J Stat Phys (2013) 152:237–274
DOI 10.1007/s10955-013-0769-x

Optimal Non-reversible Linear Drift for the Convergence to Equilibrium of a Diffusion

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Received: 4 December 2012 / Accepted: 17 May 2013 / Published online: 1 June 2013

Abstract We consider non-reversible perturbations of reversible diffusions that do not alter the invariant distribution and we ask whether there exists an optimal perturbation such that the rate of convergence to equilibrium is maximized. We solve this problem for the case of linear drift by proving the existence of such optimal perturbations and by providing an easily implementable algorithm for constructing them. We discuss in particular the role of the prefactor in the exponential convergence estimate. Our rigorous results are illustrated by numerical experiments.

Keywords Non-reversible diffusion · Convergence to equilibrium · Wick calculus

This work is supported by the Agence Nationale de la Recherche, under grant ANR-09-BLAN-0216-01 (MEGAS). This work was initiated while the two last authors had a INRIA-sabbatical semester and year in the INRIA-project team MICMAC. The research of GP is partially supported by the EPSRC under grants No. EP/H034587 and No. EP/J009636/1.

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1 Introduction

1.1 Motivation

The problem of convergence to equilibrium for diffusion processes has attracted considerable attention in recent years. In addition to the relevance of this problem for the convergence to equilibrium of some systems in statistical physics, see for example [30], such questions are also important in statistics, for example in the analysis of Markov Chain Monte Carlo (MCMC) algorithms [9]. Roughly speaking, one measure of efficiency of an MCMC algorithm is its rate of convergence to equilibrium, and increasing this rate is thus the aim of many numerical techniques (see for example [5]).

Let us recall the basic approach for a reversible diffusion. Suppose that we are interested in sampling from a probability distribution function

$$\psi_\infty = \frac{e^{-V}}{\int_{\mathbb{R}^N} e^{-V}\,dx}, \tag{1}$$

where $V:\mathbb{R}^N \to \mathbb{R}$ is a given smooth potential such that $\int_{\mathbb{R}^N} e^{-V}\,dx < \infty$. A natural dynamics to use is the reversible dynamics

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2}\,dW_t, \tag{2}$$

where W_t denotes a standard N-dimensional Brownian motion. Let us denote by ψ_t the probability density function of the process X_t at time t. It satisfies the Fokker-Planck equation

$$\partial_t \psi_t = \nabla \cdot (\nabla V \psi_t + \nabla \psi_t). \tag{3}$$

Under appropriate assumptions on the potential V (e.g. that $\frac{1}{2}|\nabla V(x)|^2 - \Delta V(x) \to +\infty$ as $|x| \to +\infty$, see [42, A.19]), the density ψ_∞ satisfies a Poincaré inequality: there exists $\lambda > 0$ such that for all probability density functions ϕ,

$$\int_{\mathbb{R}^N} \left(\frac{\phi}{\psi_\infty} - 1\right)^2 \psi_\infty\,dx \le \frac{1}{\lambda}\int_{\mathbb{R}^N} \left|\nabla\left(\frac{\phi}{\psi_\infty}\right)\right|^2 \psi_\infty dx. \tag{4}$$

The optimal parameter λ in (4) is the opposite of the smallest (in absolute value) non-zero eigenvalue of the Fokker-Planck operator $\nabla \cdot (\nabla V \cdot + \nabla \cdot)$, which is self-adjoint in $L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$ (see (7) below). Thus, λ is also called the spectral gap of the Fokker-Planck operator.

It is then standard to show that (4) is equivalent to the following inequality, which shows exponential convergence to the equilibrium for (2): for all initial conditions $\psi_0 \in L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$, for all times $t \ge 0$,

$$\|\psi_t - \psi_\infty\|_{L^2(\psi_\infty^{-1})} \le e^{-\lambda t}\|\psi_0 - \psi_\infty\|_{L^2(\psi_\infty^{-1})}, \tag{5}$$

where $\|\cdot\|_{L^2(\psi_\infty^{-1})}$ denotes the norm in $L^2(\mathbb{R}^N, \psi_\infty^{-1})$, namely $\|f\|^2_{L^2(\psi_\infty^{-1})} = \int_{\mathbb{R}^N} f^2(x)\psi_\infty^{-1}(x)\,dx$. This equivalence is a simple consequence of the following identity: if ψ_t is solution to (3), then

$$\frac{d}{dt}\|\psi_t - \psi_\infty\|^2_{L^2(\psi_\infty^{-1})} = -2\int_{\mathbb{R}^N} \left|\nabla\left(\frac{\psi_t}{\psi_\infty}\right)\right|^2 \psi_\infty dx. \tag{6}$$

In view of (5), the algorithm is efficient if λ is large, which is typically not the case if X_t is a metastable process (see [26]). A natural question is therefore how to design a Markovian dynamics which converges to the equilibrium distribution ψ_∞ (much) faster than (2). There are many approaches (importance sampling methods, constraining techniques, see for example [27]), and the focus here is on modifying the dynamics (2) to a non-reversible dynamics, which has the same invariant measure.

1.2 Non-reversible Diffusions

As noticed in [24, 25], one way to accelerate the convergence to equilibrium is to depart from reversible dynamics (see also [10] for related discussions for Markov Chains). Let us recall that the dynamics (2) is reversible in the sense that if X_0 is distributed according to $\psi_\infty(x)\,dx$, then $(X_t)_{0\le t\le T}$ and $(X_{T-t})_{0\le t\le T}$ have the same law. This is equivalent to the fact that the Fokker-Planck operator is self-adjoint in $L^2(\mathbb{R}^N, \psi_\infty^{-1}dx)$:

$$\begin{aligned}\int_{\mathbb{R}^N} \nabla\cdot(\nabla V\psi+\nabla\psi)\phi\,\psi_\infty^{-1}dx &= -\int_{\mathbb{R}^N} \nabla\big(\psi\psi_\infty^{-1}\big)\cdot\nabla\big(\phi\psi_\infty^{-1}\big)\psi_\infty dx\\ &= \int_{\mathbb{R}^N} \nabla\cdot(\nabla V\phi+\nabla\phi)\psi\,\psi_\infty^{-1}dx. \end{aligned} \tag{7}$$

Now, a natural *non-reversible* dynamics to sample from the distribution $\psi_\infty(x)\,dx$ is:

$$dX_t^b = \big(-\nabla V\big(X_t^b\big)+b\big(X_t^b\big)\big)\,dt+\sqrt{2}\,dW_t, \tag{8}$$

where b is taken to be divergence-free with respect to the invariant distribution $\psi_\infty(x)\,dx$:

$$\nabla\cdot\big(be^{-V}\big)=0, \tag{9}$$

so that $\psi_\infty(x)\,dx$ is still the invariant measure of the dynamics (8). A general way to construct such a b is to consider

$$b=J\nabla V, \tag{10}$$

where J is a constant antisymmetric matrix.

It is important to note that the dynamics (8) is non-reversible. Indeed, one can check that $(X_t^b)_{0\le t\le T}$ has the same law as $(X_{T-t}^{-b})_{0\le t\le T}$ (notice the minus sign in front of b), and thus not the same law as $(X_{T-t}^b)_{0\le t\le T}$. Likewise, Eq. (7) now becomes:

$$\int_{\mathbb{R}^N} \nabla\cdot\big((\nabla V-b)\psi+\nabla\psi\big)\phi\,\psi_\infty^{-1}dx = \int_{\mathbb{R}^N} \nabla\cdot\big((\nabla V+b)\phi+\nabla\phi\big)\psi\,\psi_\infty^{-1}dx.$$

Again, notice the change of sign in front of b.

From (10) it is clear that there are many (in fact, infinitely many) different ways to modify the reversible dynamics without changing the invariant measure. A natural question is whether the addition of a non-reversible term can improve the rate of convergence to equilibrium and, if so, whether there exists an optimal choice for the perturbation that maximizes the rate of convergence to equilibrium. The goal of this paper is to present a complete solution to this problem when the drift term in (8) is linear.

More precisely, let ψ_t^b denote the law of the process X_t^b, i.e. the solution to the Fokker-Planck equation

$$\partial_t\psi_t^b = \nabla\cdot\big((\nabla V-b)\psi_t^b+\nabla\psi_t^b\big). \tag{11}$$

Using the fact that ψ_∞ is a stationary solution to (11) (which is equivalent to (9)) and under the assumption that ψ_∞ satisfies the Poincaré inequality (4), one can check that the upper bound for the reversible dynamics (2) is still valid:

$$\left\| \psi_t^b - \psi_\infty \right\|_{L^2(\psi_\infty^{-1})} \le e^{-\lambda t} \left\| \psi_0^b - \psi_\infty \right\|_{L^2(\psi_\infty^{-1})}. \tag{12}$$

Actually, as in the reversible case, (12) (for all initial conditions ψ_0^b) is equivalent to (4). This is because (6) also holds for ψ^b solution to (11). In other words, adding a non-reversible part to the dynamics cannot be worse than the original dynamics (2) (where $b = 0$) in terms of exponential rate of convergence.

What we show below (for a linear drift) is that it is possible to choose b in order to obtain a convergence at exponential rate of the form:

$$\left\| \psi_t^b - \psi_\infty \right\|_{L^2(\psi_\infty^{-1})} \le C(V, b) e^{-\overline{\lambda} t} \left\| \psi_0^b - \psi_\infty \right\|_{L^2(\psi_\infty^{-1})}, \tag{13}$$

with $\overline{\lambda} > \lambda$ and $C(V, b) > 1$. It is important to note the presence of the constant $C(V, b)$ in the right-hand side of (13). For a reversible diffusion ($b = 0$), the spectral theorem forces the optimal $C(V, 0)$ to be equal to one, and $\overline{\lambda} = \lambda$, the Poincaré inequality constant of ψ_∞ (since (5) implies (4)). The interest in adding a non-reversible perturbation is precisely to allow for a constant $C(V, b) > 1$, which permits a rate $\overline{\lambda} > \lambda$. The difficulty is thus to design a b such that $\overline{\lambda}$ is large and $C(V, b)$ is not too large. In the following, we adopt a two-stage strategy: we first optimize b in order to get the largest possible $\overline{\lambda}$, and then we discuss how the constant $C(V, b)$ behaves for this optimal rate of convergence.

1.3 Bibliography

This problem was studied in [24] for a linear drift (namely V is quadratic and b is linear) and in [25] for the general case. It was shown in these works that the addition of a drift function b satisfying (9) helps to speed up convergence to equilibrium. Furthermore, the optimal convergence rate was obtained for the linear problem (see also Proposition 1 in the present paper) and some explicit examples were presented, for ordinary differential equations in two and three dimensions.

The behavior of the generator of the dynamics (8) under a strong non-reversible drift has also been studied [4, 6, 14]. It was shown in [14] that the spectral gap attains a finite value in the limit as the strength of the perturbation becomes infinite if and only if the operator $b \cdot \nabla$ has no eigenfunctions in an appropriate Sobolev space of index 1. These works, although relevant to our work, are not directly related to the present paper since our main focus is in obtaining the optimal perturbation rather than an asymptotic result. The effect of non-reversible perturbations to the constant in logarithmic Sobolev inequalities (LSI) for diffusions have also been studied, see [3, 13]. In these papers, examples were presented where the addition of a non-reversible perturbation can improve the constant in the LSI.

This work is also related to [16], where the authors use another idea to enhance the convergence to equilibrium. The principle is to keep a reversible diffusion, but to change the underlying Riemannian metric by considering

$$dX_t^M = -D\nabla V\left(X_t^M\right) dt + \sqrt{2D} dW_t$$

for a well chosen matrix D. More precisely, the authors apply this technique to a Hybrid Monte Carlo scheme. It would be interesting to set up some test cases in order to compare the two approaches: non-reversible drift *versus* change of the underlying metric.

Finally, we would like to mention related recent works on spectral properties of non-selfadjoint operators see for example [7, 15, 41] and references therein.

1.4 Outline of the Paper

In this paper, we study the case of a linear drift. Namely, we consider (2) with a quadratic potential

$$V(x) = \frac{1}{2} x^T S x, \tag{14}$$

where S is a positive definite $N \times N$ symmetric matrix. In the following, we denote $\mathcal{S}_N(\mathbb{R})$ the set of symmetric matrices and $\mathcal{S}_N^{>0}(\mathbb{R})$ the set of positive definite symmetric matrices. The equilibrium distribution thus has the density

$$\psi_\infty(x) = \frac{\det(S)^{1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{x^T S x}{2}\right). \tag{15}$$

It can be checked that if the vector field $b(x)$ is linear, it satisfies (9) if and only if $b = -JSx$ with $J = -J^T$ an antisymmetric real matrix, see Lemma 1. For a given S, the question is thus how to choose J in order to optimize the rate of convergence to equilibrium for the dynamics (8), which in our case becomes:

$$dX_t^J = -(I + J)SX_t^J\, dt + \sqrt{2}\, dW_t, \tag{16}$$

where I denotes the identity matrix in $\mathcal{M}_N(\mathbb{R})$, the set of $N \times N$ real valued matrices.

We provide an answer to this question. In particular:

1. We prove that it is possible to build an optimal J (denoted J_{opt}), which yields the best possible rate $\overline{\lambda}$ (denoted λ_{opt}) in (13).
2. We provide an algorithm for constructing an optimal matrix J_{opt}.
3. We obtain estimates on the constant $C(V, b) = C(S, J)$ in (13).

It appears that this procedure becomes particularly relevant in the situation when the condition number of S is large (namely for an original dynamics with multiple timescales, see Sects. 3.3 and 6). Discussions about the size of $C(S, J)$ with respect to this conditioning and to the dimension N can be carried out very accurately.

The reason why the case of linear drift is amenable to analysis is because it can be reduced to a linear algebraic problem, at least for the calculation of λ_{opt} and the construction of J_{opt}. One way to understand this is the following remark: the spectrum of an operator of the form (which is precisely the form of the generator of the dynamics (16)) $\mathcal{L} = -(Bx) \cdot \nabla + \Delta$, can be computed in terms of the eigenvalues of the matrix B. Here, B denotes any real square matrix whose eigenvalues have strictly positive real part. In [31] (see also [34, 35] and Proposition 10 below), it was indeed proven that the spectrum of $\mathcal{L}$ in L^p spaces weighted by the invariant measure of the dynamics ($p > 1$) consists of integer linear combinations of eigenvalues of B:

$$\sigma(\mathcal{L}) = \left\{ -\sum_{j=1}^{r} n_j \lambda_j, n_j \subset \mathbb{N} \right\}, \tag{17}$$

where $\{\lambda_j\}_{j=1}^r$ denote the r (distinct) eigenvalues of B. In particular, the spectral gap of the generator $\mathcal{L}$ is determined by the eigenvalues of B, and this yields a simple way to design the optimal matrix J_{opt}. On the other hand, the control of the constant $C(S,J)$ requires a more elaborate analysis, using Wick (in the sense of Wick ordered) calculus, see Sect. 5.3 below.

Compared to the related previous paper [24], our contributions are threefold: (i) we propose an algorithm to build the optimal matrix J_{opt}, (ii) we discuss how to get estimates on the constant $C(S,J)$ and (iii) we consider the longtime behavior of the partial differential equation (11) and not only of ordinary differential equations related to (16). In particular, our analysis covers also non Gaussian initial conditions for the SDE (16). Although the results that we obtain have a limited practical interest (there exist many efficient techniques to draw Gaussian random variables), we believe that this study is a first step towards further analysis, in particular for nonlinear drift terms.

The rest of the paper is organized as follows. In Sect. 1.5 we present the main results of this paper. In Sect. 2 we perform some preliminary calculations. The linear algebraic problem and the evolution of the corresponding ordinary differential equation are studied in Sect. 3. Direct computations of the expectations and the variances are performed in Sect. 4 for Gaussian initial data. The convergence to equilibrium for the non-reversible diffusion process for general initial data is then studied in Sect. 5. Results of numerical simulations are presented in Sect. 6.

1.5 Main Results

For a potential given by (14), our first result is a simple lemma which characterizes all non-reversible perturbations that satisfy the divergence-free condition (9).

Lemma 1 *Let $V(x)$ be given by (14) and let $b(x)=-Ax$ where $A\in\mathcal{M}_N(\mathbb{R})$. Then (9) is satisfied if and only if*

$$A=JS, \quad \text{with } J=-J^T. \tag{18}$$

Proof Equation (9) with $b=-Ax$ and quadratic potential (14) gives $\nabla\cdot(Ax\,e^{-\frac{x^TSx}{2}})=0$ which is equivalent to: $\forall x\in\mathbb{R}^N$, $\mathrm{Tr}(A)+(Ax)^T(Sx)=0$. This is equivalent to the conditions $\mathrm{Tr}(A)=0$ and $(A^TS)=-(A^TS)^T$. Set now $J=AS^{-1}$. We have $\mathrm{Tr}(JS)=0$ and $S(J+J^T)S=0$ which is equivalent to $J=-J^T$. □

We will denote the set of $N\times N$ real antisymmetric matrices by $\mathcal{A}_N(\mathbb{R})\subset\mathcal{M}_N(\mathbb{R})$. The following result concerns the optimization of the spectrum of the matrix $B_J=(I+J)S$, which appears in the drift of the dynamics (16) and plays a crucial role in the analysis; see Eq. (17).

Theorem 1 *Define $B_J=(I+J)S$. Then*

$$\max_{J\in\mathcal{A}_N(\mathbb{R})}\min \mathrm{Re}\big(\sigma(B_J)\big)=\frac{\mathrm{Tr}(S)}{N}. \tag{19}$$

Furthermore, there is a simple algorithm to construct matrices $J_{opt}\in\mathcal{A}_N(\mathbb{R})$ such that the maximum in (19) is attained. The matrix J_{opt} can be chosen so that the semi-group associated to $B_{J_{opt}}$ satisfies the bound

$$\big\|e^{-(I+J_{opt})St}\big\|\le C_N^{(1)}\kappa(S)^{1/2}\exp\left(-\frac{\mathrm{Tr}(S)}{N}t\right), \tag{20}$$

for all $t \geq 0$, *where the matrix norm is induced by the Euclidean norm on* $\mathbb{R}^N$ *and* $\kappa(S) = \|S\|\,\|S^{-1}\|$ *denotes the condition number.*

Theorem 1 is a straightforward consequence of Proposition 4 and Proposition 5 below, with an explicit expression for the constant $C_N^{(1)}$ given by (46). This expression allows to discuss the dependence of $C_N^{(1)}$ on the dimension N (see Remark 7 for details). The algorithm to construct the matrix J_{opt} is given in Fig. 1 below, at the end of Sect. 3.2.

The partial differential equation version of this result requires to introduce the generator

$$\mathcal{L}_J = -(B_J x) \cdot \nabla + \Delta$$

of the semigroup $(e^{t\mathcal{L}_J})_{t\geq 0}$ considered in $L^2(\mathbb{R}^N, \psi_\infty dx; \mathbb{C})$, where, we recall (see (15)),

$$\psi_\infty(x) = \frac{\det(S)^{1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{x^T S x}{2}\right).$$

Here $L^2(\mathbb{R}^N, \psi_\infty dx; \mathbb{C})$ denotes the set of functions $f : \mathbb{R}^N \to \mathbb{C}$ such that $\int_{\mathbb{R}^N} |f|^2(x)\psi_\infty(x)\,dx < \infty$.

Theorem 2 *For* $B_J = (I + J)S$ *with* $J \in \mathcal{A}_N$, *the drift-diffusion operator* $\mathcal{L}_J = -(B_J x).\nabla + \Delta$ *defined in* $L^2(\mathbb{R}^N, \psi_\infty dx; \mathbb{C})$ *with domain of definition*

$$D(\mathcal{L}_J) = \left\{u \in L^2\left(\mathbb{R}^N, \psi_\infty dx; \mathbb{C}\right),\ \mathcal{L}_J u \in L^2\left(\mathbb{R}^N, \psi_\infty dx; \mathbb{C}\right)\right\}$$

generates a contraction semigroup $(e^{t\mathcal{L}_J})_{t\geq 0}$ *and it has a compact resolvent. Optimizing its spectrum with respect to* J *gives*

$$\max_{J\in\mathcal{A}_N(\mathbb{R})} \min \mathrm{Re}\left(\sigma(-\mathcal{L}_J) \setminus \{0\}\right) = \frac{\mathrm{Tr}(S)}{N}. \tag{21}$$

Furthermore, the maximum in (21) *is attained for the matrices* $J_{opt} \in \mathcal{A}_N(\mathbb{R})$ *constructed as in Theorem* 1. *The matrix* J_{opt} *can be chosen so that*

$$\left\| e^{t\mathcal{L}_{J_{opt}}} u - \left(\int_{\mathbb{R}^N} u\psi_\infty dx\right)\right\|_{L^2(\psi_\infty)} \leq C_N^{(2)} \kappa(S)^{7/2} \exp\left(-\frac{\mathrm{Tr}(S)}{N} t\right) \left\| u - \left(\int_{\mathbb{R}^N} u\psi_\infty dx\right)\right\|_{L^2(\psi_\infty)} \tag{22}$$

holds for all $u \in L^2(\mathbb{R}^N, \psi_\infty dx; \mathbb{C})$ *and all* $t \geq 0$, *where* $\kappa(\cdot)$ *again denotes the condition number.*

Theorem 2 is a straightforward consequence of Proposition 12 below, with an explicit expression for the constant $C_N^{(2)}$ given by (64). The dependence of $C_N^{(2)}$ on the dimension N is discussed in Remark 9. A simple corollary of this result is the following:

Corollary 1 *Let us consider the Fokker Planck equation associated to the dynamics* (16) *on* X_t^J:

$$\partial_t \psi_t^J = \nabla \cdot \left(B_J x \psi_t^J + \nabla \psi_t^J\right), \tag{23}$$

where $B_J = (I + J)S$. *Let us assume that* $\psi_0^J \in L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$. *Then, by considering* $J = -J_{opt}$, *where* $J_{opt} \in \mathcal{A}_N(\mathbb{R})$ *refers to the matrix considered in Theorem* 2 *to get* (22), *the inequality*

$$\|\psi_t^J - \psi_\infty\|_{L^2(\psi_\infty^{-1})} \le C_N^{(2)} \kappa(S)^{7/2} \exp\left(-\frac{\mathrm{Tr}(S)}{N} t\right) \|\psi_0^J - \psi_\infty\|_{L^2(\psi_\infty^{-1})},$$

holds for all $t \ge 0$, *when* ψ_∞ *is defined by* (15).

Proof This result is based on the following simple remark: ψ_t^J is a solution to (23) in $L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$ if and only if $\psi_t^J \psi_\infty^{-1} = e^{t\mathcal{L}_{-J}}(\psi_0^J \psi_\infty^{-1})$ in $L^2(\mathbb{R}^N, \psi_\infty\,dx)$. Notice the minus sign in $\mathcal{L}_{-J}$. Then the exponential convergence is obtained from (22) using the equality:

$$\|\psi_t^J - \psi_\infty\|_{L^2(\psi_\infty^{-1})} = \left\| \psi_t^J \psi_\infty^{-1} - \left(\int_{\mathbb{R}^N} \psi_0^J \psi_\infty^{-1} \psi_\infty dx \right) \right\|_{L^2(\psi_\infty)}.$$

□

Remark 1 A more general result (in terms of the assumption on ψ_0^J) but with a less accurate upper bound is given in Proposition 8.

Remark 2 The partial differential equation

$$\partial_t f = \mathcal{L}_J f = -(B_J x) \cdot \nabla f + \Delta f$$

which we consider in Theorem 2 is the backward Kolmogorov equation associated with the dynamics (16). It is related to this stochastic differential equation through the Feynman-Kac formula $f(t,x) = \mathbb{E}^x(f(X_t^J))$ where X_t^J is the solution to (16) and $\mathbb{E}^x$ indicates that we consider a solution starting from $x \in \mathbb{R}^N$: $X_0^J = x$. The partial differential equation

$$\partial_t \psi_t^J = \nabla \cdot \left(B_J x \psi_t^J + \nabla \psi_t^J \right)$$

which we consider in the Corollary 1 is the Fokker Planck (or forward Kolmogorov) equation associated with (16): if $X_0^J \sim \psi_0^J(x)\,dx$, then for all times $t > 0$, ψ_t^J is the probability density function of X_t^J.

As explained in the proof of Corollary 1 above, these two partial differential equations are related through a conjugation. See also, e.g. [33, 42].

Remark 3 It would be interesting to explore extensions of this approach to the Langevin dynamics:

$$\begin{cases} dq_t = p_t\,dt, \\ dp_t = -\nabla V(q_t)\,dt - \gamma p_t\,dt + \sqrt{2\gamma}\,dW_t, \end{cases}$$

which is ergodic with respect to the measure $Z^{-1}\exp(-V(q) - |p|^2/2)\,dpdq$. For example the following modification

$$\begin{cases} dq_t = (I - J)p_t\,dt, \\ dp_t = -(I + J)\nabla V(q_t)\,dt - \gamma p_t\,dt + \sqrt{2\gamma}\,dW_t, \end{cases}$$

where J is an antisymmetric matrix leaves the measure $Z^{-1}\exp(-V(q)-|p|^2/2)\,dpdq$ stationary. In the linear case $V(x)=\frac{x^TSx}{2}$, this leads to a Kramers-Fokker-Planck operator which is a differential operator (at most) quadratic in $(q,p,\partial_q,\partial_p)$. Then the exponential decay rate can be reduced to some (more involved) linear algebra problem following [21]. About the constant prefactor in front of the decaying in time exponential, the argument based on the sectorial property used in Lemma 3 does not apply anymore. It has to be replaced by hypoelliptic estimates in the spirit of [11, 20, 21]. The reference [21] provides accurate results for differential operators with at most quadratic symbols.

2 A Useful Rescaling

The analysis will be carried out in a suitable system of coordinates which simplifies the calculations and the presentation of the intermediate results. We will perform one conjugation and a change of variables.

First, from the partial differential equation point of view, it appears to be useful to work in $L^2(\mathbb{R}^N,dx;\mathbb{C})$ instead of $L^2(\mathbb{R}^N,\psi_\infty dx;\mathbb{C})$, since this allows to use standard techniques from the spectral analysis of partial differential equations. In the following, the norm in $L^2(\mathbb{R}^N,dx;\mathbb{C})$ is simply denoted $\|\cdot\|_{L^2}$. For a general potential V, the mapping $u\mapsto\psi_\infty^{-1/2}u$ maps unitarily $L^2(\mathbb{R}^N,dx;\mathbb{C})$ into $L^2(\mathbb{R}^N,\psi_\infty dx;\mathbb{C})$ with the associated transformation rules for the differential operators:

$$e^{-\frac{V}{2}}\nabla e^{\frac{V}{2}}=\nabla+\frac{1}{2}\nabla V,\, e^{-\frac{V}{2}}\nabla^T e^{\frac{V}{2}}=\nabla^T+\frac{1}{2}\nabla V^T,$$

where ∇ and ∇^T denote the gradient and the divergence operators, respectively. Thus, the operator $\mathcal{L}=-\nabla V^T\nabla+b^T\nabla+\Delta$ is transformed into

$$\overline{\mathcal{L}}=e^{-\frac{V}{2}}\mathcal{L}e^{\frac{V}{2}}=\Delta-\frac{1}{4}|\nabla V|^2+\frac{1}{2}\Delta V+b^T\nabla+\frac{1}{2}b^T\nabla V. \tag{24}$$

In the linear case we consider in this paper, $V(x)=\frac{1}{2}x^TSx$ (where $S=S^T$ is positive definite), $b(x)=-Ax$ and $A=JS$, $J\in\mathcal{A}_N(\mathbb{R})$, (see Lemma 1), so that the operator $\mathcal{L}=\mathcal{L}_J=-(B_Jx)^T\nabla+\Delta$ with $B_J=(I+J)S$ becomes

$$\overline{\mathcal{L}_J}=\Delta-\frac{1}{4}x^TS^2x+\frac{1}{2}\mathrm{Tr}(S)+\frac{1}{2}\left(x^TSJ\nabla-\nabla^TJSx\right).$$

In the above calculation we have used $J^T=-J$, $x^TSJ^TSx=0$ and

$$\nabla^TBx=\sum_{i,j}\partial_{x_i}B_{ij}x_j=\sum_{i,j}x_jB_{ij}\partial_{x_i}+\sum_i B_{ii}=x^TB^T\nabla+\mathrm{Tr}(B)$$

with $B=SJ^T$, $B^T=-JS$ and $\mathrm{Tr}(SJ)=\mathrm{Tr}(S^{1/2}JS^{1/2})=0$. According to Lemma 1, we know that the kernel of $\overline{\mathcal{L}_J}$ is $\mathbb{C}e^{-\frac{V}{2}}=\mathbb{C}e^{-\frac{x^TSx}{4}}$. The operator $\overline{\mathcal{L}}_J$ is unitarily equivalent to the operator $\mathcal{L}_J$.

The aim of the second change of variables is to modify the kernel of the operator $\overline{\mathcal{L}}_J$ to a centered Gaussian with identity covariance matrix. Let us introduce the new coordinates $y=S^{1/2}x$, so that $\nabla_x=S^{1/2}\nabla_y$. Then the operator $\overline{\mathcal{L}_J}$ becomes:

$$\tilde{\mathcal{L}}_J=\nabla_y^TS\nabla_y-\frac{1}{4}y^TSy+\frac{1}{2}\mathrm{Tr}(S)+\frac{1}{2}\left(y^T\tilde{J}\nabla_y-\nabla^T\tilde{J}y\right) \tag{25}$$

where

$$\tilde{J} = S^{1/2} J S^{1/2} \in \mathcal{A}_N(\mathbb{R}).$$

The corresponding stochastic process is, in the new coordinate system ($Y_t = S^{1/2} X_t$):

$$dY_t = -(S + \tilde{J}) Y_t dt + \sqrt{2} S^{1/2} dW_t.$$

The L^2-normalized element of $\ker \tilde{\mathcal{L}_J}$ is now simply the standard Gaussian distribution $\frac{1}{(2\pi)^{N/4}} e^{-\frac{|y|^2}{4}}$. Notice that $\tilde{\mathcal{L}_J}$ is still acting in $L^2(\mathbb{R}^N, dx; \mathbb{C})$.

As a summary, $u(t,x)$ satisfies $\partial_t u = \mathcal{L}_J u$ if and only if $v(t,y) = \sqrt{\psi_\infty}(S^{-1/2} y)\, u(t, S^{-1/2} y)$ satisfies $\partial_t v = \tilde{\mathcal{L}}_J v$. We have $u(t,x) = e^{t\mathcal{L}_J} u_0(x)$ and $v(t,y) = e^{t\tilde{\mathcal{L}}_J} v_0(y)$ where $u_0 = u(0,\cdot)$ and $v_0 = v(0,\cdot)$ are related through $v_0(y) = \sqrt{\psi_\infty}(S^{-1/2} y)\, u_0(S^{-1/2} y)$. In particular, it is easy to check that for all $t \geq 0$,

$$\left\| e^{t\mathcal{L}_J} u_0 - \left(\int_{\mathbb{R}^N} u_0 \psi_\infty dx \right) \right\|_{L^2(\psi_\infty)} = (\det S)^{-1/4} \left\| e^{t\tilde{\mathcal{L}}_J} (I - \Pi_0) v_0 \right\|_{L^2}, \tag{26}$$

where

$$\big(\Pi_0(v_0)\big)(y) = (2\pi)^{-N/2} \left(\int_{\mathbb{R}^N} v_0(y) e^{-|y|^2/4} \, dy \right) e^{-|y|^2/4}$$

is the L^2-orthogonal projection of v_0 on the kernel $\mathbb{C} e^{-\frac{|y|^2}{4}}$ of $\tilde{\mathcal{L}}_J$. Thus, proving (22) is equivalent to proving

$$\left\| e^{t\tilde{\mathcal{L}}_{J_{opt}}} (I - \Pi_0) \right\|_{\mathcal{L}(L^2)} \leq C_N^{(2)} \kappa(S)^{7/2} \exp\left(-\frac{\operatorname{Tr}(S)}{N} t \right), \tag{27}$$

where here and in the following we use the standard operator norm

$$\|A\|_{\mathcal{L}(L^2)} = \sup_{u \in L^2(\mathbb{R}^N)} \frac{\|Au\|_{L^2}}{\|u\|_{L^2}}$$

for an arbitrary operator A.

In the following, we will mostly work with $\tilde{\mathcal{L}}_J$ and Y_t rather than with $\mathcal{L}_J$ and X_t.

3 The Linear Algebra Problem

The stochastic differential equation (8) for the linear case (quadratic potential) that we consider becomes

$$dX_t = -(I + J) S X_t \, dt + \sqrt{2} \, dW_t, \tag{28}$$

and is associated with the drift matrix

$$B_J = (I + J) S. \tag{29}$$

With the change of variables given in Sect. 2 ($Y_t = S^{1/2} X_t$), the stochastic differential equation (28) becomes

$$dY_t = -(S + \tilde{J}) Y_t \, dt + \sqrt{2} \, S^{1/2} \, dW_t.$$

The drift matrix is now

$$\tilde{B}_J = S^{1/2} B_J S^{-1/2} = (S + \tilde{J}), \tag{30}$$

where, we recall, $\tilde{J} = S^{1/2} J S^{1/2} \in \mathcal{A}_N(\mathbb{R})$. We first collect basic spectral properties of $\tilde{B}_J$ (or equivalently of B_J) when $J \in \mathcal{A}_N(\mathbb{R})$) and then show how this spectrum can be constructively optimized.

3.1 Spectrum of $\tilde{B}_J$ for a General $J \in \mathcal{A}_N(\mathbb{R})$

Proposition 1 *For $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$ (or equivalently $J = S^{-1/2}\tilde{J}S^{-1/2} \in \mathcal{A}_N(\mathbb{R})$) and $S \in \mathcal{S}_N^{>0}(\mathbb{R})$, the matrix $\tilde{B}_J = S + \tilde{J}$ has the following properties*:

(i) $\sigma(\tilde{B}_J) \subset \{z \in \mathbb{C}, \mathrm{Re}(z) > 0\}$.
(ii) $\mathrm{Tr}(\tilde{B}_J) = \mathrm{Tr}(S)$.
(iii) $\min \mathrm{Re}[\sigma(\tilde{B}_J)] \leq \frac{\mathrm{Tr}(S)}{N}$.

Notice that the properties stated above on $\tilde{B}_J$ also hold on B_J since $\sigma(\tilde{B}_J) = \sigma(B_J)$ and $\mathrm{Tr}(\tilde{B}_J) = \mathrm{Tr}(B_J)$.

Proof Let $\lambda \in \mathbb{C}$ be an eigenvalue of $\tilde{B}_J$ with corresponding (non-zero) eigenvector $x_\lambda \in \mathbb{C}^N$: $(S + \tilde{J})x_\lambda = \tilde{B}_J x_\lambda = \lambda x_\lambda$. Since S is a real matrix, the complex scalar product with x_λ gives $\lambda |x_\lambda|^2 = |S^{1/2} x_\lambda|^2 + (x_\lambda, \tilde{J} x_\lambda)_{\mathbb{C}}$. Here and in the following, the complex scalar product is taken to be right-linear and left-antilinear: for any X and Y in $\mathbb{C}^N$, $(X, Y)_{\mathbb{C}} = \overline{X}^T Y$. Using the fact that $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$, we get:

$$\mathrm{Re}(\lambda) = \frac{|S^{1/2} x_\lambda|^2}{|x_\lambda|^2} > 0.$$

This ends the proof of (i). The proof of (ii) follows immediately from the fact that the trace of the antisymmetric matrix $\tilde{J}$ is 0.

To prove (iii), let

$$\sigma(\tilde{B}_J) = \{\lambda_1, \lambda_2, \dots, \lambda_r\}$$

denote the spectrum of $\tilde{B}_J$, and let m_k denote the algebraic multiplicity of λ_k. Part (ii) says $\sum_{k=1}^r m_k \lambda_k = \mathrm{Tr}(S) \in \mathbb{R}$, and consequently:

$$\sum_{k=1}^r m_k \,\mathrm{Re}(\lambda_k) = \mathrm{Tr}(S).$$

Now, using the fact that $\sum_{k=1}^r m_k = N$, we conclude

$$\min \mathrm{Re}\big[\sigma(\tilde{B}_J)\big] = \min\big\{\mathrm{Re}(\lambda_k), k \in \{1, \dots, r\}\big\} \leq \frac{\mathrm{Tr}(S)}{N}. \qquad \square$$

3.2 Optimization of $\min \mathrm{Re}\,[\sigma(\tilde{B}_J)]$

Our goal now is to maximize $\min \mathrm{Re}[\sigma(B_J)]$ over $J \in \mathcal{A}_N(\mathbb{R})$, or equivalently, to maximize $\min \mathrm{Re}[\sigma(\tilde{B}_J)]$ over $\tilde{J} = S^{1/2} J S^{1/2} \in \mathcal{A}_N(\mathbb{R})$. Indeed, this is the quantity which will determine the exponential rate of convergence to equilibrium of the non-reversible dynamics (16) as it will become clear below.

From Proposition 1(iii), the maximum is obviously achieved if there exists a matrix $J \in \mathcal{A}_N(\mathbb{R})$ such that:

$$\forall \lambda \in \sigma(\tilde{B}_J), \quad \mathrm{Re}(\lambda) = \frac{\mathrm{Tr}(S)}{N}. \tag{31}$$

In the following proposition we obtain a characterization of the antisymmetric matrices $\tilde{J}$ (related to J through $\tilde{J} = S^{1/2} J S^{1/2}$) for which (31) is satisfied *and* $\tilde{B}_J$ is diagonalizable (see (33) below). This characterization requires to introduce a companion real symmetric positive definite matrix $Q \in \mathcal{S}_N^{>0}(\mathbb{R})$. The case of non-diagonalizable $\tilde{B}_J$ is then discussed, using an asymptotic argument. We finally show how this characterization can be used to develop an algorithm for constructing a matrix $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$ such that (31) is satisfied.

Proposition 2 *Assume that $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$ and that $S \in \mathcal{S}_N^{>0}(\mathbb{R})$. Then the following conditions are equivalent*:

(i) *The matrix $\tilde{B}_J = S + \tilde{J}$ is diagonalizable* (*in* $\mathbb{C}$) *and the spectrum of $\tilde{B}_J$ satisfies*

$$\sigma(\tilde{B}_J) \subset \frac{\mathrm{Tr}(S)}{N} + i\mathbb{R}. \tag{32}$$

(ii) *$\tilde{B}_J - \frac{\mathrm{Tr}(S)}{N} I$ is similar to an anti-adjoint matrix.*

(iii) *There exists a hermitian positive definite matrix $Q = \overline{Q}^T$ such that*

$$\tilde{J}Q - Q\tilde{J} = -QS - SQ + \frac{2\,\mathrm{Tr}(S)}{N} Q. \tag{33}$$

(iv) *There exists a real symmetric positive definite matrix $Q = Q^T$ such that* (33) *holds.*

Proof First we prove the equivalence between (i) and (ii). Equation (32) is equivalent to the statement that there exists a matrix $P \in GL_n(\mathbb{C})$ (where $GL_n(\mathbb{C})$ denotes the set of complex valued invertible matrices) such that

$$P^{-1}\left(\tilde{B}_J - \frac{\mathrm{Tr}(S)}{N} I\right) P = \mathrm{diag}(it_1, \dots, it_N)$$

for some t_k in $\mathbb{R}$, which is equivalent to statement (ii), since any anti-adjoint matrix can be diagonalized in $\mathbb{C}$.

To prove that (ii) implies (iii), we write statement (ii) as: there exists a matrix $P \in GL_n(\mathbb{C})$ such that

$$\left(\overline{P^{-1}\tilde{B}_J P}\right)^T - \frac{\mathrm{Tr}(S)}{N} I = -P^{-1}\tilde{B}_J P + \frac{\mathrm{Tr}(S)}{N} I. \tag{34}$$

Since $\tilde{B}_J = S + \tilde{J} \in \mathcal{M}_N(\mathbb{R})$ and $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$, we obtain

$$P^{-1}\tilde{J}P - \overline{P}^T \tilde{J}\left(\overline{P}^{-1}\right)^T = -\overline{P}^T S\left(\overline{P}^{-1}\right)^T - P^{-1}SP + \frac{2\,\mathrm{Tr}(S)}{N} I.$$

We multiply this equation left and right by P and $\overline{P}^T$ respectively, to obtain

$$\tilde{J}P\overline{P}^T - P\overline{P}^T\tilde{J} = -P\overline{P}^T S - SP\overline{P}^T + \frac{2\,\mathrm{Tr}(S)}{N} P\overline{P}^T. \tag{35}$$

Statement (iii) follows now by taking $Q = P\overline{P}^T$. Conversely, (iii) ⇒ (ii) follows from the writing $Q = P\overline{P}^T$, with $P \in GL_n(\mathbb{C})$ (take $P = \sqrt{Q}$) for any hermitian positive definite matrix Q. Then, one obtains (ii) by going back from (35) to (34). Finally, (iii) implies (iv) by taking the real part of (33) and using the fact that $\tilde{J}$ and S are real matrices. The converse (iv) ⇒ (iii) is obvious. This ends the proof. □

Remark 4 Notice that if $\tilde{J}$ is such that (32) is satisfied, so is $-\tilde{J}$ (and thus $\tilde{J}^T$). Indeed, if $(\tilde{J}, Q)$ satisfies (33), then $(-\tilde{J}, Q^{-1})$ also satisfies (33).

Let us give another equivalent formulation of Proposition 2(iv).

Lemma 2 *With the notation of Proposition 2, let us consider matrices $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$, $S \in \mathcal{S}_N^{>0}(\mathbb{R})$ and $Q \in \mathcal{S}_N^{>0}(\mathbb{R})$. Let us denote $\{\lambda_k\}_{k=1}^N$ the positive real eigenvalues of Q (counted with multiplicity), and $\{\psi_k\}_{k=1}^N$ the associated eigenvectors, which form an orthonormal basis of $\mathbb{R}^N$. Equation (33) is equivalent to the two conditions: for all k in $\{1, \dots, N\}$,*

$$(\psi_k, S\psi_k)_{\mathbb{R}} = \frac{\mathrm{Tr}(S)}{N} \tag{36}$$

and, for all $j \neq k$ in $\{1, \dots, N\}$,

$$(\lambda_j - \lambda_k)(\psi_j, \tilde{J}\psi_k)_{\mathbb{R}} = (\lambda_k + \lambda_j)(\psi_j, S\psi_k)_{\mathbb{R}}. \tag{37}$$

Proof Since $\{\psi_k\}_{k=1}^N$ form an orthonormal basis of $\mathbb{R}^N$, Eq. (33) is equivalent to this same equation tested against ψ_j^T on the left, and ψ_k on the right. This yields:

$$\lambda_k \psi_j^T \tilde{J}\psi_k - \lambda_j \psi_j^T \tilde{J}\psi_k = -\lambda_j \psi_j^T S\psi_k - \lambda_k \psi_j^T S\psi_k + \frac{2\,\mathrm{Tr}(S)}{N}\delta_{jk}\lambda_k,$$

where δ_{jk} is the Kronecker symbol. When $j = k$, we obtain (36) by using the antisymmetry of $\tilde{J}$, together with the fact that all eigenvalues of Q are non-zero. When $j \neq k$, we obtain (37). □

Notice that when the eigenvalues of Q are all with multiplicity one, $\tilde{J}$ is completely determined by (37): for all $j \neq k$ in $\{1, \dots, N\}$,

$$(\psi_j, \tilde{J}\psi_k)_{\mathbb{R}} = -\frac{\lambda_k + \lambda_j}{\lambda_k - \lambda_j}(\psi_j, S\psi_k)_{\mathbb{R}}. \tag{38}$$

Indeed, by the antisymmetry of $\tilde{J}$, the remaining entries are zero:

$$(\psi_j, \tilde{J}\psi_j)_{\mathbb{R}} = 0 \quad \text{for all } j \in \{1, \dots, N\}.$$

This motivates the following definition.

Definition 1 We will denote by $\mathcal{P}_{opt}(S)$ the set of pairs $(\tilde{J}, Q)$, where Q is a real symmetric positive definite matrix with N eigenvalues of multiplicity one and associated eigenvectors satisfying (36), and $\tilde{J}$ is the associated antisymmetric matrix defined by (38).

Notice that for any $(\tilde{J}, Q) \in \mathcal{P}_{opt}(S)$, $\tilde{J}$ is completely defined (by (38)) as soon as Q is chosen, so that the set $\mathcal{P}_{opt}(S)$ can be indexed by the set of matrices $Q \in \mathcal{S}_N^{>0}(\mathbb{R})$ with N eigenvalues of multiplicity one, and with eigenvectors ψ_k satisfying (36). As it will become clear below, the matrix Q of a pair $(\tilde{J}, Q) \in \mathcal{P}_{opt}(S)$ appears in the quantitative estimates of Theorem 1 and Theorem 2 through the constants $C_N^{(1)}$ and $C_N^{(2)}$. The construction of the pair $(\tilde{J}, Q)$ is also better understood by splitting the two steps: (1) construction of Q and (2) when Q is fixed, construction of $\tilde{J}$.

Remark 5 We would like to stress that the set $\mathcal{P}_{opt}(S)$ does not provide *all* the matrices $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$ such that $\sigma(\tilde{B}_J) \subset \frac{\mathrm{Tr}(S)}{N} + i\mathbb{R}$. Indeed, first, we have assumed that $\tilde{B}_J$ is diagonalizable and, second, in this case we have assumed moreover that Q has N eigenvalues of multiplicity one.

Actually the spectrum of $\tilde{B}_J$ depends continuously on $\tilde{J}$. Hence any limit $\tilde{J} = \lim_{n\to\infty} \tilde{J}_n$ in $\mathcal{A}_N(\mathbb{R})$ with $(\tilde{J}_n, Q_n) \in \mathcal{P}_{opt}(S)$ will lead to $\sigma(\tilde{B}_J) \subset \frac{\mathrm{Tr}(S)}{N} + i\mathbb{R}$. A particular case is interesting: Fix the real orthonormal basis $\{\psi_j\}_{j=1}^N$ and consider Q_α with the eigenvalues $(\alpha, \ldots, \alpha^N)$ with $\alpha > 0$. The unique associated antisymmetric matrix $\tilde{J}_\alpha$ is given by $(\psi_j, \tilde{J}_\alpha \psi_j)_\mathbb{R} = 0$ and

$$(\psi_j, \tilde{J}_\alpha \psi_k)_\mathbb{R} = -\frac{\alpha^k + \alpha^j}{\alpha^k - \alpha^j}(\psi_j, S\psi_k)_\mathbb{R}.$$

Taking the limit as $\alpha \to +\infty$ or $\alpha \to 0^+$ leads to

$$(\psi_j, \tilde{J}_\infty \psi_k)_\mathbb{R} = -\mathrm{sign}(k-j)(\psi_j, S\psi_k)_\mathbb{R}, \quad \tilde{J}_{0^+} = -\tilde{J}_\infty.$$

Actually, for such a choice $\tilde{J}_{opt} = \tilde{J}_\infty$ or $\tilde{J}_{opt} = \tilde{J}_{0^+}$, the matrix $S + \tilde{J}_{opt}$ is triangular in the basis $(\psi_j)_{1\le j\le N}$ and $\sigma(\tilde{B}_{J_{opt}}) = \{\frac{\mathrm{Tr}(S)}{N}\}$. In general (see for example Sect. 3.3), the matrix $\tilde{B}_{J_{opt}}$ may not be diagonalizable over $\mathbb{C}$ and may have Jordan blocks.

We end this section by providing a practical way to construct a couple $(\tilde{J}, Q)$ satisfying (33) (or equivalently $(\tilde{J}, Q) \in \mathcal{P}_{opt}(S)$), for a given $S \in \mathcal{S}_N^{>0}(\mathbb{R})$. The strategy is simple. We first build an orthonormal basis $\{\psi_k\}_{k=1}^N$ of $\mathbb{R}^N$ such that (36) is satisfied, then we *choose* the eigenvalues $\{\lambda_k\}_{k=1}^N$ distinct and positive, and define $\tilde{J}$ by (38). The only non-trivial task is thus to build the orthonormal basis $\{\psi_k\}_{k=1}^N$.

Proposition 3 *For every $S \in \mathcal{S}_N^{>0}(\mathbb{R})$, there exists an orthonormal basis $\{\psi_k\}_{k=1}^N$ of $\mathbb{R}^N$ such that (36) is satisfied.*

Proof We proceed by induction on N, using some Gram-Schmidt orthonormalization process. The result is obvious for $N = 1$. For a positive integer N, let us assume it is true for $N-1$ and let us consider $S \in \mathcal{S}_N^{>0}(\mathbb{R})$. Let us set $T = \frac{S}{\mathrm{Tr}(S)}$. The matrix T is in $\mathcal{S}_N^{>0}(\mathbb{R})$ with $\mathrm{Tr}(T) = 1$. Consequently $(\psi_i, T\psi_i)_\mathbb{R} > 0$, $i = 1, \ldots, N$ and $\sum_{i=1}^N (\psi_i, T\psi_i)_\mathbb{R} = 1$ for any orthonormal basis $\{\psi_i\}_{i=1}^N$ of $\mathbb{R}^N$. Assume that not all $(\psi_i, T\psi_i)_\mathbb{R}$ are equal to $1/N$. Then there exist $i_0, i_1 \in \{1, \ldots, N\}$ such that

$$(\psi_{i_0}, T\psi_{i_0})_\mathbb{R} < \frac{1}{N}, \qquad (\psi_{i_1}, T\psi_{i_1})_\mathbb{R} > \frac{1}{N}.$$

Set $\psi_t = \cos(t)\psi_{i_0} + \sin(t)\psi_{i_1}$ and consider the function $f(t) = (\psi_t, T\psi_t)_\mathbb{R}$. This function is continuous with $f(0) < 1/N$ and $f(\pi/2) > 1/N$. Consequently, there exists a $t_* \in (0, \pi/2)$

such that

$$(\psi_{t_*}, T\psi_{t_*})_{\mathbb{R}} = \frac{1}{N}. \tag{39}$$

Let now $\Pi = I - \psi_{t_*}(\psi_{t_*})^T$ denote the orthogonal projection to $\mathrm{Span}(\psi_{t_*})^{\perp}$ and define

$$T^1 = \frac{N}{N-1}\Pi T \Pi.$$

This operator is symmetric positive definite on $\mathrm{Span}(\psi_{t_*})^{\perp}$ with

$$\mathrm{Tr}\big(T^1\big) = \frac{N}{N-1}\big(\mathrm{Tr}(T) - (\psi_{t_*}, T\psi_{t_*})_{\mathbb{R}}\big) = 1.$$

It can thus be associated with a symmetric positive definite matrix in $\mathcal{M}_{N-1}(\mathbb{R})$. By the induction hypothesis there exists an orthonormal basis $(\tilde{\psi}_2, \dots, \tilde{\psi}_N)$ of $\mathrm{Span}(\psi_{t_*})^{\perp}$ such that $(\tilde{\psi}_i, T^1\tilde{\psi}_i)_{\mathbb{R}} = \frac{1}{N-1}$, $i = 2, \dots, N$. Let us consider the orthonormal basis of $\mathbb{R}^N$:

$$\tilde{\psi}_i = \begin{cases} \psi_{t_*}, & i = 1, \\ \tilde{\psi}_i, & i \geq 2. \end{cases}$$

We obtain $(\tilde{\psi}_1, T\tilde{\psi}_1)_{\mathbb{R}} = (\psi_{t_*}, T\psi_{t_*})_{\mathbb{R}} = \frac{1}{N}$ and, for $i \geq 2$, $(\tilde{\psi}_i, T\tilde{\psi}_i)_{\mathbb{R}} = \frac{N-1}{N}(\tilde{\psi}_i, T^1\tilde{\psi}_i)_{\mathbb{R}} = \frac{1}{N}$. This ends the induction argument. □

Remark 6 Finding t_* such that (39) is satisfied yields a simple algebraic problem in two dimensions. Let (i_0, i_1) be the two indices introduced in the proof. The matrix $((\psi_i, T\psi_j)_{\mathbb{R}})_{i,j\in\{i_0,i_1\}} \in \mathcal{M}_2(\mathbb{R})$ is

$$\begin{bmatrix} \alpha_0 & \beta \\ \beta & \alpha_1 \end{bmatrix} \quad \text{with} \quad \alpha_0 < \frac{1}{N}, \alpha_1 > \frac{1}{N}, \beta \in \mathbb{R}.$$

Then, $t_* \in (0, \pi/2)$ is given by

$$\tan t_* = \frac{-\beta + \sqrt{\beta^2 - (\alpha_1 - \frac{1}{N})(\alpha_0 - \frac{1}{N})}}{\alpha_1 - \frac{1}{N}}$$

and the vector ψ_{t_*} by

$$\psi_{t_*} = \frac{1}{\sqrt{1 + \tan^2 t_*}}(\psi_{i_0} + \tan t_* \psi_{i_1}).$$

The above proof and Remark 6 yield a practical algorithm, in the spirit of the Gram-Schmidt procedure, to build an orthonormal basis satisfying (36), see Fig. 1. This algorithm is used for the numerical experiments of Sect. 6. Notice that in the third step of the algorithm, only the vector ψ_{n+1} is concerned by the Gram-Schmidt procedure. The chosen vector ψ_{t_*} belongs to $\mathbb{R}\psi_n \oplus \mathbb{R}\psi_{n+1}$ and all the normalized vectors $(\psi_{n+2}, \dots, \psi_N)$ are already orthogonal to this plan.

A simple corollary of Proposition 3 is the following:

Algorithm for constructing an optimal nonreversible perturbation

Start from an arbitrary orthonormal basis $(\psi_1, \dots, \psi_N)$.

for $n = 1 : N-1$ **do**

1. Make a permutation of $(\psi_n, \dots, \psi_N)$ so that

$$(\psi_n, S\psi_n)_{\mathbb{R}} = \max_{k=n,\dots,N} (\psi_k, S\psi_k)_{\mathbb{R}} > \mathrm{Tr}(S)/N$$

and

$$(\psi_{n+1}, S\psi_{n+1})_{\mathbb{R}} = \min_{k=n,\dots,N} (\psi_k, S\psi_k)_{\mathbb{R}} < \mathrm{Tr}(S)/N.$$

2. Compute t_* such that $\psi_{t_*} = \cos(t_*)\psi_n + \sin(t_*)\psi_{n+1}$ satisfies $(\psi_{t_*}, S\psi_{t_*})_{\mathbb{R}} = \mathrm{Tr}(S)/N$ (see Remark 6 above).
3. Use a Gram-Schmidt procedure to change the set of vectors $(\psi_{t_*}, \psi_{n+1}, \dots, \psi_N)$ to an orthonormal basis $(\psi_{t_*}, \tilde{\psi}_{n+1}, \dots, \tilde{\psi}_N)$.

end

Fig. 1 Algorithm for constructing an optimal nonreversible perturbation

Proposition 4 *For every $S \in \mathcal{S}_N^{>0}(\mathbb{R})$, it is possible to build a matrix $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$ such that*

$$\frac{\mathrm{Tr}(S)}{N} = \min \mathrm{Re}\big[\sigma(\tilde{B}_J)\big] \geq \min \mathrm{Re}\big[\sigma(S)\big]$$

where $\tilde{B}_J = S + \tilde{J}$. Moreover, this holds with a strict inequality as soon as S admits two different eigenvalues.

In conclusion, the exponential rate of convergence may be improved by using a non-reversible perturbation, if and only if S is not proportional to the identity. We also refer to [24, Theorem 3.3] for another characterization of the strict inequality case.

3.3 Explicit Computations in the Two Dimensional Case

In the two dimensional case ($N = 2$), all the matrices J such that $\sigma(B_J) \subset \mathrm{Tr}(S)/N + i\mathbb{R}$ can be characterized. Accordingly, explicit accurate estimate of the exponential decay are available for the two-dimensional ordinary differential equation:

$$\frac{dx_t}{dt} = -(I + J)Sx_t \quad \text{with} \quad x_0 \text{ given in } \mathbb{R}^2. \tag{40}$$

After making the connection with our general construction of the optimal matrices J (see Definition 1), we investigate, for a given matrix $S \in \mathcal{S}_N^{>0}(\mathbb{R})$, the minimization, with respect to J, of the prefactor in the exponential decay law. We would like in particular to discuss the optimization of the constant factor in front of $\exp(-\mathrm{Tr}(S)t/2)$.

Without loss of generality, we may assume that $S = \left[\begin{smallmatrix} 1 & 0 \\ 0 & \lambda \end{smallmatrix}\right]$ and $J = \left[\begin{smallmatrix} 0 & a \\ -a & 0 \end{smallmatrix}\right]$, where $\lambda > 0$ is fixed. The eigenvalues of B_J belong to $\mathrm{Tr}(S)/2 = (1+\lambda)/2 + i\mathbb{R}$ if and only if

$$a^2 \geq \frac{(1-\lambda)^2}{4\lambda} \tag{41}$$

and then, the eigenvalues of $B_J = (I + J)S$ are $\mu_\pm = \frac{\lambda+1\pm i\sqrt{4\lambda a^2-(1-\lambda)^2}}{2}$. When the inequality (41) is strict, the associated eigenvectors are

$$u_\pm = \begin{pmatrix} 1 \\ \alpha_\pm \end{pmatrix} \quad \text{with } \alpha_\pm = \frac{\mu_\pm - 1}{a\lambda} = \frac{\lambda - 1 \pm i\sqrt{4\lambda a^2 - (1-\lambda)^2}}{2a\lambda}.$$

We have that $B_J = P\left[\begin{smallmatrix} \mu_+ & 0 \\ 0 & \mu_- \end{smallmatrix}\right]P^{-1}$ with $P = \left[\begin{smallmatrix} 1 & 1 \\ \alpha_+ & \alpha_- \end{smallmatrix}\right]$ and $P^{-1} = \frac{1}{\alpha_- - \alpha_+}\left[\begin{smallmatrix} \alpha_- & -1 \\ -\alpha_+ & 1 \end{smallmatrix}\right]$. The case $a = \pm\frac{(1-\lambda)}{2\sqrt{\lambda}}$ gives the matrix

$$B_J = \begin{bmatrix} 1 & \pm\frac{\sqrt{\lambda}(1-\lambda)}{2} \\ \mp\frac{1-\lambda}{2\sqrt{\lambda}} & \lambda \end{bmatrix}$$

which has a Jordan block when $\lambda \neq 1$. This ends the characterization of all the possible optimal J's in terms of the exponential rate.

Let us compare with the general construction of the pair $(Q, \tilde{J} = S^{\frac{1}{2}} J S^{\frac{1}{2}})$, see Definition 1. The matrix Q is diagonal in an orthonormal basis (ψ_1, ψ_2) which satisfies the relation (36). This yields $|\psi_1^1|^2 = |\psi_1^2|^2 = |\psi_2^1|^2 = |\psi_2^2|^2 = \frac{1}{2}$. Up to trivial symmetries one can fix

$$\psi_1 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \quad \text{and} \quad \psi_2 = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

Then, from (37), the eigenvalues λ_1, λ_2 of Q must satisfy

$$(\lambda_2 - \lambda_1)(-2a\sqrt{\lambda}) = (\lambda_2 + \lambda_1)(1 - \lambda)$$

and the limiting cases $a = \pm\frac{1-\lambda}{2\sqrt{\lambda}}$ are achieved after taking the limit $\frac{\lambda_2}{\lambda_1} \to +\infty$ or $\frac{\lambda_1}{\lambda_2} \to +\infty$.

Assume now $a^2 > \frac{(1-\lambda)^2}{4\lambda}$ and consider the two-dimensional Cauchy problem (40). Its solution equals $x_t = P\left[\begin{smallmatrix} \exp(-\mu_+ t) & 0 \\ 0 & \exp(-\mu_- t) \end{smallmatrix}\right]P^{-1}x_0$, which leads to

$$\|x_t\| \leq \|P\| \left\|P^{-1}\right\| \exp\left(-\frac{1+\lambda}{2}t\right)\|x_0\|,$$

when $\|\cdot\|$ denotes either the Euclidean norm on vectors or the associated matrix norm, $\|A\| = \sqrt{\max(\sigma(A^*A))}$. This yields the exponential convergence with rate $\mathrm{Tr}(S)/2 = (1 + \lambda)/2$, as soon as a satisfies $a^2 > \frac{(1-\lambda)^2}{4\lambda}$, while the degenerate case $a^2 = \frac{(1-\lambda)^2}{4\lambda}$ would give an upper bound $C(1+t)e^{-\frac{1+\lambda}{2}t}$. A more convenient matrix norm is the Frobenius norm given by $\|A\|_F^2 = \sum_{i,j=1}^2 |A_{ij}|^2 = \sum_{\alpha\in\sigma(A^*A)} \alpha$ with the equivalence in dimension 2, $\frac{1}{\sqrt{2}}\|A\|_F \leq \|A\| \leq \|A\|_F$. By recalling $\alpha_+ = \overline{\alpha_-}$, we get

$$\begin{aligned}
\|x_t\| &\leq \|P\|_F \left\|P^{-1}\right\|_F \exp\left(-\frac{1+\lambda}{2}t\right)\|x_0\| \\
&\leq 2\frac{(1+|\alpha_+|^2)}{|\alpha_- - \alpha_+|} \exp\left(-\frac{1+\lambda}{2}t\right)\|x_0\| \\
&\leq 2(\lambda+1)\frac{|a|}{\sqrt{4\lambda a^2 - (1-\lambda)^2}} \exp\left(-\frac{1+\lambda}{2}t\right)\|x_0\|.
\end{aligned}$$

Now, it is clear that the infimum of $\|P\|_F\|P^{-1}\|_F$ is obtained asymptotically as $|a| \to \infty$ and equals $\frac{\lambda+1}{\sqrt{\lambda}}$. It corresponds to an antisymmetric matrix J with infinite norm.

To end this section, we would like to discuss the situation when the original dynamics (when $J=0$) has two separated time scales, namely λ is very large or very small. In the case $\lambda \ll 1$, we observe that the optimal $\|P\|_F\|P^{-1}\|_F$ (and thus the optimal $\|P\|\|P^{-1}\|$) scales like $\frac{1}{\sqrt{\lambda}}$, and that this scaling in λ is already achieved by taking $a^2 = \frac{(1-\lambda)^2}{2\lambda}$ (twice the minimum value in (41)), since in this case, $\|P\|_F\|P^{-1}\|_F = \sqrt{2}\frac{(\lambda+1)}{\sqrt{\lambda}}$. In terms of rate of convergence to equilibrium, it means that, to get $\|x_t\|$ of the order of $\|x_0\|/2$, say, it takes a time of order $\ln(1/\lambda)$. This should be compared to the original dynamics (for $a=0$), for which this time is of order $1/\lambda$. Of course, a similar reasoning holds for $\lambda \gg 1$. Using an antisymmetric perturbation of the original dynamics, we are able to dramatically accelerate convergence to equilibrium.

4 Convergence to Equilibrium for Gaussian Laws and Applications

In this section, we use the results of the previous section in order to understand the longtime behavior of the mean and the covariance of X_t solution to (28):

$$dX_t = -(I+J)SX_t\,dt + \sqrt{2}\,dW_t.$$

In particular, if X_0 is a Gaussian random variable (including the case where X_0 is deterministic), then X_t remains a Gaussian random variable for all times, and understanding the longtime behavior of the mean $\mathbb{E}(X_t)$ and the covariance matrix $\mathrm{Var}(X_t) = \mathbb{E}(X_t \otimes X_t) - \mathbb{E}(X_t) \otimes \mathbb{E}(X_t)$ is equivalent to understanding the longtime behavior of the density of the process X_t, which is exactly Corollary 1 in a very specific case. Here and in the following, $\otimes$ denotes the tensor product: for two vectors x and y in $\mathbb{R}^N$, $x \otimes y = xy^T$ is a $N \times N$ matrix with (i,j)-component $x_i y_j$.

4.1 The Mean

Let us denote $x_t = \mathbb{E}(X_t)$, which is the solution to the ordinary differential equation

$$\frac{dx_t}{dt} = -(I+J)Sx_t, \quad x_0 = x. \tag{42}$$

The longtime behavior of x_t amounts to getting appropriate bounds on the semigroup $e^{-(I+J)St}$ or equivalently on $e^{-(S+\tilde{J})t}$.

When $J=0$, namely for the ordinary differential equation

$$\frac{dx_t}{dt} = -Sx_t, \quad x_0 = x,$$

we immediately deduce from the spectral representation of the positive symmetric matrix S that $\|x_t\| \le e^{-\rho t}\|x_0\|$ where $\rho := \min\{\sigma(S)\}$. The above bound implies that $\|e^{-St}\| \le e^{-\rho t}$, where $\|M\| = \sup_{x\in\mathbb{R}^N, x\neq 0} \frac{\|Mx\|}{\|x\|}$. Notice that $\rho \le \frac{\mathrm{Tr}(S)}{N}$.

We now derive a similar estimate for the semigroup generated by the perturbed matrix $\tilde{B}_J = S + \tilde{J}$ (or equivalently $B_J = (I+J)S$), when $(\tilde{J}, Q) \in \mathcal{P}_{opt}$, and show that a better exponential rate of convergence is obtained. As explained in the introduction, the price to pay for the improvement in the rate of convergence is the worsening of the constant (which is simply 1 in the reversible case) in front of the exponential.

Proposition 5 *For* $(\tilde{J}, Q) \in \mathcal{P}_{opt}$ *and* $J = S^{-1/2}\tilde{J}S^{-1/2}$, *the estimates*

$$\left\|e^{-(S+\tilde{J})t}\right\| \le \kappa(Q)^{1/2}\exp\left(-\frac{\mathrm{Tr}(S)}{N}t\right), \tag{43}$$

$$\left\|e^{-(I+J)St}\right\| \le \kappa\left(Q^{-1}S\right)^{1/2}\exp\left(-\frac{\mathrm{Tr}(S)}{N}t\right), \tag{44}$$

hold for every $t \ge 0$.

Proof Consider the ordinary differential equation

$$\frac{dy_t}{dt} = -(S+\tilde{J})y_t, \quad y_0 = y. \tag{45}$$

We introduce the scalar product $(\cdot,\cdot)_{Q^{-1}} := (\cdot, Q^{-1}\cdot)_{\mathbb{R}}$ on $\mathbb{R}^N$ with the corresponding norm $\|\cdot\|_{Q^{-1}}$. We calculate:

$$\begin{aligned}
\frac{d}{dt}\|y_t\|^2_{Q^{-1}} &= -2\big(y_t, Q^{-1}(S+\tilde{J})y_t\big)_{\mathbb{R}} \\
&= -\big(y_t, \big(Q^{-1}S + Q^{-1}\tilde{J} + SQ^{-1} - \tilde{J}Q^{-1}\big)y_t\big)_{\mathbb{R}} \\
&= -\left(y_t, \frac{2\,\mathrm{Tr}(S)}{N}Q^{-1}y_t\right)_{\mathbb{R}} = -\frac{2\,\mathrm{Tr}(S)}{N}\|y_t\|^2_{Q^{-1}}.
\end{aligned}$$

In the above, we have used the identity

$$Q^{-1}\tilde{J} - \tilde{J}Q^{-1} = -SQ^{-1} - Q^{-1}S + \frac{2\,\mathrm{Tr}(S)}{N}Q^{-1}$$

which follows from (33) after multiplication on the left and on the right by Q^{-1}. From the above we conclude that

$$\|y_t\|^2_{Q^{-1}} = e^{-2\frac{\mathrm{Tr}\,S}{N}t}\|y\|^2_{Q^{-1}}.$$

We now use the definition of the norm $\|\cdot\|_{Q^{-1}}$ to deduce that

$$\begin{aligned}
\|y_t\| &\le \left\|Q^{1/2}\right\|\left\|Q^{-1/2}y_t\right\| = \left\|Q^{1/2}\right\|\|y_t\|_{Q^{-1}} \\
&\le e^{-\frac{\mathrm{Tr}\,S}{N}t}\left\|Q^{1/2}\right\|\|y\|_{Q^{-1}} \le e^{-\frac{\mathrm{Tr}\,S}{N}t}\left\|Q^{1/2}\right\|\left\|Q^{-1/2}\right\|\|y\| \\
&= e^{-\frac{\mathrm{Tr}\,S}{N}t}\kappa(Q)^{1/2}\|y\|.
\end{aligned}$$

For the second estimate, we set $x_t = S^{-1/2}y_t$ and obtain

$$\begin{aligned}
\|x_t\| &\le \left\|S^{-1/2}Q^{1/2}\right\|\left\|Q^{-1/2}y_t\right\| \\
&\le e^{-\frac{\mathrm{Tr}(S)}{N}t}\left\|S^{-1/2}Q^{1/2}\right\|\left\|Q^{-1/2}y\right\| \\
&\le e^{-\frac{\mathrm{Tr}(S)}{N}t}\kappa\left(Q^{-1}S\right)^{1/2}\|x\|.
\end{aligned}$$

□

Proposition 5 shows that, for a well chosen matrix J, the mean $x_t = \mathbb{E}(X_t)$ converges to zero exponentially fast with a rate $\frac{\mathrm{Tr}(S)}{N}$. Equation (20) in Theorem 1 is a simple corollary of (44) and the inequality $\kappa(Q^{-1}S)^{1/2} \leq \kappa(Q)^{1/2}\kappa(S)^{1/2}$, so that $C_N^{(1)}$ in (20) can be chosen as

$$C_N^{(1)} = \kappa(Q)^{1/2}. \tag{46}$$

Remark 7 Using the upper bound (46), it can be shown that $C_N^{(1)}$ may be chosen independently of N, while keeping the norm of the perturbation $\tilde{J}$ under control. More precisely, for a given orthonormal basis (ψ_k) satisfying (36), let us consider the eigenvalues $\lambda_k = N + k$. On the one hand, $C_N^{(1)}$ remains small since $\kappa(Q) = 2$. On the other hand, using (38), we have

$$\begin{aligned} \|\tilde{J}\|_F^2 &= 2\sum_{j<k}\left(\frac{\lambda_k + \lambda_j}{\lambda_k - \lambda_j}\right)^2 (\psi_j, S\psi_k)_{\mathbb{R}}^2 \\ &\leq 2(4N)^2 \sum_{j<k} (\psi_j, S\psi_k)_{\mathbb{R}}^2 \leq 16N^2 \|S\|_F^2. \end{aligned}$$

Thus, the norm of $\tilde{J}$ (compared to the one of S) remains linear in N.

4.2 The Covariance

Let us again consider X_t solution to (28), and let us introduce the covariance

$$\Sigma_t = \mathbb{E}(X_t \otimes X_t) - \mathbb{E}(X_t) \otimes \mathbb{E}(X_t),$$

which satisfies the ordinary differential equation:

$$\frac{d\Sigma_t}{dt} = -(I + J)S\Sigma_t - \Sigma_t S(I - J) + 2I. \tag{47}$$

The equilibrium variance is $\Sigma_\infty = S^{-1}$.

Proposition 6 *For $(\tilde{J}, Q) \in \mathcal{P}_{opt}$ and $J = S^{-1/2}\tilde{J}S^{-1/2}$, the estimate*

$$\left\|\Sigma_t - S^{-1}\right\| \leq \kappa\left(Q^{-1}S\right) \exp\left(-2\frac{\mathrm{Tr}(S)}{N} t\right) \left\|\Sigma_0 - S^{-1}\right\| \tag{48}$$

holds for all $t \geq 0$, when the matrix norm is induced by the Euclidean norm on $\mathbb{R}^N$.

Proof The solution to (47) (see e.g. [29, 40]), Σ_t is

$$\Sigma_t = S^{-1} + e^{-tB_J}\left(\Sigma_0 - S^{-1}\right)e^{-tB_J^T}. \tag{49}$$

The result then follows from the estimate on $\|e^{-tB_J}\|$ in Proposition 5 above and $\|e^{-tB_J^T}\| = \|(e^{-tB_J})^T\| = \|e^{-tB_J}\|$. □

4.3 Gaussian Densities

As a corollary of Proposition 5 and Proposition 6, we get the following convergence to the Gaussian density (see (15))

$$\psi_\infty(x) = \frac{\det(\Sigma_\infty)^{-1/2}}{(2\pi)^{N/2}} \exp\left(-\frac{x^T \Sigma_\infty^{-1} x}{2}\right), \quad \text{with } \Sigma_\infty^{-1} = S.$$

Proposition 7 *Assume that X_t solves (28) while X_0 is a Gaussian random variable, so that X_t is a Gaussian random variable for all $t \geq 0$, with density ψ_t^J. Assume moreover that $J = S^{-1/2}\tilde{J}S^{-1/2}$, and that $(\tilde{J}, Q)$ is chosen in $\mathcal{P}_{opt}$. Then, the inequality*

$$\left\|\psi_t^J - \psi_\infty\right\|^2_{L^2(\psi_\infty^{-1})} \leq N2^N e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\left[1 + \|x_0\|^2 \exp\left(2e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x_0\|^2\right)\right],$$

holds for all times t larger than

$$t_0 = \frac{N}{2\,\mathrm{Tr}\,S}\ln\left[4\left(1 + \|S\|\right)\kappa\left(Q^{-1}S\right)\left(1 + \|S\Sigma_0\|\right)\right]. \tag{50}$$

This result is related to the result stated in Corollary 1, that will be proven in Sect. 5. Corollary 1 provides a better and uniform in time quantitative information (which has also a better behavior with respect to the dimension N according to (64) and Remark 9). On the contrary, it requires more regularity than Proposition 7 which does not assume $\psi_0^J \in L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$. Of course, with initial data outside $L^2(\mathbb{R}^N, \psi_\infty^{-1}\,dx)$, the convergence estimate makes sense only for sufficiently large times (hence the introduction of the positive time t_0 in Proposition 7).

Proof The Gaussian random vector X_t has the mean x_t, which solves (42), and the covariance Σ_t, solution to (47), so that

$$\psi_t^J(x) = \frac{\det(\Sigma_t)^{-1/2}}{(2\pi)^{N/2}}\exp\left(-\frac{(x - x_t)^T\Sigma_t^{-1}(x - x_t)}{2}\right).$$

When $t \geq t_0$, Proposition 6 gives $\|\Sigma_t - \Sigma_\infty\| \leq \frac{1}{4}\|\Sigma_\infty\|$ and thus, $\|\Sigma_\infty^{-\frac{1}{2}}\Sigma_t\Sigma_\infty^{-\frac{1}{2}} - I\| \leq \frac{1}{4}$, which yields $\frac{3}{4}\Sigma_\infty \leq \Sigma_t \leq \frac{5}{4}\Sigma_\infty$ and $\frac{4}{5}\Sigma_\infty^{-1} \leq \Sigma_t^{-1} \leq \frac{4}{3}\Sigma_\infty^{-1}$. In particular $\frac{\Sigma_t^{-1}}{2} \leq \Sigma_\infty^{-1}$ allows to compute

$$\begin{aligned}
&1 + \left\|\psi_t^J - \psi_\infty\right\|^2_{L^2(\psi_\infty^{-1})}\\
&= 1 + \int_{\mathbb{R}^N}\left(\psi_t^J - \psi_\infty\right)^2\psi_\infty^{-1} = \int_{\mathbb{R}^N}\frac{(\psi_t^J)^2}{\psi_\infty}\\
&= (2\pi)^{-N/2}\frac{\det(\Sigma_t)^{-1}}{\det(\Sigma_\infty)^{-1/2}}\int_{\mathbb{R}^N}\exp\left(-(x - x_t)^T\Sigma_t^{-1}(x - x_t) + \frac{x^T\Sigma_\infty^{-1}x}{2}\right).
\end{aligned}$$

We then use the relation, for A and B in $\mathcal{S}_N^{>0}(\mathbb{R})$,

$$\begin{aligned}
&(x - x_t)^T A(x - x_t) - x^T Bx\\
&= \left(x - \left(I - A^{-1}B\right)^{-1}x_t\right)^T(A - B)\left(x - \left(I - A^{-1}B\right)^{-1}x_t\right)\\
&\quad + x_t^T\left[A - A(A - B)^{-1}A\right]x_t,
\end{aligned}$$

with $A=\Sigma_t^{-1}$ and $B=\frac{\Sigma_\infty^{-1}}{2}$ in order to get

$$\begin{aligned}
1+&\left\|\psi_t^J-\psi_\infty\right\|^2_{L^2(\psi_\infty^{-1})}\\
&=(2\pi)^{-N/2}\frac{\det(\Sigma_t)^{-1}}{\det(\Sigma_\infty)^{-1/2}}\pi^{\frac{N}{2}}\det\left(\Sigma_t^{-1}-\frac{\Sigma_\infty^{-1}}{2}\right)^{-1/2}\\
&\quad\times\exp\left(x_t^T\left[\Sigma_t^{-1}\left(\Sigma_t^{-1}-\frac{\Sigma_\infty^{-1}}{2}\right)^{-1}\Sigma_t^{-1}-\Sigma_t^{-1}\right]x_t\right)\\
&=\frac{1}{\det(\Sigma_\infty^{-1}\Sigma_t)^{\frac12}\det(2I-\Sigma_\infty^{-1}\Sigma_t)^{\frac12}}\exp\big(x_t^T\big[2\big(2I-\Sigma_\infty^{-1}\Sigma_t\big)^{-1}-I\big]\Sigma_t^{-1}x_t\big).
\end{aligned}$$

After setting $R_t=I-\Sigma_\infty^{-1}\Sigma_t$, we deduce

$$\begin{aligned}
&\left\|\psi_t^J-\psi_\infty\right\|^2_{L^2(\psi_\infty^{-1})}\\
&\quad=\frac{1}{\det(I-R_t^2)^{\frac12}}-1\\
&\qquad+\frac{1}{\det(I-R_t^2)^{\frac12}}\times\big[\exp\big(x_t^T\big[2(I+R_t)^{-1}-I\big]\big)\Sigma_t^{-1}x_t\big)-1\big].
\end{aligned}\tag{51}$$

Let us start with the determinant $\det(I-R_t^2)$. The condition $t\geq t_0$ and Proposition 6 give

$$\|R_t\|=\left\|I-\Sigma_\infty^{-1}\Sigma_t\right\|\leq\frac{e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}}{4}\quad\text{and}\quad\left\|R_t^2\right\|\leq\frac{e^{-4\frac{\mathrm{Tr}(S)}{N}(t-t_0)}}{16}.$$

With $\|R_t^2\|\leq\frac{1}{16}$, we know

$$\left|\ln\det\big(I-R_t^2\big)\right|\leq\left|\mathrm{Tr}\big(\ln\big(I-R_t^2\big)\big)\right|\leq N\left\|\ln\big(I-R_t^2\big)\right\|\leq -N\ln\big(1-\left\|R_t^2\right\|\big).$$

We deduce

$$\frac{1}{\det(I-R_t^2)^{\frac12}}\leq\big(1-\left\|R_t^2\right\|\big)^{-\frac{N}{2}}\leq\left(\frac{16}{15}\right)^{\frac{N}{2}}\leq 2^{\frac{N}{2}}.$$

Concerning the exponential term in (51), Proposition 5 implies that the absolute value $|x_t^T[2(I+R_t)^{-1}-I]\Sigma_t^{-1}x_t|$ is smaller than

$$\big(1+2\left\|(I+R)^{-1}\right\|\big)\left\|\Sigma_t^{-1}\right\|\times\kappa\big(Q^{-1}S\big)\exp\left(-2\frac{\mathrm{Tr}(S)}{N}t\right)\|x_0\|^2.$$

The inequality $\|(1+R)^{-1}\|\leq(1-\|R\|)^{-1}\leq\frac43$ and the condition $t\geq t_0$ imply $\|\Sigma_t^{-1}\|\leq\frac43\|\Sigma_\infty^{-1}\|=\frac43\|S\|$ and

$$\left|x_t^T\big[2(I+R_t)^{-1}-I\big]\Sigma_t^{-1}x_t\right|\leq\frac{44}{9\times4}e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x_0\|^2.$$

We have proved

$$\|\psi_t^I - \psi_\infty\|^2_{L^2(\psi_\infty^{-1})} \le \left[\left(1 - \frac{e^{-4\frac{\mathrm{Tr}(S)}{N}(t-t_0)}}{16}\right)^{-\frac{N}{2}} - 1\right] + 2^{\frac{N}{2}}\left[\exp\left(\frac{11}{9}e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x_0\|^2\right) - 1\right].$$

By using $(1-x)^{-N/2} \le 1 + N2^{N/2}x$ when $x \in (0, 1/2)$ for the first term, and $e^y - 1 \le ye^y$ when $y \ge 0$ for the second term we finally obtain

$$\|\psi_t^I - \psi_\infty\|^2_{L^2(\psi_\infty^{-1})} \le N2^{\frac{N}{2}}e^{-4\frac{\mathrm{Tr}(S)}{N}(t-t_0)} + \frac{11}{9}2^{\frac{N}{2}}e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x_0\|^2\exp\left(\frac{11}{9}e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x_0\|^2\right),$$

which yields the result. □

4.4 General Initial Densities

As a corollary of Proposition 7, a convergence result for a general initial probability law can be proven by using an argument based on the conditioning by the initial data.

Proposition 8 *Let ψ_t^J satisfy the Fokker-Planck equation (23), with an initial probability law with density ψ_0^J and such that $\int_{\mathbb{R}^N} e^{\alpha\|x\|^2}\psi_0^J(x)\,dx < +\infty$ for some positive α. Assume moreover that $J = S^{-1/2}\tilde{J}S^{-1/2}$, that $(\tilde{J}, Q)$ are chosen in $\mathcal{P}_{opt}$ and that t_0 is given by (50). Then the inequality*

$$\|\psi_t^J - \psi_\infty\|^2_{L^2(\psi_\infty^{-1})} \le N2^{N+1}e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_\alpha)}\int_{\mathbb{R}^N} e^{\alpha\|x\|^2}\,\psi_0^J(x)dx, \tag{52}$$

holds for all $t \ge t_\alpha = t_0 + \frac{N}{2\,\mathrm{Tr}(S)}|\ln(\frac{\alpha}{4})|$.

Proof In all the proof, $J = S^{-1/2}\tilde{J}S^{-1/2}$ is fixed, with $(\tilde{J}, Q)$ chosen in $\mathcal{P}_{opt}$. For $x \in \mathbb{R}^N$ and $t > 0$, let us denote ϕ_t^x the density of the Gaussian process X_t^x solution to:

$$dX_t^x = -(I + J)SX_t^x\,dt + \sqrt{2}dW_t \quad \text{with } X_0^x = x.$$

Proposition 7 can be applied with $\psi_t^J = \phi_t^x$ and $\Sigma_0 = 0$, so that the time $t_0 = \frac{N}{2\,\mathrm{Tr}\,S}\ln[4(1 + \|S\|)\kappa(Q^{-1}S)]$ is fixed. With the decomposition

$$\psi_t^J(y) = \int_{\mathbb{R}^N}\phi_t^x(y)\psi_0^J(x)\,dx,$$

coming from $\phi_0^x = \delta_x$, we can write:

$$\|\psi_t^J - \psi_\infty\|^2_{L^2(\psi_\infty^{-1})} = \int_{\mathbb{R}^N}\frac{(\psi_t^J)^2(y)}{\psi_\infty(y)}\,dy - 1 = \int_{\mathbb{R}^N}\frac{1}{\psi_\infty(y)}\left(\int_{\mathbb{R}^N}\phi_t^x(y)\psi_0^J(x)\,dx\right)^2 dy - 1$$

$$
\begin{aligned}
&\le \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \frac{(\phi_t^x(y))^2}{\psi_\infty(y)}\,dy\,\psi_0^J(x)\,dx - 1\\
&= \int_{\mathbb{R}^N}\int_{\mathbb{R}^N} \left(\frac{(\phi_t^x(y))^2}{\psi_\infty(y)}\,dy - 1\right)\psi_0^J(x)\,dx.
\end{aligned}
$$

With Proposition 7, we deduce

$$
\begin{aligned}
\left\|\psi_t^J - \psi_\infty\right\|^2_{L^2(\psi_\infty^{-1})} &\le N2^N e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\\
&\quad\times\left[1 + \int_{\mathbb{R}^N}\|x\|^2 \exp\big(2e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\|x\|^2\big)\psi_0^J(x)\,dx\right]\\
&\le N2^N e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\left[1 + \frac{1}{\alpha}\int_{\mathbb{R}^N} e^{\alpha\|x\|^2}\psi_0^J(x)\,dx\right]\\
&\le N2^N e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\left(1+\frac{1}{\alpha}\right)\int_{\mathbb{R}^N} e^{\alpha\|x\|^2}\psi_0^J(x)\,dx,
\end{aligned}
$$

for $t \ge t_\alpha = t_0 + \frac{N}{2\,\mathrm{Tr}(S)}|\ln(\frac{\alpha}{4})|$. To get the second line, we used (for $t \ge t_\alpha$) $e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)} \le \frac{\alpha}{2}$ and (for $u > 0$) $ue^{\frac{\alpha}{2}u} \le \frac{2}{e\alpha}e^{\alpha u} \le \frac{1}{\alpha}e^{\alpha u}$. Writing $e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)} = e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_\alpha)}e^{-|\ln\frac{\alpha}{4}|}$ and discussing the two cases $\alpha \ge 4$ and $\alpha \le 4$ yield the result. □

The aim of the analysis using Wick calculus in Sect. 5 is to obtain more accurate and uniform in time estimates.

5 Convergence to Equilibrium for Initial Data in $L^2(\mathbb{R}^N, \psi_\infty dx)$

We shall study the spectral properties, and the norm estimates of the corresponding semigroup, for the generator $\tilde{\mathcal{L}}_J$ defined by (25) (with the dummy variable y replaced by x in the following):

$$
\tilde{\mathcal{L}}_J = \nabla^T S\nabla - \frac{1}{4}x^T Sx + \frac{1}{2}\mathrm{Tr}(S) + \frac{1}{2}\big(x^T\tilde{J}\nabla - \nabla^T\tilde{J}x\big).
$$

The operator $\tilde{\mathcal{L}}_J$ acts in $L^2(\mathbb{R}^N, dx;\mathbb{C})$ and is unitarily equivalent (when $\tilde{J} = S^{1/2}JS^{1/2}$, and after a change of variables, see Sect. 2) to

$$
\mathcal{L}_J = -(B_Jx)^T\nabla + \Delta \quad \text{with} \quad B_J = (I+J)S,\ J \in \mathcal{A}_N,
$$

acting on $L^2(\mathbb{R}^N, \psi_\infty dx;\mathbb{C})$. Since for $J \ne 0$, the operator $\tilde{\mathcal{L}}_J$ (or $\mathcal{L}_J$) is not self-adjoint, it is known (see [8, 15, 18–20, 41]) that the information about the spectrum is a first step in estimating the exponential decay of the semigroup, but that it has to be completed by estimates on the norm of the resolvent. This will be carried out by using a weighted L^2-norm associated with the construction of the matrices Q and J introduced in Sect. 3.

5.1 Additional Notation and Basic Properties of the Semigroup $e^{t\tilde{\mathcal{L}}_J}$

Let us introduce some additional notation.

- We choose the right-linear and left-antilinear convention for L^2-scalar products (or $\mathcal{S}-\mathcal{S}'$-duality products):

$$\langle f, g\rangle_{L^2} = \int_{\mathbb{R}^N} \overline{f(x)} g(x)\, dx.$$

- For a multi-index $n=(n_1,\dots,n_N)\in\mathbb{N}^N$, we will denote $n! = \prod_{j=1}^N n_j!$, $|n| = \sum_{j=1}^N n_j$ and when $X_1,\dots,X_N$ belong to a commutative algebra $X^n = \prod_{j=1}^N X_j^{n_j}$.
- The space of rapidly decaying complex valued $\mathcal{C}^\infty$ functions is

$$\mathcal{S}(\mathbb{R}^N) = \Big\{ f\in\mathcal{C}^\infty(\mathbb{R}^N),\ \forall\alpha,\beta\in\mathbb{N}^N, \exists C_{\alpha\beta}\in\mathbb{R}_+,\ \sup_{x\in\mathbb{R}^N}\big|x^\alpha\partial_x^\beta f(x)\big| \le C_{\alpha\beta}\Big\}$$

  and its dual is denoted $\mathcal{S}'(\mathbb{R}^N)$.
- The Weyl-quantization $q^W(x,D_x)$ of a symbol $q(x,\xi)\in\mathcal{S}'(\mathbb{R}^{2N}_{x,\xi})$ is an operator defined by its Schwartz-kernel

$$\big[q^W(x,D_x)\big](x,y) = \int_{\mathbb{R}^N} e^{i(x-y).\xi} q\left(\frac{x+y}{2},\xi\right)\frac{d\xi}{(2\pi)^N}.$$

  For example, for $q(x,\xi)=f(x)$, $q^W(x,D_x)$ is the multiplication by $f(x)$, for $q(x,\xi) = f(\xi)$, $q^W(x,D_x)$ is the convolution operator $f(-i\nabla)$, and for $q(x,\xi)=x^T\xi$, $q^W(x,D_x)$ is $\frac{1}{2i}(x^T\nabla+\nabla^T x)$.
- The Wick-quantization of a polynomial symbols of the variables $(z,\overline{z})$, where $z\in\mathbb{C}^N$ is an operator defined by replacing z_j with the so-called annihilation operator $a_j=\partial_{x_j}+\frac{x_j}{2}$ and $\overline{z}_j$ with the so-called creation operator $a_j^* = -\partial_{x_j}+\frac{x_j}{2}$. Wick's rule implies that for monomials involving both z and $\overline{z}$, the annihilation operators are gathered on the right-hand side and the creation operators on the left-hand side: For given multi-indices $\alpha,\beta\in\mathbb{N}^N$, the monomial $\overline{z}^\alpha z^\beta$ becomes $(a^*)^\alpha a^\beta$. A general presentation of the Wick calculus may be found in [1, 2]. In the following, we will use direct calculation based on the canonical commutation relation $[a_i,a_j^*]=\delta_{ij}$. We shall also use the vectorial notation $a=(a_1,\dots,a_N)^T$ and $a^*=(a_1^*,\dots,a_N^*)^T$.
- The orthogonal projection from $L^2(\mathbb{R}^N,dx;\mathbb{C})$ onto $\mathbb{C}e^{-\frac{|x|^2}{4}}$ will be denoted by Π_0.

Let us now recall a few basic properties of the semigroup $e^{t\tilde{\mathcal{L}}_J}$. The Weyl symbol of

$$-\tilde{\mathcal{L}}_J + \frac{\mathrm{Tr}(S)}{2} = -\nabla^T S\nabla + \frac{1}{4}x^T Sx - \frac{1}{2}\big(x^T\tilde{J}\nabla - \nabla^T\tilde{J}x\big)$$

is (using the fact that $\tilde{J}$ is antisymmetric)

$$q_J(x,\xi) = \xi^T S\xi + \frac{x^T Sx}{4} - \frac{i}{2}\big(x^T\tilde{J}\xi - \xi^T\tilde{J}x\big) = \xi^T S\xi + \frac{x^T Sx}{4} - ix^T\tilde{J}\xi, \tag{53}$$

which is a complex quadratic form on $\mathbb{R}^{2N}_{x,\xi}$. Besides, the operator $-\tilde{\mathcal{L}}_J$ is the Wick quantization of a quadratic polynomial since

$$\begin{aligned}-\tilde{\mathcal{L}}_J &= -\nabla^T S\nabla + \frac{1}{4}x^T Sx - \frac{1}{2}\mathrm{Tr}(S) - \frac{1}{2}\big(x^T\tilde{J}\nabla - \nabla^T\tilde{J}x\big)\\ &= a^{*,T}(S-\tilde{J})a.\end{aligned} \tag{54}$$

Proposition 9 *The differential operator $-\tilde{\mathcal{L}}_J$ is continuous from $\mathcal{S}(\mathbb{R}^N)$ into itself and from $\mathcal{S}'(\mathbb{R}^N)$ into itself. Its formal adjoint is $-\tilde{\mathcal{L}}_{-J}$. With the domain $D(-\tilde{\mathcal{L}}_J) = \{u \in L^2(\mathbb{R}^N, dx; \mathbb{C}), -\tilde{\mathcal{L}}_J u \in L^2(\mathbb{R}^N, dx; \mathbb{C})\}$, the operator $-\tilde{\mathcal{L}}_J$ is a maximal accretive and sectorial operator in $L^2(\mathbb{R}^N, dx; \mathbb{C})$. Its resolvent is compact and its kernel equals $\mathbb{C}e^{-\frac{|x|^2}{4}}$. The associated semigroup $(e^{t\tilde{\mathcal{L}}_J})_{t\geq 0}$ has the following properties*:

- *For any $u \in \mathcal{S}(\mathbb{R}^N)$ (resp. any $u \in \mathcal{S}'(\mathbb{R}^N)$), the map $[0, +\infty) \ni t \mapsto e^{t\tilde{\mathcal{L}}_J}u$ is a $\mathcal{S}(\mathbb{R}^N)$-valued (resp. $\mathcal{S}'(\mathbb{R}^N)$-valued) $\mathcal{C}^\infty$ function.*
- *For any $t > 0$, the operator $e^{t\tilde{\mathcal{L}}_J}$ maps continuously $\mathcal{S}'(\mathbb{R}^N)$ into $\mathcal{S}(\mathbb{R}^N)$.*
- *In the orthogonal decomposition $L^2(\mathbb{R}^N, dx; \mathbb{C}) = \bigoplus_{k\in\mathbb{N}}^{\perp} \mathcal{D}_k$ into the finite dimensional vector spaces spanned by Hermite functions with degree k:*

$$\mathcal{D}_k = \mathrm{Span}\left\{\left(a^*\right)^n e^{-\frac{|x|^2}{4}},\ n \in \mathbb{N}^N, |n| = k\right\},$$

the semigroup has a block diagonal decomposition

$$e^{t\tilde{\mathcal{L}}_J} = \bigoplus_{k\in\mathbb{N}}^{\perp} e^{t\tilde{\mathcal{L}}_J}\Big|_{\mathcal{D}_k}.$$

Proof As a differential operator with a polynomial Weyl symbol, $-\tilde{\mathcal{L}}_J$ is continuous from $\mathcal{S}(\mathbb{R}^N)$ (resp. $\mathcal{S}'(\mathbb{R}^N)$) into itself. Its formal adjoints has the Weyl symbols $\overline{q_J(x,\xi)} = q_{-J}(x,\xi)$ and equals $-\tilde{\mathcal{L}}_{-J}$. For $k \in \mathbb{N}$, set

$$\mathcal{H}^k = \left\{u \in L^2\left(\mathbb{R}^N, dx; \mathbb{C}\right), x^\alpha D_x^\beta u \in L^2\left(\mathbb{R}^N, dx; \mathbb{C}\right),\right.$$
$$\left.\text{for all } \alpha, \beta \in \mathbb{N}^N\ s.t.\ |\alpha| + |\beta| \leq k\right\}$$

and let $\mathcal{H}^{-k}$ be its dual space. They satisfy $\bigcap_{k\in\mathbb{Z}} \mathcal{H}^k = \mathcal{S}(\mathbb{R}^N)$ and $\bigcup_{k\in\mathbb{Z}} \mathcal{H}^k = \mathcal{S}'(\mathbb{R}^N)$. Since S is a real symmetric positive definite matrix, the inequality

$$\left|q_J(x,\xi)\right| \geq \xi^T S\xi + \frac{x^T Sx}{4} \geq C_S\left(|\xi|^2 + |x|^2\right)$$

implies that the operator $-\tilde{\mathcal{L}}_J$ is globally elliptic (see [17, 36, 37, 39]). Therefore, it is a bijection from $\mathcal{H}^k$ onto $\mathcal{H}^{k-2}$ for any $k \in \mathbb{Z}$. This provides the compactness of the resolvent and the maximality property. The sectorial property (see [38, Chap. VIII]) comes from

$$\langle u, -\tilde{\mathcal{L}}_J u\rangle_{L^2} = \left\langle u, a^{*,T} Sau\right\rangle_{L^2} - \left\langle u, a^{*,T} \tilde{J}au\right\rangle_{L^2}, \quad \text{with}$$
$$\left|\left\langle u,\ a^{*,T} \tilde{J}au\right\rangle_{L^2}\right| \leq \frac{\|\tilde{J}\|}{\min\sigma(S)}\left\langle u, a^{*,T} Sau\right\rangle_{L^2}.$$

This yields (using the fact that $\mathrm{Re}(\langle u, -\tilde{\mathcal{L}}_J u\rangle_{L^2}) = \langle u, a^{*,T} Sau\rangle_{L^2}$ and $\mathrm{Im}(\langle u, -\tilde{\mathcal{L}}_J u\rangle_{L^2}) = -\langle u, a^{*,T} \tilde{J}au\rangle_{L^2}$)

$$\forall u \in \mathcal{S}\left(\mathbb{R}^N\right), \quad \left|\arg\langle u, -\tilde{\mathcal{L}}_J u\rangle_{L^2}\right| \leq \theta, \tag{55}$$

with $0 \leq \tan(\theta) \leq \frac{\|\tilde{J}\|}{\min\sigma(S)} < +\infty$. Here and in the following, $\arg(z)$ denotes the argument of a complex number z.

Then the usual contour integration technique for sectorial operators (see for example [38, Theorem X.52] and its two corollaries) implies that $(-\tilde{\mathcal{L}}_J)^k e^{t\tilde{\mathcal{L}}_J}$ is bounded for any $k \in \mathbb{N}$

and any $t > 0$. Combined with the global ellipticity of $-\tilde{\mathcal{L}}_J$, this provides all our regularity results.

The orthogonal decomposition $L^2(\mathbb{R}^N, dx; \mathbb{C}) = \bigoplus_{k\in\mathbb{N}}^{\perp} \mathcal{D}_k$ is actually the spectral decomposition for the harmonic oscillator Hamiltonian $a^{*T}a$. From the Wick calculus (use either $[a_i, a_j^*] = \delta_{ij}$ or the general formula in [1, Proposition 2.7]), we deduce

$$\left[a^{*,T}a,\, a^{*,T}(S-\tilde{J})a\right] = a^{*,T}\left[I,\, (S-\tilde{J})\right]a = 0.$$

This implies that the spectral subspaces $\mathcal{D}_k$, $k \in \mathbb{N}$, are indeed invariant by the semigroup $e^{t\tilde{\mathcal{L}}_J}$. □

Note that with the last property, the question of estimating the convergence to equilibrium stated in Theorem 2 is equivalent to estimating the decay of the semigroup $e^{t\tilde{\mathcal{L}}_J}(I - \Pi_0)$ or $e^{t\tilde{\mathcal{L}}_J}|_{\mathcal{D}_0^{\perp}}$ where Π_0 is the orthogonal projection onto $\mathbb{C}e^{-\frac{|x|^2}{4}} = \mathcal{D}_0$ (see also (27)).

5.2 Spectrum of $\tilde{\mathcal{L}}_J$

The result of this section is a direct application of the general results of [21, 36, 37] developed after [22, 39]. See also [34, 35] where these general results are used in order to compute the spectrum of the generator of a linear SDE with, possibly degenerate diffusion matrix. This result was first obtained in [31] using different techniques.

Proposition 10 *The spectrum of the operator $-\tilde{\mathcal{L}}_J$ equals*

$$\sigma(-\tilde{\mathcal{L}}_J) = \left\{ \sum_{\lambda\in\sigma(\tilde{B}_J)} k_\lambda \lambda,\, k_\lambda \in \mathbb{N} \right\},$$

and its kernel is $\mathbb{C}e^{-\frac{|x|^2}{4}}$.

Proof The spectrum of the operator $q_J^W(x, D_x) = -\tilde{\mathcal{L}}_J + \frac{\mathrm{Tr}(S)}{2}$ associated with the elliptic quadratic Weyl symbol $q_J(x, \xi)$ defined by (53) equals, according to [21, Theorem 1.2.2],

$$\sigma\left(q_J^W(x, D_x)\right) = \left\{ \sum_{\substack{\lambda\in\sigma(F)\\ \mathrm{Im}\,\lambda\geq 0}} -i\lambda(r_\lambda + 2k_\lambda),\, k_\lambda \in \mathbb{N} \right\},$$

where F is the so-called Hamilton map associated with q_J, and r_λ is the algebraic multiplicity of $\lambda \in \sigma(F)$, i.e. the dimension of the characteristic space. The Hamilton map is the $\mathbb{C}$-linear map $F : \mathbb{C}^{2N} \to \mathbb{C}^{2N}$ associated with the matrix

$$F = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix} M_{q_J}, \quad \text{where } M_{q_J} = \begin{bmatrix} \frac{S}{4} & -\frac{i}{2}\tilde{J} \\ \frac{i}{2}\tilde{J} & S \end{bmatrix} \in \mathcal{M}_{2N}(\mathbb{C})$$

is the matrix of the $\mathbb{C}$-bilinear form associated with q_J. The matrix F is similar to $\tilde{F}$ defined by

$$\tilde{F} = \begin{bmatrix} \frac{1}{\sqrt{2}} & 0 \\ 0 & \sqrt{2} \end{bmatrix} F \begin{bmatrix} \sqrt{2} & 0 \\ 0 & \frac{1}{\sqrt{2}} \end{bmatrix} = \frac{1}{2}\begin{bmatrix} i\tilde{J} & S \\ -S & i\tilde{J} \end{bmatrix}.$$

Thus, the characteristic polynomial of F can be computed by

$$\begin{aligned}\det(F-\lambda I)=\det(\tilde F-\lambda I)&=2^{-2N}\begin{vmatrix} i\tilde J-2\lambda I & S\\ -S & i\tilde J-2\lambda I\end{vmatrix}\\ &=2^{-2N}\begin{vmatrix} i\tilde J-2\lambda I & S\\ -S-\tilde J-i2\lambda I & i(\tilde J+S+i2\lambda I)\end{vmatrix}\\ &=2^{-2N}\begin{vmatrix} i(\tilde J-S+i2\lambda I) & S\\ 0 & i(\tilde J+S+i2\lambda I)\end{vmatrix}\\ &=2^{-2N}\det(S-\tilde J-i2\lambda I)\det(S+\tilde J+i2\lambda I)\\ &=2^{-2N}\det(S+\tilde J-i2\lambda I)\det(S+\tilde J+i2\lambda I),\end{aligned}$$

where we used $\det(M)=\det(M^T)$ for $M=S-\tilde J-i2\lambda I$ in the last line. Using the fact that $\mathrm{Re}(\sigma(\tilde B_J))\geq 0$, we thus obtain that $\sigma(F)\cap\{\lambda,\mathrm{Im}\,\lambda\geq 0\}$ equals $\frac{i}{2}\sigma(S+\tilde J)=\frac{i}{2}\sigma(\tilde B_J)$. In particular one gets,

$$\sum_{\substack{\lambda\in\sigma(F)\\ \mathrm{Im}\,\lambda\geq 0}}-i\lambda 2k_\lambda=\sum_{\mu\in\sigma(\tilde B_J)}k_{i\mu/2}\mu$$

and

$$\sum_{\substack{\lambda\in\sigma(F)\\ \mathrm{Im}\,\lambda\geq 0}}-i\lambda r_\lambda=\frac{1}{2}\mathrm{Tr}(\tilde B_J)=\frac{\mathrm{Tr}(S)}{2}.$$

This concludes the proof. □

The Gearhart-Prüss theorem (see [12, 19, 41]) provides the following corollary.

Corollary 2 *When the pair $(\tilde J,Q)$ belongs to $\mathcal{P}_{opt}$, the spectrum of $-\tilde{\mathcal{L}}_J$ is contained in*

$$\{0\}\cup\left\{z\in\mathbb{C},\mathrm{Re}\,z\geq\frac{\mathrm{Tr}(S)}{N}\right\}$$

and

$$\lim_{t\to\infty}\frac{1}{t}\ln\left\|e^{t\tilde{\mathcal{L}}_J}(I-\Pi_0)\right\|_{\mathcal{L}(L^2)}=-\frac{\mathrm{Tr}(S)}{N},$$

where, we recall, $\|e^{t\tilde{\mathcal{L}}_J}(I-\Pi_0)\|_{\mathcal{L}(L^2)}=\sup_{u\in\mathcal{D}_0^\perp}\frac{\|e^{t\tilde{\mathcal{L}}_J}u\|_{L^2}}{\|u\|_{L^2}}$.

The above logarithmic convergence is weaker than an estimate $\|e^{t\tilde{\mathcal{L}}_J}\|\leq Ce^{-\frac{\mathrm{Tr}(S)}{N}}$ with a good control of the constant C. Obtaining such a control is not an easy task for general semigroups with non self-adjoint generators (see [15, 18–20]). This is the subject of the next section.

5.3 Convergence to Equilibrium for $e^{t\tilde{\mathcal{L}}_J}$

Consider a pair $(\tilde{J}, Q) \in \mathcal{P}_{opt}$ according to Definition 1. We recall that $(\tilde{J}, Q) \in \mathcal{P}_{opt}$ satisfies (33). We associate to the matrix Q the operator

$$C_Q = a^{*,T} Qa \tag{56}$$

which will be used to define a natural functional space to study the norm of $e^{t\tilde{\mathcal{L}}_J}$ in Proposition 11 below. The operator C_Q is the Wick-quantization of the polynomial $\overline{z}^T Qz$ and it has the following properties:

- It is continuous from $\mathcal{S}(\mathbb{R}^N)$ into itself and from $\mathcal{S}'(\mathbb{R}^N)$ into itself.
- It is globally elliptic (see [17, 36]) and it has a compact resolvent.
- It is a non negative self-adjoint operator in $L^2(\mathbb{R}^N, dx; \mathbb{C})$ with the domain $D(C_Q) = \{u \in L^2(\mathbb{R}^N, dx; \mathbb{C}), C_Q u \in L^2(\mathbb{R}^N, dx; \mathbb{C})\}$.
- Its kernel is $\mathbb{C}e^{-\frac{|x|^2}{4}}$.
- It is block diagonal in the decomposition $L^2(\mathbb{R}^N, dx; \mathbb{C}) = \bigoplus_{k\in\mathbb{N}}^{\perp} \mathcal{D}_k$:

$$\forall t \in \mathbb{R}, \quad e^{itC_Q} = \bigoplus_{k\in\mathbb{N}}^{\perp} e^{itC_Q}|_{\mathcal{D}_k}. \tag{57}$$

Let us introduce the two Hilbert spaces:

- $\mathcal{H}_Q^1 = \{u \in L^2(\mathbb{R}^N, dx; \mathbb{C}), \langle u, C_Q u\rangle_{L^2} < +\infty\}$, naturally endowed with the scalar product

$$\langle u, v\rangle_{\mathcal{H}_Q^1} = \langle u, v\rangle_{L^2} + \langle u, C_Q v\rangle_{L^2};$$

- $\dot{\mathcal{H}}_Q^1 = \mathcal{H}_Q^1 \cap \mathcal{D}_0^{\perp}$ (where, we recall, $\mathcal{D}_0 = \mathbb{C}e^{-\frac{|x|^2}{4}}$) endowed with the scalar product

$$\langle u, v\rangle_{\dot{\mathcal{H}}_Q^1} = \langle u, C_Q v\rangle_{L^2}.$$

Proposition 11 *Assume that the pair $(\tilde{J}, Q)$ belongs to $\mathcal{P}_{opt}$. Then the semigroup $(e^{t\tilde{\mathcal{L}}_J})_{t\geq 0}$ is a contraction semigroup on $\mathcal{H}_Q^1$ satisfying the following estimate*:

$$\forall t \geq 0, \quad \left\| e^{t\tilde{\mathcal{L}}_J}(I - \Pi_0)\right\|_{\mathcal{L}(\dot{\mathcal{H}}_Q^1)} \leq e^{-\frac{\mathrm{Tr}(S)}{N}t}, \tag{58}$$

where $\|e^{t\tilde{\mathcal{L}}_J}(I - \Pi_0)\|_{\mathcal{L}(\dot{\mathcal{H}}_Q^1)} = \sup_{u\in\dot{\mathcal{H}}_Q^1} \frac{\|e^{t\tilde{\mathcal{L}}_J}u\|_{\dot{\mathcal{H}}_Q^1}}{\|u\|_{\dot{\mathcal{H}}_Q^1}}$.

Proof The operator $e^{t\tilde{\mathcal{L}}_j}$ is block diagonal (see Proposition 9) in the decomposition $\mathcal{D}_0 \oplus^{\perp} \mathcal{D}_0^{\perp} = \bigoplus_{k\in\mathbb{N}}^{\perp} \mathcal{D}_k$ which is an orthogonal decomposition in $L^2(\mathbb{R}^N, dx; \mathbb{C})$ and also in $\mathcal{H}_Q^1$ owing to (57). With $e^{t\tilde{\mathcal{L}}_J}e^{-\frac{|x|^2}{4}} = e^{-\frac{|x|^2}{4}}$, the semigroup property on $\mathcal{H}^1$ is thus a consequence of the estimate (58) in $\dot{\mathcal{H}}_Q^1$.

Using the relation (33) together with the inequality (65) of Lemma 4 proved at the end of this section, we have: for all $u \in \mathcal{D} = \mathbb{C}[x_1, \ldots, x_N]e^{-\frac{|x|^2}{4}} \cap \mathcal{D}_0^{\perp}$,

$$\left\langle u, \left(-\tilde{\mathcal{L}}_J^* C_Q - C_Q\tilde{\mathcal{L}}_J\right)u\right\rangle_{L^2} \geq \frac{2\,\mathrm{Tr}(S)}{N}\langle u, C_Q u\rangle_{L^2}.$$

Since the semigroup $(e^{t\tilde{\mathcal{L}}_J})_{t\geq 0}$ is a strongly $\mathcal{C}^1$ semigroup on $\mathcal{S}(\mathbb{R}^N)$ and leaves $\mathcal{D} \subset \mathcal{S}(\mathbb{R}^N)$ invariant, we can compute for any $u \in \mathcal{D}$,

$$\begin{aligned}\frac{d}{dt}\big\langle e^{t\tilde{\mathcal{L}}_J}u, C_Q e^{t\tilde{\mathcal{L}}_J}u\big\rangle_{L^2} &= \big\langle e^{t\tilde{\mathcal{L}}_J}u, \big(\tilde{\mathcal{L}}_J^* C_Q + C_Q\tilde{\mathcal{L}}_J\big)e^{t\tilde{\mathcal{L}}_J}u\big\rangle_{L^2} \\ &\leq -\frac{2\,\mathrm{Tr}(S)}{N}\big\langle e^{t\tilde{\mathcal{L}}_J}u,\, C_Q e^{t\tilde{\mathcal{L}}_J}u\big\rangle_{L^2}.\end{aligned}$$

The proof is then completed using the density of $\mathcal{D}$ in $\dot{\mathcal{H}}^1_Q$. □

We are now in position to state the main result of this section.

Proposition 12 *Assume that the pair $(\tilde{J}, Q)$ belongs to $\mathcal{P}_{opt}$. Then the semigroup $(e^{t\tilde{\mathcal{L}}_J})_{t\geq 0}$ satisfies*:

$$\begin{aligned}\forall t \geq 0,\quad &\big\|e^{t\tilde{\mathcal{L}}_J}(I - \Pi_0)\big\|_{\mathcal{L}(L^2)} \\ &\leq 2^5 N\kappa(Q)^{1/2}\left(\frac{\max\sigma(Q)}{\min_{\lambda,\lambda'\in\sigma(Q),\,\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2 \kappa(S)^{7/2} e^{-\frac{\mathrm{Tr}(S)}{N}t}.\end{aligned}$$

Proof From the inequalities on real symmetric matrices $\min\sigma(Q)\, I \leq Q \leq \max\sigma(Q)\, I$ and $\min\sigma(S)\, I \leq S \leq \max\sigma(S)\, I$ and from

$$C_Q = \sum_{i,j=1}^N a_i^* Q_{ij} a_j, \qquad -\frac{\mathcal{L}_J + \mathcal{L}_J^*}{2} = \sum_{i,j=1}^N a_i^* S_{ij} a_j,$$

we deduce the following inequalities on self-adjoint operators:

$$\begin{aligned}&\min\sigma(Q) a^{*,T} a \leq C_Q \leq \max\sigma(Q) a^{*,T} a, \\ &\min\sigma(S) a^{*,T} a \leq -\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2} \leq \max\sigma(S) a^{*,T} a, \quad \text{and} \\ &-\frac{\min\sigma(Q)}{\max\sigma(S)}\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2} \leq C_Q \leq -\frac{\max\sigma(Q)}{\min\sigma(S)}\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2}.\end{aligned}$$

Here, we have used the fact that $-\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2}$ is the Wick quantization of $(z, Sz)_{\mathbb{C}}$. Hence, using Proposition 11, the following inequalities hold: for any $u \in \dot{\mathcal{H}}^1_Q$ and any $t \geq t_0 > 0$,

$$\begin{aligned}&\left\langle e^{t\tilde{\mathcal{L}}_J}u, -\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2} e^{t\tilde{\mathcal{L}}_J}u\right\rangle_{L^2} \\ &\leq \frac{\max\sigma(S)}{\min\sigma(Q)}\big\|e^{t\tilde{\mathcal{L}}_J}u\big\|^2_{\dot{\mathcal{H}}^1_Q} \\ &\leq \frac{\max\sigma(S)}{\min\sigma(Q)} e^{-2\frac{\mathrm{Tr}(S)}{N}(t-t_0)}\big\|e^{t_0\tilde{\mathcal{L}}_J}u\big\|^2_{\dot{\mathcal{H}}^1_Q} \\ &\leq \kappa(Q)\kappa(S) e^{-2\frac{\mathrm{Tr}(S)}{N}t} e^{2\frac{\mathrm{Tr}(S)}{N}t_0}\left\langle e^{t_0\tilde{\mathcal{L}}_J}u, -\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2} e^{t_0\tilde{\mathcal{L}}_J}u\right\rangle_{L^2}\end{aligned}$$

$$\leq \kappa(Q)\kappa(S)e^{-2\frac{\mathrm{Tr}(S)}{N}t}e^{2\frac{\mathrm{Tr}(S)}{N}t_0}\left\|e^{t_0\tilde{\mathcal{L}}_J}u\right\|_{L^2}\left\|\tilde{\mathcal{L}}_J e^{t_0\tilde{\mathcal{L}}_J}u\right\|_{L^2}.$$

Using the inequalities

$$\forall v \in \mathcal{D}_0^\perp, \quad \min\sigma(S)\|v\|_{L^2}^2 \leq \left\langle v, -\frac{\tilde{\mathcal{L}}_J + \tilde{\mathcal{L}}_J^*}{2}v\right\rangle_{L^2} \leq \|v\|_{L^2}\|\tilde{\mathcal{L}}_J v\|_{L^2},$$

with $v = e^{t\tilde{\mathcal{L}}_J}u$ and $v = e^{t_0\tilde{\mathcal{L}}_J}u$, we deduce

$$\left\|e^{t\tilde{\mathcal{L}}_J}u\right\|_{L^2}^2 \leq \kappa(Q)\kappa(S)e^{-2\frac{\mathrm{Tr}(S)}{N}t}\frac{e^{2\frac{\mathrm{Tr}(S)}{N}t_0}}{t_0^2\min\sigma(S)^2}\left\|t_0\tilde{\mathcal{L}}_J e^{t_0\tilde{\mathcal{L}}_J}u\right\|_{L^2}^2.$$

By taking $t_0 = \frac{N}{\mathrm{Tr}(S)} \geq \frac{1}{\max\sigma(S)}$, we obtain, for all $u \in \dot{\mathcal{H}}_Q^1$,

$$\left\|e^{t\tilde{\mathcal{L}}_J}u\right\|_{L^2}^2 \leq \kappa(Q)\kappa(S)^3 e^{-2\frac{\mathrm{Tr}(S)}{N}t}e^2\sup_{t'>0}\left\|t'\tilde{\mathcal{L}}_J e^{t'\tilde{\mathcal{L}}_J}\right\|_{\mathcal{L}(L^2)}^2\|u\|_{L^2}^2. \tag{59}$$

The Lemma 3 below provides the bound

$$\sup_{t'>0}\left\|t'\tilde{\mathcal{L}}_J e^{t'\tilde{\mathcal{L}}_J}\right\|_{\mathcal{L}(L^2)}^2 \leq \frac{1}{\pi^2\sin^4\alpha} \tag{60}$$

with $\alpha \in (0, \pi/4)$ defined by

$$\tan\left(\frac{\pi}{2} - 2\alpha\right) = \sup_{u\in D(\tilde{\mathcal{L}}_J)}\frac{|\mathrm{Im}\langle u, \tilde{\mathcal{L}}_J u\rangle_{L^2}|}{|\mathrm{Re}\langle u, \tilde{\mathcal{L}}_J u\rangle_{L^2}|} \leq \frac{\|\tilde{J}\|}{\min\sigma(S)}.$$

The last inequality was proven in (55) above. We thus obtain

$$\frac{1}{\sin\alpha} \leq \frac{2\cos\alpha}{\cos(2\alpha)}\frac{\|\tilde{J}\|}{\min\sigma(S)}.$$

In view of (60), one can assume that $\alpha \in (0, \pi/8)$ (up to changing α by $\min(\alpha, \pi/8)$) so that

$$\frac{1}{\sin\alpha} \leq 2\sqrt{2}\frac{\|\tilde{J}\|}{\min\sigma(S)}. \tag{61}$$

When $(\tilde{J}, Q) \in \mathcal{P}_{opt}$ (see Definition 1), the relation (38) provides an expression of the linear mapping associated with $\tilde{J}$ in the orthonormal basis $(\psi_k)_{1\leq k\leq N}$. In this basis, the Frobenius norm can be computed and we get

$$\begin{aligned}\|\tilde{J}\|^2 \leq \|\tilde{J}\|_F^2 &\leq 2\left(\frac{\max\sigma(Q)}{\min_{\lambda,\lambda'\in\sigma(Q),\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2\|S\|_F^2 \\ &\leq 2\left(\frac{\max\sigma(Q)}{\min_{\lambda,\lambda'\in\sigma(Q),\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2 N\max\big(\sigma(S)\big)^2. \end{aligned} \tag{62}$$

By gathering (59)–(60)–(61)–(62), we finally obtain the expected upper bound when $t \geq t_0$:

$$\left\|e^{t\tilde{\mathcal{L}}_J}u\right\|_{L^2}^2 \leq 2^{10}N^2\kappa(Q)\left(\frac{\max\sigma(Q)}{\min_{\lambda,\lambda'\in\sigma(Q),\,\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^4\kappa(S)^7 e^{-2\frac{\mathrm{Tr}(S)}{N}t}\|u\|_{L^2}^2,$$

for all $u \in \dot{\mathcal{H}}^1_Q$ and by density for all $u \in \mathcal{D}_0^\perp$. When $t \le t_0 = \frac{N}{\operatorname{Tr} S}$, simply use

$$\left\| e^{t\tilde{\mathcal{L}}_J}(I - \Pi_0)\right\|_{\mathcal{L}(L^2)} \le 1 \le \frac{2^5 N}{e}\kappa(Q)^{\frac{1}{2}}\left(\frac{\max \sigma(Q)}{\min_{\lambda\neq\lambda'\in\sigma(Q)}|\lambda-\lambda'|}\right)^2 \kappa(S)^{\frac{7}{2}}. \qquad \square$$

Remark 8 A lower bound can be given for $\|\tilde{J}\|$ with

$$\|\tilde{J}\|^2 \ge \frac{1}{N}\|\tilde{J}\|_F^2 \ge \frac{2}{N}\left(\frac{\min \sigma(Q)}{\max_{\lambda,\lambda'\in\sigma(Q),\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2 \|S\|_F^2$$
$$= \frac{2}{N}\left(\frac{\min \sigma(Q)}{\max_{\lambda,\lambda'\in\sigma(Q),\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2 \operatorname{Tr}\big(S^2\big).$$

Thus, we have

$$\|\tilde{J}\| \ge \sqrt{2}\frac{\min \sigma(Q)\min \sigma(S)}{\max_{\lambda,\lambda'\in\sigma(Q),\lambda\neq\lambda'}|\lambda-\lambda'|}. \tag{63}$$

In view of (27), Proposition 12 yields the estimate (22) in Theorem 2 with a constant

$$C_N^{(2)} = 2^5 N\kappa(Q)^{1/2}\left(\frac{\max \sigma(Q)}{\min_{\lambda,\lambda'\in\sigma(Q),\,\lambda\neq\lambda'}|\lambda-\lambda'|}\right)^2. \tag{64}$$

Let us comment on the way $C_N^{(2)}$ behaves.

Remark 9 In view of the upper bound (64), using the same construction as in Remark 7, we again notice that it is possible to have $C_N^{(2)} = \mathcal{O}(N^3)$ while keeping a reasonable perturbation $\tilde{J}$ (with a Frobenius norm estimated by $\|\tilde{J}\|_F \le 4N\|S\|_F$). Contrary to the case of the ordinary differential equation discussed in Remark 7 our estimate does not provide a uniform in N constant.

We conclude this section with two technical lemma which were respectively used in the proof of Proposition 12 and of Proposition 11.

Lemma 3 *Let* $(L, D(L))$ *be a maximal accretive and sectorial operator in a Hilbert space* $\mathcal{H}$ *with*

$$\forall u \in D(L), \quad \big|\arg\langle u, Lu\rangle_{\mathcal{H}}\big| \le \theta = \frac{\pi}{2} - 2\alpha \quad \textit{with } \alpha > 0,$$

where, we recall, $\arg(z)$ *denotes the argument of a complex number* z*. Then, the associated semigroup satisfies*

$$\forall t \ge 0, \quad \left\| tLe^{-tL}\right\|_{\mathcal{L}(\mathcal{H})} \le \frac{1}{\pi \sin^2\alpha}.$$

Proof The case $t = 0$ is obvious. For $t > 0$, e^{-tL} maps $\mathcal{H}$ into $D(L)$ so that tLe^{-tL} belongs to $\mathcal{L}(\mathcal{H})$. Consider first the case when $0 \notin \sigma(L)$. Our assumptions with $\alpha > 0$, ensure that the operator tLe^{-tL} is given by the convergent contour integral

$$tLe^{-tL} = \frac{1}{2i\pi}\int_\Gamma tze^{-tz}(z-L)^{-1}\,dz,$$

where Γ is the union of the two half lines with arguments $\frac{\pi}{2}-\alpha$ and $-\frac{\pi}{2}+\alpha$. For $z = x \pm i\frac{x}{\tan\alpha} \in \Gamma$ with $x > 0$ the resolvent $(z-L)^{-1}$ satisfies (see for example [38, Chap. VIII.17]) $\|(z-L)^{-1}\|_{\mathcal{L}(\mathcal{H})} \le \frac{1}{x}$. Moreover, $|dz| = \sqrt{1+\frac{1}{\tan^2\alpha}}dx = \frac{dx}{\sin\alpha}$ and $|e^{-tz}| = e^{-tx}$. From these estimates, we deduce

$$\left\|tLe^{-tL}\right\|_{\mathcal{H}} \le \frac{2}{2\pi}\int_0^{+\infty}\frac{tx}{\sin\alpha}e^{-tx}\frac{1}{x}\frac{dx}{\sin\alpha} = \frac{1}{\pi\sin^2\alpha}\int_0^{\infty}te^{-tx}\,dx = \frac{1}{\pi\sin^2\alpha}.$$

When $0 \in \sigma(L)$ it suffices to replace L by $\varepsilon + L$ which satisfies the same assumptions as L with the same α with $0 \notin \sigma(\varepsilon + L)$. The identity

$$t(\varepsilon+L)e^{-t(\varepsilon+L)} - Le^{-tL} = t\varepsilon e^{-\varepsilon t}e^{-tL} + \left(e^{-\varepsilon t}-1\right)tLe^{-tL}$$

with $t > 0$ fixed and $e^{-tL}, tLe^{-tL} \in \mathcal{L}(\mathcal{H})$ implies $\lim_{\varepsilon\to 0}\|t(\varepsilon+L)e^{-t(\varepsilon+L)} - tLe^{-tL}\|_{\mathcal{L}(\mathcal{H})} = 0$, which yields the result in the general case. □

Lemma 4 *Let $S, Q, \tilde{J}$ be real matrices such that $S \in \mathcal{S}_N^{\geq 0}(\mathbb{R})$, $Q \in \mathcal{S}_N^{>0}(\mathbb{R})$ and $\tilde{J} \in \mathcal{A}_N(\mathbb{R})$. Let us consider the operator $L = -\tilde{\mathcal{L}}_J$ (see Eq. (25) for the definition) and $C = C_Q$ (see Eq. (56)). The operator L (respectively C) is the Wick quantization of the polynomial $\ell(z) = (z, Sz)_{\mathbb{C}} - (z, \tilde{J}z)_{\mathbb{C}}$ (respectively $p(z) = (z, Qz)_{\mathbb{C}}$). Moreover, we have the following estimate: $\forall \varphi \in \mathcal{D} = \mathbb{C}[x_1, \ldots, x_N]e^{-\frac{|x|^2}{4}} \cap \mathcal{D}_0^{\perp}$,*

$$\left\langle\varphi, \left(L^*C + CL\right)\varphi\right\rangle_{L^2} \ge \left\langle\varphi, \left(\left(z, [SQ + QS + \tilde{J}Q - Q\tilde{J}]z\right)_{\mathbb{C}}\right)^{Wick}\varphi\right\rangle_{L^2}. \tag{65}$$

Proof The fact that $L = (\ell(z))^{Wick}$ and $C = (p(z))^{Wick}$ is easy to check. Both operator are block diagonal in the orthogonal decomposition $\mathcal{D}_0 \oplus^{\perp} \mathcal{D}_0^{\perp} = \bigoplus_{k\in\mathbb{N}}^{\perp}\mathcal{D}_k$ valid in $L^2(\mathbb{R}^N, dx; \mathbb{C})$ and in $\mathcal{H}_Q^1$. Hence the composed operator $L^*C + CL$ is well defined on $\mathcal{D}$ which is the algebraic direct sum $\mathcal{D} = \bigoplus_{n\in\mathbb{N}^*}^{alg}\mathcal{D}_k$. Notice that the polynomials ℓ and p satisfy

$$\mathrm{Re}\,\ell(z) = (z, Sz)_{\mathbb{C}}, \qquad \mathrm{Im}\,\ell(z) = -\frac{1}{i}(z, \tilde{J}z)_{\mathbb{C}}, \qquad \overline{p(z)} = p(z).$$

We are looking for a lower bound for $L^*C + CL$. Using the general formula of [1, Proposition 2.7] or by direct calculation using the relation $[a_i, a_j^*] = \delta_{ij}$, the Wick symbol of $L^*C + CL$ is

$$\begin{aligned}&\overline{\ell(z)}p(z) + p(z)\ell(z) + \partial_z\overline{\ell(z)}.\partial_{\overline{z}}p(z) + \partial_z p(z).\partial_{\overline{z}}\ell(z)\\ &\quad = \left(z^{\otimes 2}, (S\otimes Q + Q\otimes S)z^{\otimes 2}\right)_{\mathbb{C}} + \left(z, (SQ + QS + \tilde{J}Q - Q\tilde{J})z\right)_{\mathbb{C}}.\end{aligned}$$

Since S and Q are non negative matrices, we deduce that $S\otimes Q$ and $Q\otimes S$ are non negative and so is the sum $S\otimes Q + Q\otimes S$. When $B = (B_{(i,j),(k,\ell)})_{1\le i,j,k,\ell\le N}$ is a non negative matrix on $\mathbb{C}^{N^2}$ with the symmetries $B_{(i,j),(k,\ell)} = B_{(i,j),(\ell,k)} = B_{(j,i),(k,\ell)}$, the operator

$$b^{Wick} = \sum_{i,j,k,\ell} a_i^* a_i^* B_{(i,j),(k,\ell)}a_k a_\ell$$

associated with the symbol $b(z) = (z^{\otimes 2}, Bz^{\otimes 2})_{\mathbb{C}}$ is non negative. This can be checked by direct calculation of

$$\left\langle\varphi, b^{Wick}\varphi\right\rangle = \sum_{1\le i,j,k,\ell\le N}\int_{\mathbb{R}^N}\overline{\varphi_{(i,j)}(x)}B_{(i,j),(k,\ell)}\varphi_{(k,\ell)}(x)\,dx$$

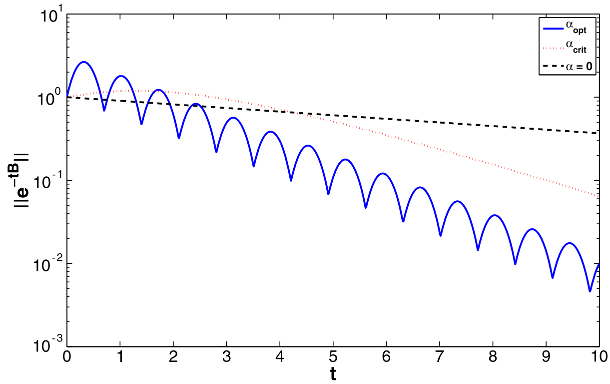

Fig. 2 Norms of the matrix exponentials for the 2×2 diagonal matrix (66) and optimal nonreversible perturbations

where $\varphi_{(i,j)} = a_i a_j \varphi$. We refer the reader to [2], precisely relation (8) after Proposition 2.2, for a general statement. □

Notice that the inequality (65) cannot be obtained neither by using the non negative anti-Wick quantization (see [28]) nor the sharp Garding or Feffermann-Phong inequalities (see [23]).

6 Numerical Experiments

In this section we present some numerical experiments, based on the algorithm presented as a pseudo-code in Fig. 1. The numerical computations presented in this section are based on the following steps:

1. Calculate the orthonormal basis $\{\psi_k\}_{k=1}^N$ using the algorithm presented in Fig. 1.
2. Choose the eigenvalues of the matrix Q, $\{\lambda_k\}_{k=1}^N$, e.g. according to Remark 7.
3. Calculate the optimal perturbation J using (38) and the formula $J = S^{-1/2}\tilde{J}S^{-1/2}$.
4. Calculate the optimally perturbed matrix $B_J = (I + J)S$.
5. Calculate the matrix exponentials e^{-tB} and e^{-tB_J} and their norms.

In Fig. 2 we present the results for a two dimensional problem, for which all results can be performed analytically, see Sect. 3.3. We consider the case where the matrix B has a spectral gap,

$$S = \mathrm{diag}(1, 0.1). \tag{66}$$

In the figure we plot the norms of the matrix exponentials for the symmetric case, an optimal perturbation and the critical value, see Eq. (41).

In Fig. 3 we present results for a three dimensional problem with the symmetric matrix

$$S = \mathrm{diag}(1, 0.1, 0.01). \tag{67}$$

The spectral gap of the optimally perturbed nonreversible matrix (and of the generator of the semigroup) is given by $\frac{\mathrm{Tr}\, S}{3} = 0.37$, which is a substantial improvement over that of S, namely 0.01.

In Fig. 4 we consider a 100×100 diagonal matrix with random entries, uniformly distributed on [0, 1]. For our example the minimum diagonal element (spectral gap) is 0.0012. On the contrary, the spectral gap of B_J with $J = J_{opt}$ is 0.4762.

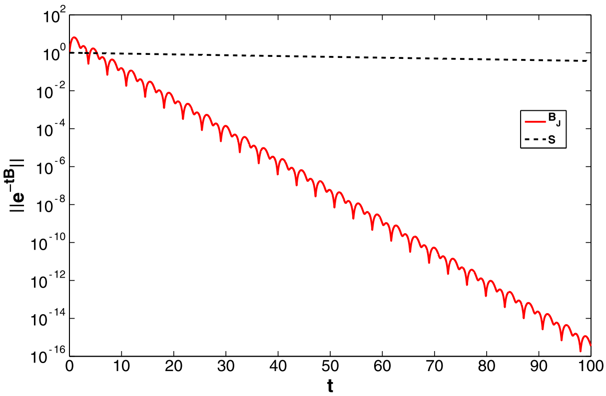

Fig. 3 Norms of the matrix exponentials for the 3×3 diagonal matrix (67) and its optimal nonreversible perturbation

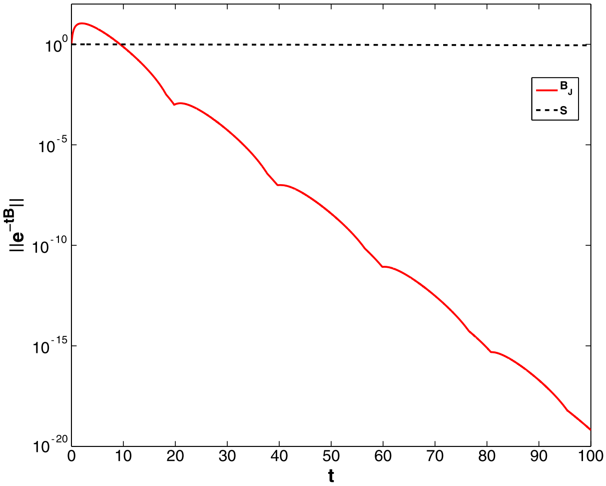

Fig. 4 Norms of the matrix exponentials for a diagonal matrix with random uniformly distributed entries and its optimal nonreversible perturbation for $N = 100$

Finally, in Fig. 5 we consider a drift that is a (high dimensional) finite difference approximation of the Laplacian with periodic boundary conditions. More precisely, consider the drift matrix

$$B_{ii} = 2, \qquad B_{i,i+1} = B_{i-1,i} = -1,$$

with $N = 100$. In this case the improvement on the convergence rate is over three orders of magnitude, since

$$\min\bigl(\sigma(B)\bigr) = 9.67 \times 10^{-4}, \quad \text{whereas} \quad \mathrm{Re}\bigl(\sigma(B_J)\bigr) = \frac{\mathrm{Tr}\, S}{100} = 2.$$

We can think of this example in connection of sampling from a Gaussian random field using a finite difference approximation of the stochastic heat equation $\partial_t u = \partial_x^2 u + \xi$ in [0, 1] with periodic boundary conditions, and where ξ denotes space-time white noise. Since the computational cost of calculating the optimal nonreversible perturbation is very low, we believe that the algorithm developed in this paper can be used for sampling Gaussian distributions in infinite dimensions.

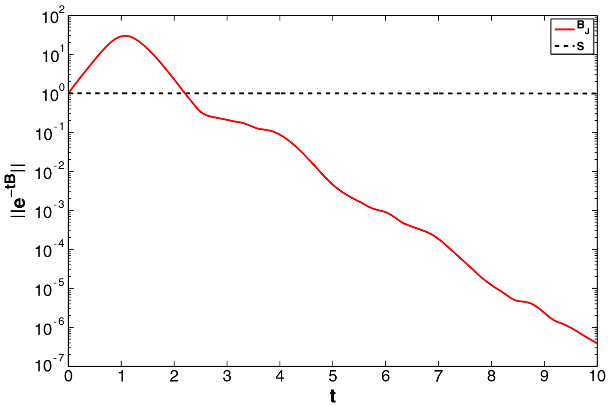

Fig. 5 Norms of the matrix exponentials for the discrete Laplacian and its optimal nonreversible perturbation for $N = 100$

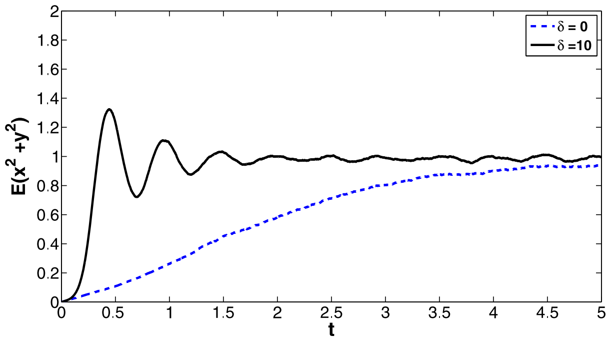

Fig. 6 Second moment as a function of time for (68) with the potential (69). We take 0 as an initial condition and $\beta^{-1} = 0.1$

The algorithm developed in this paper provides us with the optimal nonreversible perturbation only in the case of linear drift. However, even for nonlinear problems it is always the case that the addition of a nonreversible perturbation can accelerate the convergence to equilibrium, as mentioned in the introduction. This is particularly the case for systems with metastable states and/or multiscale structure [26]; for such systems, a "clever" choice of the nonreversible perturbation can lead to a very significant increase in the rate of convergence to equilibrium. A systematic methodology for obtaining the optimal nonreversible perturbation for general reversible diffusions (i.e. not necessarily with a linear drift) will be developed elsewhere.

We illustrate the advantage of adding a nonreversible perturbation to the dynamics by considering a simple two-dimensional example. In particular, we consider the nonreversible dynamics

$$dX_t = (-I + \delta J)\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t, \tag{68}$$

with $\delta \in \mathbb{R}$ and J the standard 2×2 antisymmetric matrix, i.e. $J_{12} = 1,\ J_{21} = -1$. For this class of nonreversible perturbations the parameter that we wish to choose in an optimal way is δ. Based on our numerical experiments we can conclude that even a non-optimal choice of δ significantly accelerates convergence to equilibrium. To illustrate the effect of adding a nonreversible perturbation, we solve numerically (68) using the Euler-Maruyama method with a sufficiently small time step and for a sufficiently large number of realizations of the noise. We then compute the expectation value of observables of the solution, in particular, the second moment by averaging over all the trajectories that we have generated.

We use one of the potentials that were considered in [32], namely

$$V(x, y) = \frac{1}{4}\left(x^2 - 1\right)^2 + \frac{1}{2}y^2. \tag{69}$$

In Fig. 6 we present the convergence of the second moment to its equilibrium value for $\beta^{-1} = 0.1$. Even in this very simple example, the addition of a nonreversible perturbation, with $\delta = 10$, speeds up convergence to equilibrium. Notice also that, as expected, the non-reversible perturbation leads to an oscillatory transient behavior.

Acknowledgement We would like to thank Matthieu Dubois for preliminary numerical experiments.

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