \right)$ and $\bar{M} = (\check{M}, \hat{M})$.

Since the variation in $\tau = t$ is given by $v_n = (v_{vn}, 0)$, because of the boundary conditions satisfied by the mixed minimizer $q^{DN}(\tau)$, we can write Eq. (D1) as

$$\varepsilon \sum_{j=0}^{n} \delta^2 S(q^{DN}, v)_j = \frac{1}{\varepsilon} \sum_{j=1}^{n-1} \left[v_j^T (G_j + G_{j+1} + \varepsilon^2 V_j^{DN}) v_j - v_j^T U_j^{DN} v_{j-1} - v_{j-1}^T (U_j^{DN})^T v_j \right]$$

$$+ \frac{1}{\varepsilon} \left[v_{vn}^T (\check{G}_n + \varepsilon \check{A}_n^{DN} + \varepsilon^2 \check{V}_n^{DN}) v_{vn} - v_{vn}^T \bar{U}_n^{DN} v_{vn-1} - v_{vn-1}^T (\bar{U}_n^{DN})^T v_{vn} \right]. \tag{D2}$$

At this point, we perform a change of variables. We define the transformation (with unit Jacobian) $\phi_j := v_j - \beta_j^{DN} v_{j-1} \in \mathbb{R}^d$ for $j = 1, \ldots, n-1$ and $\phi_n := v_{vn} - \beta_n^{DN} v_{n-1} \in \mathbb{R}^l$, where the matrices β_j^{DN} are given recursively by the following construction:

$$\alpha_n^{DN} := \check{G}_n + \varepsilon \frac{\check{A}_n^{DN} + (\check{A}_n^{DN})^T}{2} + \varepsilon^2 \check{V}_n^{DN} \in \mathbb{R}^{l \times l}, \tag{D3a}$$

$$\alpha_j^{DN} := G_j + G_{j+1} + \varepsilon^2 V_j^{DN} - (\beta_{j+1}^{DN})^T \alpha_{j+1}^{DN} \beta_{j+1}^{DN} \in \mathbb{R}^{d \times d} \quad \text{for } j = n-1, \ldots, 1, \tag{D3b}$$

$$\bar{U}_n^{DN} = \alpha_n^{DN} \beta_n^{DN} \in \mathbb{R}^{l \times d}, \tag{D3c}$$

$$U_j^{DN} = \alpha_j^{DN} \beta_j^{DN} \in \mathbb{R}^{d \times d} \quad \text{for } j = 1, \ldots, n-1. \tag{D3d}$$

These expressions are motivated by the fact that they allow one to express Eq. (D2) as a sum of quadratic forms, which is desired in view of a Gaussian integration, namely,

$$\varepsilon \sum_{j=0}^{n} \delta^2 S(q^{DN}, v)_j = \frac{1}{\varepsilon} \sum_{j=1}^{n} \phi_j^T \alpha_j^{DN} \phi_j. \tag{D4}$$

We then define $F_j^{DN} := \alpha_j^{DN} G_j^{-1}$ for $j = 1, \ldots, n-1$, and we compute the Gaussian integrals as

$$I_n^{DN} = \int_{v(t_0)=0}^{v_F(t)=0} \prod_{j=1}^{n} \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d} \right]^{\frac{1}{2}} \prod_{j=1}^{n-1} dv_j dv_{vn} e^{-\frac{\varepsilon}{2} \sum_{j=0}^{n} \delta^2 S(q^{DN}, v)_j}$$

$$= \int \prod_{j=1}^{n} \left[\frac{\det(G_j)}{(2\pi\varepsilon)^d} \right]^{\frac{1}{2}} d\phi_j e^{-\frac{1}{2\varepsilon} \sum_{j=1}^{n} \phi_j^T \alpha_j^{DN} \phi_j} = \left[(2\pi\varepsilon)^{d-l} \det(\alpha_n^{DN}) \right]^{-\frac{1}{2}} \det \left[G_n^{-1} \prod_{j=1}^{n-1} F_j^{DN} \right]^{-\frac{1}{2}}. \tag{D5}$$

Equation (28) is finally recovered by making the choice (which substantially simplifies the calculations in the next section)

$$F_n^{DN} := \begin{pmatrix} \alpha_n^{DN} & \hat{G}_n \\ \mathbb{0} & \varepsilon \mathbb{1}_{d-l \times d-l} \end{pmatrix} G_n^{-1}. \tag{D6}$$

2. Derivation of Eq. (29)

In order to derive Eq. (29) we need to compute the limit in Eq. (26). We notice that the recurrence relations exploited in Appendix A 2 are the same here, thus leading to the same differential equation, Eq. (15). Namely, we can define $D_{n-k}^{DN} := \prod_{j=0}^{k} F_{n-j}^{DN}$ for $k = 0, 1, \ldots, n-1$ and provide the following iterative method for D^{DN} and α^{DN}: initial condition, $D_n^{DN} = F_n^{DN}$; iteration scheme, $D_{n-(k+1)}^{DN} = D_{n-k}^{DN} \alpha_{n-(k+1)}^{DN} G_{n-(k+1)}^{-1}$ for $k = 0, 1, \ldots, n-2$; and initial condition, $\alpha_n^{DN} = \check{G}_n + \varepsilon \frac{\check{A}_n^{DN} + (\check{A}_n^{DN})^T}{2} + \varepsilon^2 \check{V}_n^{DN}$; iteration scheme, $\alpha_{n-(k+1)}^{DN} = G_{n-(k+1)} + G_{n-k} + \varepsilon^2 V_{n-(k+1)}^{DN} - (\beta_{n-k}^{DN})^T \alpha_{n-k}^{DN} \beta_{n-k}^{DN}$ for $k = 0, 1, \ldots, n-2$. Therefore, the only step left is the computation of the boundary conditions for Eq. (A10).

Using the block matrix inversion formula

$$G_n^{-1} = \begin{pmatrix} \breve{G}_n & \hat{G}_n \\ \hat{G}_n^T & \tilde{G}_n \end{pmatrix}^{-1} = \begin{pmatrix} \breve{G}_n^{-1} + \breve{G}_n^{-1}\hat{G}_n Z_n^{-1}\hat{G}_n^T \breve{G}_n^{-1} & -\breve{G}_n^{-1}\hat{G} Z_n^{-1} \\ -Z_n^{-1}\hat{G}_n^T \breve{G}_n^{-1} & Z_n^{-1} \end{pmatrix}, \quad Z = \tilde{G} - \hat{G}^T \breve{G}^{-1}\hat{G}, \tag{D7}$$

and the fact that $\alpha_n^{DN} \to \breve{G}_n$ for $\varepsilon \to 0$, the following expression is easily obtained

$$D_n^{DN} = \begin{pmatrix} \alpha_n^{DN} & \hat{G}_n \\ \mathbb{0} & \varepsilon\mathbb{1}_{d-l \times d-l} \end{pmatrix} G_n^{-1} \to \begin{pmatrix} \mathbb{1}_{l \times l} & \mathbb{0}_{l \times d-l} \\ \mathbb{0}_{d-l \times l} & \mathbb{0}_{d-l \times d-l} \end{pmatrix}, \quad \varepsilon \to 0, \tag{D8}$$

so that for Eq. (15) we get $D^{DN}(t) = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{0} \end{pmatrix}$. Moreover, the derivative at the boundary is discretized as

$$\frac{D_{n-1}^{DN} - D_n^{DN}}{\varepsilon} = \frac{D_n^{DN}(\alpha_{n-1}^{DN} G_{n-1}^{-1} - \mathbb{1})}{\varepsilon}, \tag{D9}$$

where the term $\varepsilon^{-1}(\alpha_{n-1}^{DN} G_{n-1}^{-1} - \mathbb{1}) \sim \varepsilon^{-1}(G_n - (\beta_n^{DN})^T \alpha_n^{DN}\beta_n^{DN})G_{n-1}^{-1}$ is evaluated by computing

$$\begin{aligned}(\beta_n^{DN})^T \alpha_n^{DN}\beta_n^{DN} &= (\bar{U}_n^{DN})^T (\alpha_n^{DN})^{-1}\bar{U}_n^{DN} \\ &= \left\{ \bar{G}_j + \frac{\varepsilon}{2}\big[\overline{(A_j^{DN})^T} - \bar{A}_{j-1}^{DN}\big] \right\}^T (\alpha_n^{DN})^{-1}\left\{ \bar{G}_j + \frac{\varepsilon}{2}\big[\overline{(A_j^{DN})^T} - \bar{A}_{j-1}^{DN}\big] \right\} \\ &\sim G_n^\alpha + \varepsilon\frac{T_n + T_n^T}{2}, \end{aligned} \tag{D10}$$

with

$$G_n^\alpha := \begin{pmatrix} \breve{G}_n(\alpha_n^{DN})^{-1}\breve{G}_n & \breve{G}_n(\alpha_n^{DN})^{-1}\hat{G}_n \\ \hat{G}_n^T(\alpha_n^{DN})^{-1}\breve{G}_n & \hat{G}_n^T(\alpha_n^{DN})^{-1}\hat{G}_n \end{pmatrix}, \quad T_n := \begin{pmatrix} [\breve{A}_n^{DN} - (\breve{A}_{n-1}^{DN})^T](\alpha_n^{DN})^{-1}\breve{G}_n & [\breve{A}_n^{DN} - (\breve{A}_{n-1}^{DN})^T](\alpha_n^{DN})^{-1}\hat{G}_n \\ [\hat{A}_n^{DN} - (\hat{A}_{n-1}^{DN})^T](\alpha_n^{DN})^{-1}\breve{G}_n & [\hat{A}_n^{DN} - (\hat{A}_{n-1}^{DN})^T](\alpha_n^{DN})^{-1}\hat{G}_n \end{pmatrix}. \tag{D11}$$

To conclude, we have

$$\frac{D_{n-1}^{DN} - D_n^{DN}}{\varepsilon} \sim D_n^{DN}\frac{(G_n - G_n^\alpha)}{\varepsilon} G_{n-1}^{-1} - D_n^{DN}\frac{T_n + T_n^T}{2} G_{n-1}^{-1}. \tag{D12}$$

From the definition $T(t) := \lim_{\varepsilon \to 0} T_n$, and noting that $\frac{\mathbb{1} - \breve{G}_n(\alpha_n^{DN})^{-1}}{\varepsilon} \to \frac{\breve{A}^{DN} + (\breve{A}^{DN})^T}{2}\breve{G}^{-1}(t)$ for $\varepsilon \to 0$, we perform the necessary computations that take into account a minus sign when transforming the derivative from Eq. (A10) to Eq. (15), and finally we obtain

$$\dot{D}^{DN}(t) = \begin{pmatrix} -\frac{\breve{A}^{DN} + (\breve{A}^{DN})^T}{2}[\breve{G}^{-1} + \breve{G}^{-1}\hat{G} Z^{-1}\hat{G}^T \breve{G}^{-1}] & \frac{\breve{A}^{DN} + (\breve{A}^{DN})^T}{2}\breve{G}^{-1}\hat{G} Z^{-1} \\ Z^{-1}\hat{G}^T \breve{G}^{-1} & -Z^{-1} \end{pmatrix}(t) + \begin{pmatrix} \overline{\frac{T + T^T}{2} G^{-1}} \\ \mathbb{0} \end{pmatrix}(t). \tag{D13}$$

3. Boundary conditions for the Jacobi fields

As discussed in Appendix C for the previous cases, the solutions D of Eq. (15) and L of Eq. (24) are related by the nonlinear transformation Eq. (25) presented in Ref. [17]. Here we explain in detail how the boundary conditions for D translate into boundary conditions for L for the general problem of marginal distributions and how to recover Eq. (10).

Equation (25) gives us a mapping between L^{DN} and D^{DN}, as far as they are invertible. If we assume L^{DN} and D^{DN} to be invertible for all $\tau \neq t$ (no conjugate points), the transformation is valid except for $\tau = t$, where D^{DN} is singular because of the boundary conditions. Therefore, the first step is to find the Taylor expansion (with singular term) of $(D^{DN})^{-1}(\tau)$ around $\tau = t$, arising from Eqs. (D8) and (D13), which leads to

$$(D^{DN})^{-1}(\tau) = P\frac{1}{\tau - t} + R + O(\tau - t), \quad P = \begin{pmatrix} \breve{P} & \hat{P} \\ \grave{P} & \tilde{P} \end{pmatrix} = \begin{pmatrix} \mathbb{0} & \mathbb{0} \\ \mathbb{0} & -Z(t) \end{pmatrix}, \quad R = \begin{pmatrix} \breve{R} & \hat{R} \\ \grave{R} & \tilde{R} \end{pmatrix} = \begin{pmatrix} \mathbb{1} & * \\ * & * \end{pmatrix}, \tag{D14}$$

where the entries denoted by "$*$" are unnecessary for the derivation of the results.

Furthermore, Eq. (25) allows us to write $\dot{L}^{DN} = L^{DN}(D^{DN})^{-1}\dot{D}^{DN} + L^{DN}(A^{DN})^{(a)}G^{-1}$ for $\tau \neq t$. As a consequence, in order to obtain a finite boundary condition for $\dot{L}^{DN}$, we necessarily want

$$L^{DN}(D^{DN})^{-1} \to X \quad \text{as} \quad \tau \to t, \tag{D15}$$

where X is a finite-valued matrix.

Since around $\tau = t$ we can also write $L^{DN}(\tau) = L^{DN}(t) + \dot{L}^{DN}(t)(\tau - t) + O(\tau - t)^2$, then for Eq. (D15) to be true we necessarily want $L^{DN}(t) = Y$, with $\hat{Y} = \mathbb{0}$, $\tilde{Y} = \mathbb{0}$, $\breve{X} = \breve{Y}$, and $\grave{X} = \grave{Y}$, so that

$$\lim_{\tau \to t} L^{DN}(D^{DN})^{-1} = \begin{pmatrix} \breve{Y} & \hat{X} \\ \grave{Y} & \tilde{X} \end{pmatrix}. \tag{D16}$$

At this point, we use the observation that $\det L = c \det D$ for all τ, where c is a constant [17]. In order to make the transformation unique (up to invertible matrices sharing the same determinant), we impose $c = 1$ by choosing $\check{Y} = \mathbb{1}$, $\tilde{X} = \mathbb{1}$, $\grave{Y} = \mathbb{0}$, and $\hat{X} = [(\grave{A}^{DN})^T + \frac{\check{A}^{DN} - (\check{A}^{DN})^T}{2}\check{G}^{-1}\hat{G}](t)$. The latter choice will be the key element for deriving the boundary conditions appearing in Eq. (10). We obtain $L^{DN}(t) = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{0} \end{pmatrix}$ and, after some algebra, we arrive at

$$\dot{L}^{DN}(t) = \begin{pmatrix} \mathbb{1} & (\grave{A}^{DN})^T + \frac{\check{A}^{DN} - (\check{A}^{DN})^T}{2}\check{G}^{-1}\hat{G} \\ \mathbb{0} & \mathbb{1} \end{pmatrix} \dot{D}^{DN}(t) + \begin{pmatrix} \overline{(A^{DN})^{(a)}G^{-1}} \\ 0 \end{pmatrix}(t),$$

$$= \begin{pmatrix} -(\check{A}^{DN})^T(\check{G}^{-1} + \check{G}^{-1}\hat{G}Z^{-1}\hat{G}^T\check{G}^{-1}) + (\grave{A}^{DN})^T Z^{-1}\hat{G}^T\check{G}^{-1} & (\check{A}^{DN})^T\check{G}^{-1}\hat{G}Z^{-1} - (\grave{A}^{DN})^T Z^{-1} \\ Z^{-1}\hat{G}^T\check{G}^{-1} & -Z^{-1} \end{pmatrix}(t). \quad (D17)$$

To conclude, reminding that $W^{DN} = (L^{DN})^T$ and that the conjugate variable under the Legendre transform for the Hamiltonian form of the Jacobi equation is given by $M^{DN} = G\dot{W}^{DN} + A^{DN}W^{DN}$, we recover the boundary conditions for Eq. (10):

$$W^{DN}(t) = \begin{pmatrix} \mathbb{1} & \mathbb{0} \\ \mathbb{0} & \mathbb{0} \end{pmatrix}, \quad M^{DN}(t) = \begin{pmatrix} \mathbb{0} & \mathbb{0} \\ \mathbb{0} & -\mathbb{1} \end{pmatrix}. \quad (D18)$$

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