Brownian motion in trapping enclosures: Steep potential wells and false bistability of affiliated Schrödinger type systems

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Langevin and Fokker-Planck equations for the Brownian motion in steep (extremally anharmonic) potential wells of the form $U(x) = x^m/m, m = 2n, n > 1$ are interpreted as reliable approximations of the reflected Brownian motion in the interval, as the potential steepness grows indefinitely. We investigate a familiar transformation of the involved Fokker-Planck operator to the Hermitian (eventually self-adjoint) Schrödinger-type one $-\Delta + V$, with the two-well (bistable) potential $V(x) = V_n(x) = (x^{m-2}/2)(x^m/2 + (1 - m))$. We analyze and resolve somewhat puzzling issue of the absence of negative eigenvalues in such looking-bistable dynamical systems, and that of the existence of spectrally isolated zero-energy ground states, whose squares actually coincide with Boltzmann-type equilibria $\rho_*(x) \sim \exp(-x^m/m)$ of the related steep-well Langevin (Fokker-Planck) problems. Limits of validity of the spectral "closeness" of $-\Delta + V$ (with $m$ large) and the Neumann Laplacian $(-\Delta)_N$ in the interval are established.

I. MOTIVATION.

Classic problems of Brownian motion in the interval with Dirichlet (absorption) or Neumann (reflection) boundary conditions directly involve spectral solutions of Laplacian operators properly restricted to that interval, and here denoted $(-\Delta)_D$ and $(-\Delta)_N$, respectively. In the literature there exist many proposals on how to approximate Brownian motion in the interval by means of strongly confining random model systems, both on the Langevin (thus Fokker-Planck) and Schrödinger type (semigroups, generalized diffusion equations) levels of description. Typically one employs either a sequence of finite well potentials with an increasing height of the barrier, or a sequence of strongly anharmonic potentials, alternatively $\sim x^{2n}, \sim x^{2n}/2n$ with $n$ growing indefinitely (plus a number of other alternatives).

The limiting properties of dynamical problems (Langevin, Fokker-Planck and related Schrödinger type evolutions) with steep potential wells have been addressed before in the Brownian motion framework and e.g. it is known how to get a satisfactory approximation of the Dirichlet (infinite well/finite interval-restricted) operator $(-\Delta)_D$, both on the Fokker-Planck and Schrödinger-type (generalised diffusion equation, spectral convergence) levels of description, see also [7]. Although there still remain some mathematical obstacles that annoy physicists. [8].

To the contrary, the reflected Brownian motion in the interval has been left somewhat aside. In the current literature, it is taken for granted (see [12-13] and references there-in) that the Brownian motion in extremely anharmonic potentials (while considered in terms of Langevin and Fokker-Planck equations) is a reliable approximation of the reflected Brownian motion in the interval. This statement needs to be reconciled with the fact that the formal realization of the latter motion is provided in terms of the spectral solution for the Laplacian with Neumann boundary conditions, here denoted $(-\Delta)_N$, c.f. [9-11], and actually being the generator of the pertinent (reflected) motion. This task (approximating sequences of Schrödinger-type operators and their limiting properties) has never been accomplished nor duly addressed.

Our basic aim in the present paper is to examine the standard theory of the Brownian motion in steep potential wells, with an emphasis on the familiar link between the Langevin (and hence Fokker-Planck) dynamics and that governed by to the affiliated Schrödinger semigroup. Here, we have in mind a transformation of the Fokker-Planck operator into the Hermitian, eventually self-adjoint one, of the Schrödinger type, c.f. [2]. In this reformulation, the relationship (eventual affinity) between the semigroup generator and the Neumann generator $(-\Delta)_N$, expected to arise in a suitable (extremal potential steepness) limit, can be carefully examined.

Newtonian forces (explicitly present in Langevin and Fokker-Planck equations) stem from potentials of the form $U(x) = x^m/m, m = 2n, n \geq 1$. The asymptotic stationary probability densities, to which the dynamical system relaxes, have the Boltzmann form $\rho_*(x) \sim \exp(-x^m/m)$ The affiliated t Schrödinger operators $-\Delta + V$ include manifestly bistable (two-well) potentials $V_n(x) = (x^{m-2}/2)(x^m/2 + (1 - m))$, and somewhat surprisingly, there is no bistability impact upon the functional form of ground state functions $\psi_0(x) \sim \exp(-x^m/2m)$.

These eigenfunctions correspond to the eigenvalue zero of the Schrödinger operator (the problem of spectrally isolated zero energy bound states continually reappears in the literature, [14-20]). Although the local minima of our bistable potentials have values that are below zero, negative energy bound states are conspicuously absent. At the first glance, this slightly puzzling property seems to contradict standard intuitions underlying the concept of bistability and the related tunnelling-through-the-barrier analyses in quantum theory (c.f. a "canonical" discussion.
of the negative eigenvalues splitting in case of the familiar double-well potential, \cite{27}). This point will shall amply address in below.

II. THERMODYNAMICS OF BROWNIAN MOTION AND RELAXATION TO EQUILIBRIUM

A. Boltzmann-type equilibria for Smoluchowski diffusion processes.

Let us consider a one-dimensional diffusion process \cite{2}, with the Langevin representation

\[ \dot{x} = b(x, t) + \sqrt{2DB}(t), \]

where \( \langle B(s) \rangle = 0, \langle B(s)B(s') \rangle = \delta(s - s') \) and \( b(x) \) is a forward drift of the process having the gradient form \( b = 2D\nabla\Phi \), where \( D \) stands for a diffusion constant.

If an initial probability density \( \rho_0(x) \) is given, then the diffusion process obeys the Fokker-Planck equation

\[ \partial_t \rho = D\Delta \rho - \nabla (b \cdot \rho). \]

We introduce an osmotic velocity field \( u = D\ln \rho \), together with the current velocity field \( v = b - u \). The latter directly enters the continuity equation \( \partial_t \rho = -\nabla j \), where \( j = v \cdot \rho \) has a standard interpretation of a probability current.

We restrict further discussion to time-independent drifts, that are induced by external (conservative, Newtonian) force fields \( f = -\nabla V \). One arrives at Smoluchowski diffusion processes by setting

\[ b = f/m\beta = -\frac{1}{m\beta} \nabla V. \]

This expression accounts for the fully-fledged phase-space derivation of the spatial process, in the large friction \( \beta \) regime. It is taken for granted that the fluctuation-dissipation balance gives rise to the standard form \( D = k_B T/m\beta \) of the diffusion coefficient, \cite{2, 14}.

Let us consider a stationary asymptotic regime, where \( j \to j_* = 0 \). We denote \( \rho_* = \rho_*(x) \) a strictly positive probability density, to which \( \rho(x, t) \) is presumed to relax as \( t \to \infty \). Accordingly in that regime \( v \to v_* = 0 \). Since \( b = f/m\beta \) is time-independent, there holds

\[ b = u = D\nabla \ln \rho_. \]

Consequently, we have

\[ \rho_*(x) = (1/Z) \exp[-V(x)/k_B T] = \exp[(F_* - V)/k_B T], \]

where \( 1/Z \) is a normalization constant. Our outcome has the familiar Gibbs-Boltzmann form.

In passing, we note that here \( F_* = -k_B T \ln Z \) is the minimal value of the time dependent Helmholtz free energy of the random motion \( F = F(t) = \langle V + k_B T \ln \rho \rangle \), to which \( F(t) \) relaxes as \( t \to \infty \). \cite{14}, \( \langle \cdot \rangle \) denotes the mean value with respect to \( \rho(x, t) \).

B. Schrödinger semigroup reformulation of the Fokker-Planck dynamics.

Following a standard procedure \cite{1, 2, 13, 16}, given a stationary density \( \rho_*(x) \), one can transform the Fokker-Planck dynamics, Eq. (2) into an associated Hermitian (Schrödinger-type) dynamical problem by means of a redefinition

\[ \rho(x, t) = \Psi(x, t)\rho_*^{1/2}(x). \]

Indeed, the Fokker-Planck evolution (2) of \( \rho(x, t) \) implies the validity (and in reverse, given (6)) of the generalized diffusion equation,

\[ \partial_t \Psi = D\Delta \Psi - V\Psi; \]

for \( \Psi(x, t) \). Note that \( \rho(x, t) \to \rho_*(x) \) as \( t \to \infty \) property, induces \( \Psi(x, t) \to \rho_*^{1/2}(x) \).
The potential function $\mathcal{V}(x)$ derives, as a function of the drift $b(x)$, Eq. (3), from a compatibility condition

$$\mathcal{V}(x) = \frac{1}{2} \left( \frac{b^2}{2D} + \nabla b \right).$$

(8)

In view of Eq. (4), an equivalent form of $\mathcal{V}(x)$ reads

$$\mathcal{V}(x) = D \frac{\Delta \rho_s^{1/2}}{\rho_s^{1/2}}.$$  

(9)

It is important to mention that the Fokker-Planck dynamics (2) (given $\rho_s(x)$, (6)) can be recast in another form, being a direct consequence of the semigroup dynamics (7):

$$\partial_t \rho = \rho_s^{1/2} \partial_t \Psi = D \left[ \rho_s^{1/2} \Delta (\rho_s^{-1/2} \rho) - \rho_s^{-1/2} (\Delta \rho_s^{1/2} \rho) \right].$$

(10)

If the $(1/2mD$ rescaled) Schrödinger-type Hamiltonian $\hat{H} = -D\Delta + \mathcal{V}$ is a bounded from below, self-adjoint operator in a suitable Hilbert space, then one arrives at a dynamical semigroup $\exp(-t\hat{H})$, which implies $\Psi(x,t) = [\exp(-t\hat{H})\Psi](x,0)$. We note that, in our particular F-P context, one is bound to choose $\Psi(x,0) = \rho_0(x)/\rho_s^{1/2}(x)$, with $\rho_0(x)$ being an initial probability density for Eq. (2). $\Psi(x,0)$ is presumed to be the $L^2(\mathbb{R})$ function. In general we have $\|\Psi(t)\|^2 \geq 1$ for $t \geq 0$, and a normalization to 1 is achieved only in the $t \to \infty$ limit.

It is clear that with $\mathcal{V}$ given by (9), the square root $\rho_s^{1/2}(x)$ of the invariant density (5) is a particular solution of the eigenvalue equation for $\hat{H}$, [17-20]:

$$\hat{H}\psi(x) = [-D\Delta + \mathcal{V}]\psi(x) = \epsilon\psi(x).$$

(11)

corresponding to the eigenvalue zero: $\hat{H}\rho_s^{1/2} = 0$. The separation ansatz $\Psi(x,t) = \psi(x) \exp(-\epsilon t)$ converts Eq. (7) into $\hat{H}\psi = \epsilon\psi$. Note that traditional physical dimensions can be restored by passing from $\hat{H}$ to $(2mD)\hat{H}$. Then $E = (2mD)\epsilon$ becomes a legitimate energy eigenvalue.

Concerning the generalised diffusion equation equation (7), let us make an assumption that the auxiliary potential function $\mathcal{V}$ is a continuous function that is bounded from below. Then, we can introduce the positive symmetric integral kernel $k(t,x,y) = k(t,y,x)$ of the semigroup operator $\exp(-t(\hat{H}))$ (given e.g. by the Feynman-Kac formula, with an explicit $\mathcal{V}$ entry), c.f. [1, 31, 32].

Accordingly, Eq. (10) can be rewritten in the form:

$$\partial_t \rho(x) = \rho_s^{1/2}(x) \partial_t \Psi(x,t) = \rho_s^{1/2}(x) \int k(t,x,y)\Psi(y)\,dy = \int k(t,x,y)\rho_s^{1/2}(x)\rho(y)\,dy = \int p(t,x,y)\rho(y)\,dy$$

(12)

which in the self-defining manner identifies [1], the transition probability density $p(t,x,y)$ of the Markovian diffusion process, which underlies the transport equation (10). In contrast to the semigroup kernel $k(t,x,y)$, then transition pdf $p(t,x,y)$ is not a symmetric function of spatial arguments.

The outlined procedure may be regarded as a reconstruction of the semigroup dynamics from an eigenstate (here, ground state function), [21]. It is an alternative to another, reverse engineering procedure [10] (termed also targeted stochasticity), whose main goal is to reconstruct the random motion (the Fokker-Planck equation) which is compatible with a priori a given equilibrium function (e.g. the stationary pdf).

III. METHODOLOGY EXEMPLIFIED.

A. Ornstein-Uhlenbeck process vs harmonic oscillator semigroup.

Since, the explicit presence of dimensional constants somewhat blurs a connection between the Langevin equation-induced Fokker-Planck) dynamics (1)-(5), the inferred semigroup one (6)-(9) and the emergent spectral problem (11), we shall discuss in some detail the case of the standard harmonic attraction $V(x) = kx^2/2$.

The drift $b(x) = -(k/m\beta)x = -\kappa x$ defines the Ornstein-Uhlenbeck process, for which the semigroup potential (8) takes the form:

$$\mathcal{V}(x) = \frac{\kappa^2 x^2}{4D} - \frac{\kappa}{2}$$

(13)
Since a multiplication by $2mD$ restores the standard dimensional version (Joule as the energy unit) of the potential, we realize that upon setting $\omega = \kappa$, the potential
\begin{equation}
2mD\mathcal{V}(x) = \frac{m\omega^2x^2}{2} - 2mD\frac{\kappa}{2} \tag{14}
\end{equation}
can be interpreted as that of a harmonic oscillator system, with an $mD\omega$ subtracted. One should not confuse this $\omega$ with a natural frequency $\sqrt{k/m}$ of the potential $V(x) = kx^2/2$ which has been a departure point for our present discussion.

By means of a formal identification $D \equiv \hbar/2m$ where $\hbar$ is the reduced Planck constant, we give $2mD\hat{H}$ the familiar form:
\begin{equation}
2mD\hat{H} \equiv -\frac{\hbar^2}{2m} \Delta + \frac{m\omega^2x^2}{2} - \frac{\hbar\omega}{2} \tag{15}
\end{equation}
of the quantum harmonic oscillator Hamiltonian with a ground state energy renormalization. More general discussion of this subtraction issue can be found in Refs. [1,20,30,32], see also Section 3 in Ref. [34] for spectral aspects of the relationship between the OU process and the harmonic oscillator semigroups.

We know that the eigenvalue problem (10), while promoted to the operator (13) has the spectral solution in $L^2(R)$, with eigenvalues $(2mD)\lambda_n = E_n - E_0 = \hbar\omega n$, $n \geq 0$ and the lowest eigenvalue equal zero.

The $L^2(R)$-normalized (ground state) eigenfunction of the operator (13) reads:
\begin{equation}
\phi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \exp\left[-\frac{m\omega x^2}{2\hbar}\right] = \left(\frac{k}{2\pi k_B T}\right)^{1/4} \exp\left[-\frac{V(x)}{2k_B T}\right] = \rho_0^{1/2}(x), \tag{16}
\end{equation}
where $V(x) = kx^2/2$, and to recover the functional form (5) of the invariant density $\rho_\kappa(x)$, we have reintroduced the "thermal" notation, e.g. $\hbar \equiv 2mD$, $D = k_B T/m\beta$ and $\omega = \kappa = k/m\beta$. Accordingly $F_\kappa = (1/2)\ln(k/2\pi k_B T)$.

### B. Eigenfunction expansions.

At this point we come back to the (notorious) harmonic oscillator spectral problem for the energy operator with subtraction (13). We note that if the energy is measured in units of $\hbar\omega$, while the distance in units of $\sqrt{\hbar/m\omega}$, the rescaled energy operator with subtraction takes the form
\begin{equation}
\hat{H} = \frac{1}{2}(-\Delta + x^2 - 1), \tag{17}
\end{equation}
with the spectrum $E_n = n$, $n \geq 0$ and the ground state function $\phi_0(x) = \pi^{-1/4} \exp(-x^2/2)$. Note that the spectrum of $2\hat{H} = -\Delta + x^2 - 1$ coincides with $2E_n = 2n$ and begins from the eigenvalue zero.

Consider the (rescaled, without subtraction) harmonic oscillator problem defined by $\hat{H} = (1/2)(-\Delta + x^2)$. Its spectral solution comprises a sequence of eigenvalues $\epsilon_n = n + \frac{1}{2}$ and corresponding eigenfunctions $\phi_n(x) = \left[4^n(n!)^2\pi\right]^{-1/4} \exp(-x^2/2) H_n(x)$ which are $L^2(R)$ normalized. Here $H_n(x)$ is the $n$-th Hermite polynomial $H_n(x) = (-1)^n \exp(x^2) \frac{d^n}{dx^n} \exp(-x^2)$. Consequently $\phi_0(x) = \pi^{-1/4} \exp(-x^2/2)$ and $\epsilon_0 = 1/2$. It is well known that the integral kernel of $\exp(-t\hat{H})$:
\begin{equation}
k(t, x, y) = k(t, y, x) = \sum_j \exp(-\epsilon_j t) \phi_j(y)\phi_j(x). \tag{18}
\end{equation}
is a transition density of the diffusion-type process with killing, c.f. Ref. [1]. We note that the kernel sets the semigroup propagation rule as follows: $\Psi(x, t) = [\exp(-\hat{H}t)\Psi](x) = \int_R k(t, x, y)\Psi(y)dy$.

The integral kernel of the "renormalized" energy operator $\hat{H} - 1/2 = (1/2)(-\Delta + x^2 - 1)$ has the form:
\begin{equation}
k_{ren}(t, x, y) = \exp(+\epsilon_0 t) k(t, x, y) = \phi_0(x)\phi_0(y) + \sum_{j=1}^{\infty} \exp[-(\epsilon_j - \epsilon_0)t] \phi_j(y)\phi_j(x), \tag{19}
\end{equation}
with a conspicuously time-independent ground state contribution. We note that any suitable $\Psi(x) = \sum_j \alpha_j \phi_j(x)$ evolves in time according to $\Psi(x,t) = \alpha_0 \phi_0(x) + \sum_{j=1}^{\infty} \exp[-(\epsilon_j - \epsilon_0)t] \alpha_j \phi_j(x)$.

The asymptotic demand $\Psi(x,t) \to \phi_0 = \rho_0^{1/2}$ can be met only if $\alpha_0 = 1$. Hence, a proper form for $\Psi(x)$ of interest is

$$\Psi(x) = \phi_0(x) + \sum_{j=1}^{\infty} \alpha_j \phi_j(x).$$

(20)

In principle, one can work with any $\Psi \in L^2(R)$. The form (20) can be reintroduced, if $\Psi$ is not orthogonal to $\phi_0$. Then, $(\Psi, \phi_0) = \alpha_0 \neq 0$ entails the replacement of $\Psi$ by $(1/\alpha_0)\Psi$, which does the job.

C. Transition densities.

The link with the Fokker-Planck dynamics of $\rho(x,t)$ for the Ornstein-Uhlenbeck process, while in the present notation, is restored as follows. To comply with Eq. (6), we identify $\rho_\ast(x) = |\phi_0(x)|^2$ and set $\Psi(x) \phi_0(x) = \rho(x,0)$.

The Fokker-Planck operator takes the form $L_{FP} = (1/2)\Delta - \nabla [b(x) \cdot \nabla] \phi_0(x)$ and $b(x) = -x$, (the diffusion constant $D$ is here replaced by $1/2$). The asymptotic (invariant, stationary) probability density of the pertinent process reads $\rho_\ast(x) = \phi_0^2(x) = (1/\pi)^{1/2} \exp(-x^2)$.

We note that the stationary density $\rho_\ast(x)$ of the F-P equation $\partial_t \rho = D \Delta \rho - \nabla [b(x) \cdot \nabla] \rho$, where $b = \nabla U = D \nabla \ln \rho_\ast$, has the form $\rho_\ast \sim \exp(-U(x)/D)$. It is the choice of $D = 1/2$ and $U(x) = x^2/2$, which gives rise to the above $\rho_\ast(x) \sim \exp(-x^2)$.

We have $b(x) = (1/2)\nabla \rho_\ast(x) = \nabla \ln \phi_0(x) = -x$ and $\mathcal{V} = (1/2)(x^2 - 1)$. Let us add that (not "renormalized") operator $\hat{H} = (1/2)(-\Delta + x^2)$ determines the semigroup of the process with killing.\[1, 31, 32].

In passing, we note that the choice of $D = 1$ and $U = x^2/2$ implies $\rho_\ast(x) \sim \exp(-x^2/2)$. Then, we have $b(x) = \nabla \ln \rho_\ast(x) = -x$ and $\mathcal{V} = (1/2)(x^2/2 - 1)$. Eq. (7) takes the form $\partial_t \Psi = \Delta \Psi - \mathcal{V} \Psi$, quite often exploited in the literature,\[12, 43].

We can give a detailed explanation of links the between transition densities $k(t,x,y)$ and $p(t,x,y)$, we have introduced in subsection II.B; specifically in connection with the transport equation (12) form $\rho(x,t)$. Namely,\[1], the integral kernel of $\exp(-t\hat{H})$ with $\hat{H} = (1/2)(-\Delta + x^2)$. is given by the Mehler formula:

$$k(x,y,t) = \exp(-t\hat{H})(y,x) = \frac{1}{\sqrt{\pi}} \exp[-(x^2 + y^2)/2] \sum_{n=0}^{\infty} \frac{1}{2^n n!} H_n(y) H_n(x) \exp(-\epsilon_n t) =$$

$$\exp(-t/2) (\pi[1 - \exp(-2t)])^{-1/2} \exp \left[ \frac{1}{2} (x^2 - y^2) - \frac{\left(x - e^{-t} y\right)^2}{1 - e^{-2t}} \right].$$

(21)

Note a conspicuous presence of the time-dependent factor $\exp(-t/2)$, comprising the contribution from the lowest eigenvalue $1/2$ of $\hat{H}$.

The transition probability density of the process governed by Eq. (12), while adopted to the present case, reads:

$$p(t-s,x,y) = k(t-s,x,y) \phi_0(y) \phi_0(y) e^{(t-s)/2} = [\pi (1 - e^{-2(t-s)})]^{-1/2} \exp \left[ -\frac{(x - e^{-(t-s)} y)^2}{1 - e^{-2(t-s)}} \right].$$

(22)

where $\phi_0(x) = \rho_\ast^{1/2}(x)$. Eq. (22) reproduces the transition density of the familiar Ornstein-Uhlenbeck process in $R$.

We recall that $k(t,x,y)$ refers to a process with killing,\[1, 22], while $k(t,x,y) \exp(+t/2) = k_{ren}(t,x,y)$, Eq. (19), is a principal building block of the transition probability density Eq. (12).

IV. STEEP POTENTIAL WELLS IN THE BROWNIAN MOTION.

A. Langevin driving.

It is a folk wisdom, that a sequence of symmetric single well (superharmonic) potentials

$$V_{2n}(x) = \frac{(x_L)^{2n}}{2n},$$

(23)
FIG. 1: Left panel: $U(x) = x^m/m$ for $m = 2, 10, 50, 100$. Right panel: $\rho(x) = A \exp[-U(x)]$, with $1/A = \int_\infty^\infty \exp[-U(x)] \, dx$. In passing we note that $U(\pm 1) = 1/m$ for $m < \infty$ and sets at 0 as $m \to \infty$.

FIG. 2: For comparative purposes (with regard to slightly different convergence features) we depict $U(x) = x^m/m$, $m = 2n$, (left panel) and related (dimensionless) Boltzmann-Gibbs pdfs (right panel). For $m = 50$ and $m = 100$ the maximum "plateau" is set almost at 1/2. We note that irrespective of what $m$ is, the depicted curves have two common intersection points at the value $U(\pm 1) = 1$. There is no continuous transition to the infinite well on the level of $U(x)$ alone.

with the growth of their steepness (i.e. for large values of $n$), can be used as an approximation of the infinite well rectangular potential well with reflecting (sometimes renamed as impenetrable) boundaries located at $x = \pm L$. For computational purposes it is convenient to pass to the dimensionless notation $x/L \to x$ so that $U(x) = x^{2n}/2n$ becomes an approximant of the infinite well supported on $[-1, 1]$, as $n \to \infty$.

We point out that the impenetrability issue needs some care, since that is closely related to the proper implementation of boundary conditions (Dirichlet, Neumann, alternatively - absorbing or reflecting) for the random motion on the interval, [37-40]. An apparent spectral link of quantum mechanical anharmonic oscillators and the infinite well problem, [4-6] and [1, 2] needs to be observed as well.

Let us denote $\rho(x) = A \exp[-U(x)]$, where $U(x) \equiv U_m(x) = x^m/m$, $m = 2n$. The normalization condition
\( A \int_{\mathbb{R}} \exp[-x^m/m] \, dx = 1, \) upon a substitution \( y = x^m/m, \) gives rise to

\[
1 = 2A(m)^{(1-m)/m} \int_0^\infty \exp(-y) y^{1/m-1} \, dy, \tag{24}
\]

where the integral expression is recognizable as the Euler Gamma function \( \Gamma(z) = \int_0^\infty x^{z-1} e^{-x} \, dx. \) Accordingly, we have:

\[
A \equiv A_m = \frac{1}{2m^{(1-m)/m} \Gamma(1/m)} = \frac{1}{2m^{1/m} \Gamma(1 + 1/m)}. \tag{25}
\]

The analogous normalization coefficient \( B \) for the case of \( U_m(x) = x^m, \) \( m = 2n, \) is the \( m^{1/m} \) multiple of that in Eq. (22): \( B = m^{1/m} A. \) Since \( m^{1/m} \to 1 \) with \( m \to \infty, \) the limiting behavior (convergence rate) in both cases is similar.

We note however that \( A \equiv A_m \) approaches the limiting value \( 1/2 \) from below as a growing function, while \( B \equiv B_m \) approaches \( 1/2 \) from above as a decreasing function. For illustration we give approximate values of the normalization coefficients for \( m = 50 \) and \( m = 100. \) We have \( B_{50} \approx 1/1.9777 \) and \( B_{100} \approx 1/1.9886 \) while \( A_{50} \approx 1/2.1386 \) and \( A_{100} \approx 1/2.0824. \) Since \( \rho(0) = A \) or \( B \) respectively, we realize that the pertinent normalization coefficients actually set the value of an asymptotic "plateau", with \( 1/2 \) referring to a uniform probability distribution on the interval \([−1, 1]\), whose length equals 2. See e.g. Figs. 1 and 2. It seems instructive to have visualized the dependence of \( \rho(x) \) on \( m \) in the close vicinity of boundary points \( x = \pm 1. \) That is depicted in Fig.3 for \( x = 0.99, 1, 1.01. \)

**B. The reference problem: Reflected Brownian motion on \([-1, 1].\)**

The uniform probability distribution on the interval \([-1, 1]\) is a signature of reflecting (Neumann) boundary data and that of the reflecting Brownian motion on the interval, \([9, 10, 12]\). We emphasize that nothing is here said about the exterior \( R\setminus[-1, 1]. \) of the pertinent interval.

An exact solution of the latter problem refers to the standard Laplacian, while constrained to the interval and subject to reflecting (e.g. Neumann) boundary conditions. Solutions of the diffusion equation \( \partial_t \Psi(x,t) = \Delta_{\mathbb{R}} \Psi(x,t) \) in \([-1, 1], \) need to respect \( (\partial_x \Psi)(-1,t) = (\partial_x \Psi)(+1,t) \) for all \( t. \) The pertinent transition density reads, \([10]:\)

\[
k_N(t, x, y) = \frac{1}{2} + \sum_{n=1}^\infty \cos \left( \frac{n\pi}{2} (x + 1) \right) \cos \left( \frac{n\pi}{2} (y + 1) \right) \exp \left( -\frac{n^2 \pi^2}{4} t \right) \tag{26}
\]
and is an integral kernel of the reflecting semigroup $\exp(t\Delta_N)$. The operator $-\Delta_N$ admits the eigenvalue 0 at the bottom of its spectrum, the corresponding eigenfunction being a constant $1/\sqrt{2}$, whose square actually stands for a uniform probability distribution on the interval of length 2.

Solutions of the diffusion equation with reflection at the boundaries of $D = [-1, 1]$ can be modeled by setting $p(x, t) = k_N(t, x, x_0)$, while remembering that $p(x, 0) = \delta(x - x_0)$. We can as well resort to $\Psi(x, t) = \int_D k_N(t, x, y)\Psi(y)dy$. Note that all $n \geq 1$ eigenvalues coincide with those of the absorbing case, and (up to dimensional constants) coincide with eigenvalues $((n\pi/2)^2$ of the standard (quantum mechanical) infinite well problem, with Dirichlet boundary data. The eigenfunctions respect Neumann conditions, and do not vanish at the boundary points (that would be the Dirichlet case).

The direct path-wise description of the reflected Brownian motion belongs to a non-standard inventory, if compared with the standard Langevin modeling. It involves the so-called Skorokhod problem and a class of stochastic differential equations with reflection, [10, 11]. This problem is avoided (or circumvented) in the pragmatic approach to the reflection issue via computer simulations of sample paths, where it is the boundary behavior (proper handling of the instantaneous reflection) that alters the statistical features of propagation of the otherwise free Brownian motion, [39, 41, 42].

C. Superharmonic approximations of the reflecting well in $\mathbb{R}$: Violation of the Neumann boundary condition.

![Graphical insight into where (on $\mathbb{R}$) and when (large $m$) $-\nabla U(x)$ may be considered as vanishing. Upper row: all $-\nabla U(x) = -x^{m-1}$ data are depicted for $m=50$; left, $x \in \mathbb{R}$ (we emphasize that for any finite $m$ we have a residual tail of $-x^{m-1}$ which extends to infinity); middle, in this scale the behavior of $-\nabla U(x)$ in the vicinity of $x = 1$ is blurred, we need to remember that for any finite $m$, we have $-\nabla U(1) = -1$; right, the real state of affairs is depicted in the enlarged segment located in the interval $[0.98, 1.02]$. Lower row: details of the curve $-\nabla U(x)$ in the segment $x \in [0.98, 1.02]$, left, $m=100$; middle, $m=200$; right $m=300$. Note scale indications on the vertical axis and keep in memory that $-\nabla U(1) = -1$.

As long as we prefer to deal with traditional Langevin-type methods of analysis, it is of some pragmatic interest to know, how reliable is an approximation of the reflected Brownian motion in $[-1, 1]$ by means of the attractive Langevin driving (and thence the Fokker-Planck equation), with force terms (e.g. drifts) coming from extremally anharmonic (steep) potential wells.

The main obstacle, we encounter here is that a “naive” $m = 2n \rightarrow \infty$ limit is singular and cannot be safely executed on the level of potentials proper. We note that for any finite $m$, irrespective of how large $m$ actually is, we deal with
FIG. 5: Graphical insight into when (large m) and where (vicinity of ±1) we can interpret \( \nabla \rho_\ast(x) \) as vanishing. Upper row from the left: \( \nabla \rho_\ast(x) = -A x^{m-1} \exp(-x^m/m) \) for \( m = 50, \) next \( m = 100, 200, 300 \). Second row from the left: details of \( \nabla \rho_\ast(x) \) in the vicinity of the point +1 for \( m = 50, 100, 200, 300 \). We note that the minimum of \( \nabla \rho_\ast(x) \) is located at \( x = (m - 1)^{1/m} > 1 \), while a maximum at \( x = -(m - 1)^{1/m} < -1 \). Third row reports comparatively the behavior of \( \nabla \rho_{1/2}(x) \), whose minimum is located at \( x = [2(m - 1)]^{1/m} > (m - 1)^{1/m} > 1 \).

a continuous and infinitely differentiable potential and likewise, the Boltzmann-Gibbs pdf as a consequence of (1)-(5).

On the informal, graphical level (Figs. 1 and 2) we can anticipate that the limiting pdf, is a constant \( \frac{1}{2} \) in the closed interval (uniform distribution on the interval) and vanishes identically for \( |x| > 1 \):

\[
\rho_{\ast,\text{well}}(x) = \lim_{m \to \infty} \rho_{\ast m}(x) = \begin{cases} 
\frac{1}{2}, & |x| \leq 1; \\
0, & |x| > 1,
\end{cases}
\]

(27)

This is consistent with the formal limiting behavior of \( U_m(x) \) (with \( U_m \) explicitly present in the exponent of the BG density), as \( m \to \infty \), only if one ultimately arrives at the infinite well potential, \([44]\):

\[
U_{\text{well}} = \begin{cases} 
0, & |x| \leq 1; \\
\infty, & |x| > 1,
\end{cases}
\]

(28)

whose infinite-valuedness everywhere beyond \([-1,1]\) is an essential complement to potential shapes depicted in Figs. 1 and 2.

If (28) is taken literally as a (more or less legal) limit of a sequence of superharmonic potentials, there is an obstacle to be overcome or bypassed. Namely, differentiability properties of resultant (limiting) functions \( U \) and \( \rho_\ast \) are lost at the interval \([-1,1]\) endpoints. We emphasize that an infinite differentiability is a valid property of \( U(x), \rho_\ast(x) \) and \( \rho_{1/2}(x) \) for all \( 2 \leq m < \infty \), irrespective of how large \( m \) actually is.

Let us consider in more detail the properties of \( -\nabla U_m \) and \( \nabla \rho_{\ast m} \) in \( R \), for large \( m = 2n \), in the vicinity of ±1. We
focus here on the emergent reflecting behavior and that of (interior) Neumann boundary conditions for the infinite well potential (25).

In the superharmonic Langevin-type regime we have \( b(x) = -\nabla U(x) = \nabla \ln \rho_*(x) = -x^{m-1} \). Since \( \nabla \rho_*(x) = -Ax^{m-1} \exp(-x^m/m) \), we readily infer the location of its minimum in the vicinity of \( x = 1 \):

\[
x^m = m - 1 \Rightarrow x = (m - 1)^{1/m}
\]

which, for large \( m \), can be safely replaced by \( x = m^{1/m} \). One may infer, c.f. \[33\], a useful estimate for the actual location of the considered minimum for finite but large values of \( m \):

\[
1 < \frac{m}{m-1} \leq m^{1/m} \leq 1 + \frac{2}{\sqrt{m}}
\]

with a limiting property \( \lim_{m \to \infty} m^{1/m} = 1 \) as \( m \to \infty \).

Accordingly for all finite values of \( m \), irrespective of how large \( m \) is, there is a lot to happen (in the lore of turned over sample paths) in the narrow zone of thickness \( 4/\sqrt{m} \), beyond the interval boundaries set at \( \pm 1 \) on \( R \).

| \( m \) | \( x = 0.99 \) | \( x = 1 \) | \( x = 1.01 \) | \( x = 0.99 \) | \( x = 1 \) | \( x = 1.01 \) |
|-----|-----|-----|-----|-----|-----|-----|
| 50  | -0.6111 | -1 | -1.6283 | -0.2823 | -0.4583 | -0.7368 |
| 100 | -0.3697 | -1 | -2.6780 | -0.1769 | -0.4754 | -1.2517 |
| 200 | -0.1533 | -1 | -7.2436 | -0.0660 | -0.4859 | -3.4102 |
| 300 | -0.04954 | -1 | -19.5925 | -0.0243 | -0.4899 | -9.0155 |
| 600 | -0.0024 | -1 | -387.706 | -0.0012 | -0.4943 | -99.9590 |
| 800 | -0.000325 | -1 | -2836.47 | -0.0002 | -0.4956 | -39.1928 |
| \( \infty \) | 0 | -1 | -\infty | 0 | -0.5 | 0 |

TABLE I: The vicinity \( [0.99, 1.01] \) of \( x = 1 \). The approximation accuracy of the value zero, for three gradient functions, may be regarded satisfactory (fapp - for all practical purposes) in the half-open interval \( [0.99, 1) \), but not at \( 1 \), for \( m \geq 300 \).

The smoothness properties of \( \nabla \rho^{1/2}_*(x) \) (and the limiting behavior for \( m \gg 1 \)) can be read out from the formula \( (\nabla \rho^{1/2}_*)(1) = -(A^{1/2}/2) \exp(-1/2m) \), where \( A = A_m \), c.f. Eq. (25). A detailed insight into the approximation accuracy of the infinite well enclosure with Neumann boundary conditions, while in terms of superharmonic traps, is provided in Table I. Beginning from \( m = 300 \), the considered gradient functions are fapp (for all practical purposes) equal zero in the interior of the well (e.g. \( x < 1 \)). Nonetheless, irrespective of how large \( m \) is, we have \(-\nabla U(1) = -1 \). This gradient function rapidly varies for \( |x| > 1 \), in a narrowing "window" close to \( |x| = 1 \), c.f. Fig. 4.

Both \( \rho_*(x) \) and \( \rho^{1/2}_*(x) \) have nonvanishing gradients at \( \pm 1 \). We note that \( (\nabla \rho^{1/2}_*)(1) = -(A^{1/2}/2) \exp(-1/2m) \) is nonvanishing for all \( m \), including the \( m \to \infty \) limit. Indeed, since \( A = A_m \), Eq. (25), converges to \( 1/2 \) with \( m \to \infty \), we get the (point-wise) limit \( \nabla \rho^{1/2}_*(\pm) \to -1/2\sqrt{2} \). This shows that the (expected to hold true) Neumann boundary condition is violated. Albeit \( \nabla \rho^{1/2}_*(x) \equiv 0 \) in an arbitrarily close vicinity of \( \pm 1 \), while in the interior of \( [-1, 1] \), see e.g. Table I.

V. SCHRÖDINGER SEMIGROUP TRANSCRIPT OF THE FOKKER-PLANCK DYNAMICS IN STEEP POTENTIAL WELLS.

A. Reconstruction of the Schrödinger-type dynamics from an eigenstate of the motion generator.

While inspired by the targeted stochasticity concept of Ref. \[13\], we follow a procedure described in \[13\] to infer the Schrödinger semigroup from a given a priori invariant probability density function (strictly speaking, from its square root). The semigroup dynamics is to deduced from the knowledge of the strictly positive zero energy eigenstate \( \rho^{1/2}_*(x) \sim \exp(-U(x)/2), U(x) = x^m/m, m = 2n \geq 2 \) of the sought for (semigroup) motion generator, see e.g. also \[13, 20 \] for rudiments of the reverse engineering concept and this of the targeted stochasticity.

By setting \( D = 1 \) in Eqs. (7)-(10), we interpret the introduced \( m \)-family of \( \rho^{1/2}_*(x) \sim \exp(-x^m/2m) \) as ground-state solutions of the generalised diffusion equation

\[
\partial_t \Psi = \Delta \Psi - \nabla \Psi = -\dot{H} \Psi
\]

(31)
FIG. 6: $U(x)$, $\rho_\ast(x)$ and $\rho^{1/2}_\ast(x)$ for $m = 2, 4, 20, 100$. In the left panel, the dashed line depicts the infinite well potential contour. Each of the depicted $\rho^{1/2}_\ast(x)$ is an eigenfunction of $-\Delta + V(x)$ corresponding to the eigenvalue zero. Shapes of $V(x)$ for selected values of $m$ are depicted below, in Fig.6.

FIG. 7: $V(x) = V_m(x) = \frac{m^2 - 2}{2} \left[ \frac{x^m}{2} + (1 - m) \right]$ for $m = 20, 40, 100$. Note significant scale differences along the vertical axis. Minima of the semigroup potential are located at points $x = \pm[(m - 2)/m]^{1/m}$ i.e. $|x| \sim m^{1/m} > 1$.

with $\hat{H} = -\Delta + V$, where the reconstructed (semigroup, Feynman-Kac) potential actually reads

$$V(x) = V_m(x) = \frac{x^{m-2}}{2} \left[ \frac{x^m}{2} + (1 - m) \right]. \quad (32)$$

In the literature, slightly less restrictive reconstruction problems for the Schrödinger-type dynamics have been considered. Namely, \[20, 21\], one may depart as well from the eigenvalue problem in $L^2(R)$

$$[\hat{H} - E]\psi_0(x) = -\Delta\psi_0(x) + [V(x) - E]\psi_0(x) \Rightarrow \mathcal{V}(x) - E = \frac{\Delta\psi_0(x)}{\psi_0(x)} \quad (33)$$

with the given a priori $L^2(R)$ eigenfunction $\psi_0(x)$ (typically free of nodes, albeit it is not the must, see Remark in below), and ask for the well behaved potential function which makes the eigenvalue problem well defined and solvable. This is in fact the main idea behind the "reconstruction of the dynamics form the eigenstate".

It is clearly an inversion of the standard logic, where one first selects the appropriate potential and then seeks solutions (and eigensolutions) of the Schrödinger or Schrödinger-type (generalized diffusion one, our case) equation.

Remark: It is customary to reconstruct the dynamics from the strictly positive function, which is interpreted as the ground state of the sought for motion generator. However, it is not a must. One may as well admit other eigenfunctions, that lead to non-negative probability densities, instead of the strictly positive one. It is possible to
handle the problem of zeroes. A detailed analysis of the harmonic oscillator case in this regard (evaluation of drifts and related semigroup potentials of the form (8) from excited eigenstates) is provided in the text between formulas (46) and (50) of Ref. [?]. See also Ref. [20].

The functional form (32) of $V(x)$ looks quite intriguing, if compared with the familiar anharmonic expression $x^m$, often employed in the quantum theory literature as the potential function, [6]. In fact, the operator $-\Delta + x^m$ is known to provide a fairly accurate spectral approximation of the standard infinite well problem, with Dirichlet boundary data, as $m \to \infty$, see e.g. [3–5].

In the present paper, we are interested in the large $m$ behavior of the potential (31), and specifically to what extent the reconstructed semigroup spectral problem might be perceived as "close" to that related to the Neumann Laplacian $\Delta_N$, compare e.g. Subsection IV.B.

B. On the spectral affinity ($m \gg 2$ regime) with the reflecting Brownian motion on the interval.

Rather specific functional form of the deduced semigroup potential (32) and its increasingly singular behavior at the boundaries of $[-1, 1]$, with the growth of $m$, makes problematic a direct computer-assisted evaluation of higher level eigenvalues and eigenfunctions.

The level of difficulties present here has been noted before [21] in connection with the particular example of the sextic potential $V(x) = ax^6 - bx^2$. The corresponding spectral problem for $-\Delta + V(x)$ has been associated with the broader class of quasi-exactly solvable Schrödinger equations, whose solutions are not amenable to standard algebraic methods and basically unknown, except for very few examples. We mention a discussion of decatic potentials in Ref. [24, 25], as a complementary record of various curiosities concerning the solvability of related spectral problems.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{Fig8.png}
\caption{The $m$-dependence of $V(x) = V_m(x) = \frac{m^2}{2} \left( \frac{m^2}{2} + (1 - m) \right)$ at $x = 0.9, 0.99, 0.999, 0.9999$ and $x = 1$. Two different scales are employed. The convergence properties for $x = 0.9$ and $x = 0.99$ suggest that the link with the reflecting Brownian motion may be considered reliable at best within the interval $[-0.99, +0.99]$.}
\end{figure}

Let us consider the eigenvalue problem

$$H\psi = -\Delta \psi + V\psi = \lambda \psi, \quad (34)$$

where $V(x)$ has the two-well functional form (32). Since we are interested in testing whether with the growth of $m$ one may relate the corresponding semigroup generator with the Neumann Laplacian in $L^2([-1, 1])$.

Let us choose the Neumann basis on $[-1, 1]$, c.f. [1, 13] and Section IV.B:

$$\psi_n(x) = \cos \left( \frac{n\pi}{2} (x + 1) \right), \quad n = 0, 1, \ldots \quad (35)$$

Presuming that it is the reference basis system, we make a hypothesis that any eigenfunction $\psi(x)$ in Eq. (34), for large $m$, should be "close" to the corresponding Neumann eigenfunction. Likewise, we expect the same "closeness" property from the corresponding eigenvalue (in the large $m$ regime).
If (32) is a valid eigenvalue problem, the eigenvalues should follow from the $L^2(R)$ expectation value

$$\lambda_{n,m} = <\psi_n|H\psi_n>, \quad (36)$$

that needs to be approximated by the expectation values in $L^2([-1,1])$ with respect to the Neumann basis.

According to Fig. 8, for $|x| > 0.99$ the singular behavior of $V(x)$, in the large $m$ regime, is incompatible with the Neumann basis properties at the interval boundaries. If the boundary parameter $a$ goes to 1, we need to take into account the term $(m-1)x^{m-2}$, which does not vanish at $\pm 1$ and gives a large input at the boundary, in the numerically assisted integration procedure.

Therefore, instead of extending the involved integration to whole of $[-1,1]$, we restrict the interval boundaries to $[-a,a]$, $a < 1$. Accordingly, we disregard the misbehaving part of the integral (this misbehavior is a consequence of replacing/approximating the "true" eigenfunction by of the Neumann one). Moreover, we isolate a leading term $(n\pi/2)^2$, $n \geq 1$ which is characteristic for the Neumann well spectral solution. The remaining integral expression is expected to decay to 0 as $m \to \infty$:

$$\lambda_{n,m} \sim \left(\frac{n\pi}{2}\right)^2 + \int_{-a}^{a} V(x) \cos^2\left(\frac{n\pi}{2}(x+1)\right) dx. \quad (37)$$

In Table II we collect the pertinent integral values for a couple of $m$ values, for specific choices of the integration parameter $a = 0.9, 0.99$ and $a = 0.999$, with reference to the first excited level, i.e. $n = 1$.

| $m$  | $a = 0.9$       | $a = 0.99$       | $a = 0.999$      |
|------|-----------------|------------------|------------------|
| 10   | -0.345908       | -0.849936        | -0.923367        |
| 20   | -0.127473       | -0.806033        | -0.957354        |
| 30   | -0.045061       | -0.737262        | -0.958168        |
| 50   | -0.005528       | -0.607352        | -0.945658        |
| 100  | -2.87 \cdot 10^{-5} | -0.368941 | -0.903151        |
| 200  | -7.63 \cdot 10^{-10} | -0.135228 | -0.818505        |
| 300  | -2.03 \cdot 10^{-14} | -0.049511  | -0.740936        |
| 500  | -1.43 \cdot 10^{-23} | -0.006634 | -0.606782        |
| 1000 | -1.89 \cdot 10^{-46} | -4.36 \cdot 10^{-5} | -0.368025        |

TABLE II: Computed values of the integral term in Eq. (37), for $n = 1$, and selected choices of $a$ and $m$. The conspicuous decay of this term with $m \to \infty$ is confirmed for $a \leq 0.99$.

Remark: The approximation accuracy of the "true" eigenfunction $\psi_1(x)$ by the Neumann eigenfunction $\cos(\pi(x+1)/2)$ is excellent up to $a = 0.99$ and improves with $m \to \infty$. The approximation finesse surely breaks down for $a > 0.99$, if while approaching the boundary value 1 we do not exceed $m = 1000$. See, e.g. Table II at the column corresponding to 0.999. In fact for any $a < 1$, say 0.999999, for each value of $m$ we can evaluate the integral. As $m \to \infty$ the integral will (possibly discouragingly slowly) converge to 0. For example, if we take $a = 0.999$, at $m = 1000$ the integral value is $-0.135332$. If we would have evaluated the integral for $m = 2000, 3000, 5000, 10000$, the respective values would read: $-0.135332, -0.0238809, -0.00336391, -0.0000226092$. The convergence to 0 is obvious.

We can convince ourselves with regard to the reported signatures of the spectral affinity in the interval $[-a,a]$ for $a \leq 0.99$, by presenting the detuning diagram, i.e. the plot of $|H\psi_1 - \lambda_{1,m}\psi_1|$ for $a = 0.9$ and $m = 10, 30, 100$, as a function of $x$, provided $\psi_1(x) \equiv \cos(\pi(x+1)/2)$ in $[-a,a]$. The detuning can be made arbitrarily small with the growth of $m$.

VI. FALSE BISTABILITY IN SCHRÖDINGER TWO-WELL SYSTEMS.

A. The enigma of the eigenvalue zero for two-well systems or: why there is no signatures of bistability?

Double-well potentials in the classic (quartic) double-well version have received an ample coverage in the literature, specifically in connection with effects of tunneling through the barrier, which gives rise to a splitting of otherwise
degenerate negative energy (might be positive, but then necessarily with energies below the top of the central double-well barrier i.e. below the local maximum of the potential). A standard procedure, employed to analyze the low-lying spectrum, amounts to a local approximation of each well by a suitable harmonic oscillator potential.\cite{27}

Let us consider the general eigenvalue problem for a Hermitian (eventually self-adjoint) Schrödinger type operator

\[ -\Delta \psi + V \psi = \lambda \psi \]  

We presume the potential to be bounded from below and symmetric (this assumption does not harm the generality of further arguments). Let \( V(x) \) has a minimum (in the least a local minimum) at \( x_0 \in \mathbb{R} \) and consider a Taylor expansion of \( V(x) \), which in a sufficiently close vicinity of \( x_0 \) may be reduced to

\[ V(x) = V(x_0) + \frac{1}{2} V''(x_0)(x - x_0)^2. \]  

Let us furthermore assume that \( V(x_0) < 0 \) in the vicinity of \( x_0 \) and at \( x_0 \).

Inserting an approximate expression \( V(x) \) to the eigenvalue equation \( \psi \), we arrive at an approximate eigenvalue problem:

\[ -\Delta \psi(x) + \frac{1}{2} V''(x_0)(x - x_0)^2 \psi(x) = (\lambda - V(x_0)) \psi(x) \]  

Setting \( z = x - x_0 \), \( dz = dx \) we arrive at

\[ -\Delta \psi(z) + \frac{1}{2} V''(x_0) z^2 \psi(z) = (\lambda - V(x_0)) \psi(z). \]  

This expression can be readily compared with the standard harmonic oscillator spectral problem. Indeed, since we have:

\[ -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} \psi(z) + \frac{1}{2} m\omega^2 z^2 \psi(z) = E \psi(z), \]  

Eqs. \( 37 \) and \( 38 \) become compatible upon formal constants (and units) rearrangements (we need \( V''(x_0) > 0 \))

\[ \frac{\hbar^2}{2m} = 1, \quad \frac{m\omega^2}{2} = \frac{V''(x_0)}{2}, \quad E = \lambda - V(x_0). \]  

While keeping in mind that \( \frac{\hbar^2}{2m} = 1 \), we get

\[ \frac{\hbar^2}{2m} \frac{m\omega^2}{2} = \frac{\hbar^2\omega^2}{4} = \frac{V''(x_0)}{2}. \]
Since for the quantum harmonic oscillator \((E_n = (n + 1/2)\hbar\omega)\), the ground state eigenvalue \(n = 0\) is \(E_0 = \hbar\omega/2\), we can infer a corresponding \(\lambda_0\) from the (approximate) identity \(E_0 = \lambda_0 - \mathcal{V}(x_0)\), so arriving at

\[
\lambda_0 = \frac{\hbar\omega}{2} + \mathcal{V}(x_0).
\] (45)

Our assumption that in the vicinity of the local minimum \(\mathcal{V}(x_0)\), our potential function \(\mathcal{V}(x)\) is negative, implies a (rough) sufficient condition for the existence of negative eigenvalues in the two wells potential case. Indeed, a demand \(\lambda_0 < 0\) enforces

\[
\frac{\hbar\omega}{2} < -\mathcal{V}(x_0).
\] (46)

Both sides of the inequality are positive, hence after taking the square and employing (40) we can rewrite a condition for the negativity of \(\lambda_0\) as the restriction upon the curvature of the two well potential \(\mathcal{V}(x)\) at \(x_0\) by the twice the squared local minimum value:

\[
\mathcal{V}''(x_0) < 2[\mathcal{V}(x_0)]^2.
\] (47)

We work with a special subclass in the two-parameter family of two well potentials:

\[
\mathcal{V}(x) = ax^{2m-2} - bx^{m-2}, \quad a, b > 0, \quad m > 2
\] (48)

for which two local (well) minima are symmetrically located at \(\pm x_0\), where

\[
x_0 = \left(\frac{(m - 2)b}{2(m - 1)a}\right)^{1/m}.
\] (49)

Note that assuming \(b > 3a\), for all \(m\) we have \(x_0 > 1\), while for \(b < 2a\) the minima are located in the interior of \([-1, 1]\).

Our specific case of the two-well potential Eq. (32) is identified by setting \(a = 1/4\), \(b = (m - 1)/2\) and assuming \(m = 2n, n > 1\) (we recall that the case \(n = 1\) refers to the standard harmonic oscillator potential with ground state energy subtracted, \([1, 32]\)). This implies \(x_0 = (m - 2)\gamma/m\).

Further calculation is performed for our two-well potential (32). We have:

\[
\mathcal{V}''(x_0) = \frac{m(m - 1)}{2}(m - 2)^{(2m-4)/m},
\] (50)

and

\[
[\mathcal{V}(x_0)]^2 = \frac{m^2}{16}(m - 2)^{(2m-4)/m}.
\] (51)

This implies a sharp inequality

\[
\frac{m(m - 1)}{2} < 2 \cdot \frac{m^2}{16} \Rightarrow m < 4/3.
\] (52)

Since we assume \(m > 2\), the condition \(m < 4/3\) is violated from the start, which excludes negative eigenvalues for the Schrödinger operator \(-\Delta + \mathcal{V}\) with the two-well potential in the form given by Eq. (32).

Clearly, even while ignoring the derivations of Section I.B (which imply the existence of the eigenvalue zero for (31), (32)), the presented argument (provided we take for granted the validity of the harmonic oscillator approximation at local minima of the looking-bistable potential) excludes the existence of negative eigenvalues for \(m = 2n, n > 1\).

### B. Bistability versus false bistability for two-well potentials, or when (why) negative eigenvalues cease to exist.

#### 1. Quartic double-well

Although the widely studied in the literature quartic double-well case does not belong to our \(m = 2n\) family of two-well potentials, it may serve as a useful credibility test of our methods. Arguments of the previous subsection can be readily adopted to this familiar example. Let us consider

\[
\mathcal{V}(x) = ax^4 - bx^2
\] (53)
FIG. 10: Double-well $V(x) = x^4 - 2\alpha^2 x^2$ (black) for $\alpha = 1$ (left panel) and $\alpha = 2$ (right panel) with an approximating parabola $V(x) = 4\alpha^2 (x - \alpha)^2 - \alpha^4$ (red) at the bottom of the $x_0 = \alpha$ well. Note that $2\alpha$ is a distance between two local minima. We point out that scales on vertical and horizontal axis are different.

FIG. 11: Ground state function $\psi_0(x)$ for $-\Delta + V$ with the double-well potential $V(x) = x^4 - 2\alpha^2 x^2$. Eigenfunction shapes are depicted for $\alpha = 1, 1.2, 2$ and a fitted ”transitional” value $\alpha_{fit} = 1.0564$ around which the eigenfunction topology changes from unimodal to bimodal. The corresponding (numerically computed) ground state eigenvalues read: $+0.137786$ ($\alpha = 1$), $-0.489604$ ($\alpha = 1.2$), $-12.1363$ ($\alpha = 2$). For $\alpha = 1.1$ we have the eigenvalue $-0.135576$. According to an independent reasoning of Ref. 22, the ground state eigenvalue zero should appear for $\alpha_{critical} \sim 1.0534677$.

and investigate how the the existence or non-existence of negative eigenvalues for $-\Delta + V$ depends on the mutual balance of steering parameters $a$ and $b$. We note that the local maximum is located at 0, two local minima at $\pm x_0$ with $x_0 = \sqrt{b/2a}$, and the distance between the minima (effective width of the central barrier) equals $2\sqrt{b/2a}$.

An approximation of the double-well by harmonic oscillator (parabolic) potentials placed at local minima implies a previously derived sufficient condition (47) under which the existence of negative eigenvalues is permitted. To check the reliability of the procedure leading to (47), we need to evaluate the local minimum value of $V(x_0)$ and the
curvature of the potential $V''(x_0)$.

These read: $V(x_0) = -b^2/4a$ and $V''(x_0) = 4b$. Accordingly, our rough (in the local harmonic oscillator approximation) condition for the existence of negative eigenvalues takes the form $4b < 2(b^2/4a)^2$, i.e $b^3 > 32a^2$.

Let us examine this restriction for a simple but popular in the literature double well example:

$$V(x_0) = \frac{-b^2}{4a}$$

$$V''(x_0) = 4b$$

with two minima at $\pm \alpha, \alpha > 0$ (the effective width of the central barrier equals $2\alpha$). The subtracted term actually sets the depth of each well (alternatively - height of the central barrier with a local maximum at $x = 0$ equal zero). A passage from the previous notation involves substitutions: $a = 1, b = 2\alpha^2$.

We have $V(\pm \alpha) = -\alpha^4$ and $V''(\pm \alpha) = 8\alpha^2$ and to have undoubtedly accommodated the negative eigenvalues we need $\alpha > 2^{1/3} \sim 1.25992$. In terms of $V = ax^4 - bx^2$ this amounts to $a = 1$ and $b > 3.1747$.

Accordingly, the bistability of two-well potentials (and the double-well in this number) may not be reflected in the topological properties of ground state eigenfunctions. These functions may be unimodal or bimodal, depending on the value of $\alpha$, and there is a transitional value $\alpha_{\text{critical}}$ which results in the eigenvalue zero of the operator $-\Delta + V$.

For $\alpha < \alpha_{\text{critical}}$ the ground state eigenvalues are positive, while for $\alpha > \alpha_{\text{critical}}$ negative ground state eigenvalues are admitted. Thus, the topology change of the ground state function form unimodal to bimodal shape is reflected in the sign change of related eigenvalues.

Zero energy eigenvalue corresponds to the "transitional shape", where the associated $\alpha_{\text{critical}}$ stands for a bifurcation point: the local maximum of the unimodal function degenerates and bifurcates into twin local maxima of the bimodal one. The local maxima existence is the signature of bistability and the presence of negative eigenvalues for $-\Delta + V$.

2. Sextic two-well potential

In contrast to the quartic double-well the sextic two-well potential

$$V(x) = ax^6 - bx^2,$$

upon identifications $a = 1/4$ and $b = 3/2$, becomes a member of our family (32).

Coming back to the notation (55), we realize that the extrema are located at 0 and $\pm x_0$ where $x_0 = (b/3a)^{1/4}$. Accordingly we have $V(x_0) = -\frac{2b}{3} \left(\frac{b}{3a}\right)^{1/2}$ and $V''(x_0) = 8b$. Accordingly, a sufficient condition for the existence of negative eigenvalues takes the form $27a < b^2$. 

![Figure 12: Left panel: quartic double-well $V(x) = x^4 - bx^2$, $b=2$ (black) - only positive eigenvalues, $b=4$ (red) - negative eigenvalue, $b=6$ (green) negative eigenvalue. Right panel: sextic double well $V(x) = x^6 - bx^2$, depicted for $b = 3$ (black) and $b = 7$ (red), the corresponding eigenvalues are displayed in terms of horizontal lines. For comparison, on the same panel we depict quartic double well potentials: $b = 2$ (green) and $b = 4$ (blue).]
In passing we note that in our case (Eq. 32), which corresponds to the bottom eigenvalue zero, the pertinent inequality does not hold true.

In Ref. [21] a one-parameter family of sextic potentials

\[ \mathcal{V}(x) = \alpha^2 x^6 - 3ax^2 \]  

(56) has been introduced (\( \alpha > 0 \) is presumed). By inspection one can verify that for each member of this family the operator \(-\Delta + \mathcal{V}\) has the energy zero eigensolution of the form \( \psi_0(x) \sim \exp(-\alpha x^4/4)\).

We can readily verify that (identify \( a = \alpha^2 \) and \( b = 3a \)) the sufficient condition for the existence of negative eigenvalues \( 27a < b^2 \) does not hold true.

Plugging \( \alpha = 1 \) we get \( \mathcal{V}(x) = x^6 - 3x^2 \) with the related \( \psi_0(x) \sim \exp(-x^4/4)\). Not that the exponent \( x^4/4 \) is twice the exponent \( x^4/8 \) (inferred from \( \rho^{1/2} \)), which we have associated with the potential function (32) i.e. \( \mathcal{V}(x) = x^6/4 - (3/2)x^2 \).

In Ref. [21], and example is given of the sextic potential \( \mathcal{V}(x) = x^7 - 7x^2 \), for which by inspection we can verify that \(-\Delta + \mathcal{V}\) has two explicitly known eigenfunctions and eigenvalues. Namely, the ground state eigenfunction (yet unnormalized) \( \psi_0(x) = (2x^2 - \sqrt{2}) \exp(-x^2/4) \) corresponds to the negative eigenvalue \( E_0 = -2\sqrt{2} \), while \( \psi_2(x) = (2x^2 + \sqrt{2}) \exp(-x^2/4) \) corresponds to the positive eigenvalue \( E_0 = 2\sqrt{2} \) (it is not the first, but the second excited eigenfunction, has the same parity as the ground state). Plugging \( a = 1 \) and \( b = 7 \) we readily verify that the condition \( 27a < b^2 \) in the present case holds true, as expected.

VII. OUTLOOK

Our present investigation has been motivated by that of Ref. [13], where somewhat puzzling features of jump-type processes in the presence of steep potential wells were reported. Namely, while departing from the Langevin picture of the Lévy-type motion in steep potential wells \( x^m/m, m = 2n, n > 1 \), one arrives at fractional Fokker-Planck equations, whose limiting properties as \( m \to \infty \) are ultimately interpreted in terms of reflected Lévy flights in an interval \([-1, 1]\).

We have identified a number of obstacles and curiosities of the argument, that hamper this formally straightforward interpretation.

Since in case of the Brownian motion, the analogous limiting behavior (with a reflecting Brownian motion as a limit) is taken for granted, we have turned back to the "obvious" issue, with a focus on a transformation of the Fokker-Planck operator to the Schrödinger type one.

The expected outcome should have been a possibly "smooth" limiting behavior (this however has proved not to be the case) of Schrödinger-type operators \(-\Delta + \mathcal{V}(m)\) as \( m \to \infty \) that would justify a reliable approximation of the reflected Brownian motion with the generator \((-\Delta)_{\alpha} \) by the Brownian motion in extremally steep anharmonic potentials.

The present paper is a preparatory step to tackle problems arising in the description of Lévy-type processes that actually has been carried out along the similar (Langevin motion in steep anharmonic potentials) lines and is an active research topic, [31-40], see also [13].

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