On the Generalised Langevin Equation for Simulated Annealing

Martin Chak · Nikolas Kantas · Grigorios A. Pavliotis

Received: date / Accepted: date

Abstract In this paper, we consider the generalised (higher order) Langevin equation for the purpose of simulated annealing and optimisation of nonconvex functions. Our approach modifies the underdamped Langevin equation by replacing the Brownian noise with an appropriate Ornstein-Uhlenbeck process to account for memory in the system. Under reasonable conditions on the loss function and the annealing schedule, we establish convergence of the continuous time dynamics to a global minimum. In addition, we investigate the performance numerically and show better performance and higher exploration of the state space compared to the underdamped and overdamped Langevin dynamics with the same annealing schedule.

Keywords nonconvex optimization \cdot generalized Langevin equation \cdot simulated annealing

Mathematics Subject Classification (2010) 60J25, 46N10, 60J60

1 Introduction

Algorithms for optimisation have received significant interest in recent years due to applications in machine learning, data science and molecular dynamics. Models in machine learning are formulated to have some loss function and parameters with respect to which it is to be minimised, where use of optimisation techniques is heavily relied upon. We refer to [8,71] for related discussions. Many models, for instance neural networks, use parameters that vary over a continuous space, where gradient-based optimisation methods can be used to find good parameters that generate effective predictive ability. As such, the design and analysis of such algorithms for global optimisation has been the subject of considerable research [69] and it has proved useful to study algorithms for global optimisation using tools from the theory of stochastic processes and dynamical systems. A paradigm of the use of stochastic dynamics for the design of algorithms for global optimisation is one of simulated annealing, where overdamped Langevin dynamics with a time dependent temperature (1.1) that decreases with an appropriate cooling schedule is used to guarantee the global minimum of a nonconvex loss function $U : \mathbb{R}^n \to \mathbb{R}$:

$$dX_t = -\nabla U(X_t) \, dt + \sqrt{2T_t} \, dW_t. \tag{1.1}$$

Here W_t is a standard *n*-dimensional Wiener process and $T_t : \mathbb{R}_+ \to \mathbb{R}$ is an appropriate deterministic function of time often referred to as the annealing or cooling schedule. For fixed $T_t = T > 0$, this is the dynamics used for the related problem of sampling from a possibly high dimensional probability measure, for example in the unadjusted Langevin algorithm [21]. Gradually decreasing T_t to zero balances the exploration-exploitation trade-off by allowing at early times larger noise to drive X_t and hence sufficient mixing to escape local minima. Designing an appropriate annealing schedule is well-understood. We briefly mention classical references [17,30,31,33,34,38,39,43], as well as the more recent [42,50,65], where one can find details and convergence results. In this paper we aim to consider generalised versions of (1.1) for the same purpose.

Department of Mathematics, Imperial College London, SW72AZ

E-mail: martin.chak14@imperial.ac.uk · n.kantas@imperial.ac.uk · g.pavliotis@imperial.ac.uk

Using dynamics such as (1.1) has clear connections with sampling. When $T_t = T$ is a constant function, the invariant distribution of X is proportional to $\exp(-\frac{U(x)}{T})dx$. In addition, when T_t decreases with time, the probability measure $\nu_t(dx) \propto \exp(-\frac{U(x)}{T_t})dx$ converges weakly to the set of global minima based on the Laplace principle [41]. One can expect that if one replaces (1.1) with a stochastic process that mixes faster and maintains the same invariant distribution for constant temperatures, then the superior speed of convergence should improve performance in optimisation due to the increased exploration of the state space. Indeed, it is well known that many different dynamics can be used in order to sample from a given probability distribution, or for finding the minima of a function when the dynamics is combined with an appropriate cooling schedule for the temperature. Different kinds of dynamics have already been considered for sampling, e.g. nonreversible dynamics, preconditioned unadjusted Langevin dynamics [2,4,48,62], as well as for optimisation, e.g. interacting Langevin dynamics [74], consensus based optimisation [10,11,66], to name a few.

A natural candidate in this direction is to use the underdamped or kinetic Langevin dynamics:

$$dX_t = Y_t \, dt \tag{1.2a}$$

$$dY_t = -\nabla U(X_t) \, dt - T_t^{-1} \mu Y_t \, dt + \sqrt{2\mu} \, dW_t \tag{1.2b}$$

Here the reversibility property of (1.1) has been lost; the improvement from breaking reversibility in both the context of sampling and that of optimisation investigated in [19,47] and [27] respectively. When $T_t = T$, (1.2) can converge faster than (1.1) to its invariant distribution

$$\rho(dx, dy) \propto \exp\left(-\frac{1}{T}\left(U(x) + \frac{|y|^2}{2}\right)\right) dx \, dy,$$

see [22] or Section 6.3 of [63] for particular comparisons and also [5,6] for more applications using variants of (1.2). In the context of simulated annealing, using this set of dynamics has recently been studied rigorously in [55], where the author established convergence to global minima using the generalised Γ -calculus [56] framework that is based on Bakry-Emery theory. Note that (1.2b) uses the temperature in the drift rather than the diffusion constant in the noise as in (1.1). Both formulations admit the same invariant measure when $T_t = T$. In the remainder of the paper, we adopt this formulation to be closer to [55].

In this paper we will consider an extension of the kinetic Langevin equation by adding an additional auxiliary variable that accounts for the memory in the system. To the best of the authors' knowledge, this has not been attempted before in the context of simulated annealing and global optimisation. In particular we consider the Markovian approximation to the generalised Langevin equation:

$$dX_t = Y_t \, dt \tag{1.3a}$$

$$dY_t = -\nabla U(X_t) \, dt + \lambda^\top Z_t \, dt \tag{1.3b}$$

$$dZ_t = -\lambda Y_t \, dt - T_t^{-1} A Z_t \, dt + \Sigma \, dW_t, \tag{1.3c}$$

where $A \in \mathbb{R}^{m \times m}$ is symmetric positive definite matrix, meaning that there exists a constant $A_c > 0$ such that

$$z^{\top}Az \ge A_c|z|^2$$

for all $z \in \mathbb{R}^m$, $\Sigma \in \mathbb{R}^{m \times m}$ satisfies

 $\varSigma \varSigma^\top = 2A$

and W_t is now *m*-dimensional. Here $X_t, Y_t \in \mathbb{R}^n$ and $Z_t \in \mathbb{R}^m$ (with $m \ge n$), M^{\top} denotes the transpose of a matrix $M, \lambda \in \mathbb{R}^{m \times n}$ is a rank *n* matrix with a left inverse $\lambda^{-1} \in \mathbb{R}^{n \times m}$.

Our aim is to establish convergence using similar techniques as [55] and investigate the improvements in performance. Equation (1.3) is related to the generalised Langevin equation, where memory is added to (1.2) by integrating over past velocities with a kernel $\Gamma : \mathbb{R}_+ \to \mathbb{R}^{n \times n}$:

$$\ddot{x} = -\nabla U(x) - \int_0^t \Gamma(t-s)\dot{x}(s)\,ds + F_t \tag{1.4}$$

with F_t being a zero mean stationary Gaussian process with an autocorrelation matrix given by the fluctuationdissipation theorem

$$\mathbb{E}(F_t F_s^{\top}) = T_t \Gamma(t-s)$$

When $T_t = T$, (1.4) is equivalent to (1.3) when setting

$$\Gamma(t) = \lambda^{\top} e^{-At} \lambda, \tag{1.5}$$

and the invariant distribution becomes

$$\rho(dx, dy, dz) \propto \exp\left(-\frac{1}{T}\left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2}\right)\right) dx \, dy \, dz,$$

see Section 8.2 of [63] for details¹. In the spirit of adding a momentum variable in (1.1) to get (1.2), (1.3) adds an additional auxiliary variable to the Langevin system whilst preserving the invariant distribution in the x marginal. In the constant temperature context, (1.4) is natural from the point of statistical mechanics and has already been considered as a sampling tool in [12, 13, 14, 58] with considerable success. We will demonstrate numerically that the additional tuning parameters can improve performance; see also [57] for recent work demonstrating advantages of using (1.4) compared to using (1.2) when sampling from a log concave density. A detailed study of the Markovian approximation (1.3) of the generalised Langevin dynamics in (1.4) can be found in [60].

To motivate the use of (1.3), consider the quadratic case where $U = \alpha x^2$ and $0 < \alpha < 1$. This case allows for explicit or numerical calculation of the spectral gaps of the generators in (1.1)-(1.3) in order to compare the rate of convergence to equilibrium; see [53,61] for details. For a given T, it is possible to choose λ and A, such that the spectral gap of the generator of (1.3) is much larger than that of (1.2) with the best possible choice of μ being used. The latter is already larger than that of the overdamped dynamics in (1.1). We will later demonstrate numerically that this will translate to better exploration in simulated annealing (when T_t is decreasing in time).

Use of (1.4) is also motivated by parallels with accelerated gradient descent algorithms. When the noise is removed from (1.2), the second order differential equation can be loosely considered as a continuous time version of Nesterov's algorithm [73]. The latter is commonly preferred to discretising the first order differential equation given by the noiseless version of (1.1), because in the high dimensional and low iterations setting it achieves the optimal rate of convergence for convex optimisation; see Chapter 2 in [59] and also [32] for a nonconvex setting. Here we would like to investigate the effect of adding another auxiliary variable, which would correspond to a third order differential equation when noise is removed. When noise is added for the fixed temperature case, [26] has studied the long time behaviour and stability for different choices of a memory kernel as in (1.4). Finally, we note that generalised Langevin dynamics in (1.4) have additionally been studied in related areas such as sampling problems in molecular dynamics from chemical modelling [1,12,13,14,58,77], see also [44] for work determining the kernel Γ in the generalised system (1.4) from data.

Our theoretical results will focus only on the continuous time dynamics and follow the approach in [55]. The main requirement in terms of assumptions are quadratic upper and lower bounds on U and bounded second derivatives. This is different to classical references such as [31], [33] or [39]. These works also rely on the Poincaré inequality, an approach which will be mirrored here (and in [55] for the underdamped case) using a log-Sobolev inequality; see also [38] for the relationship between such functional inequalities and the annealing schedule in the finite state space case. We will also present detailed numerical results for different choices of U. There are many possibilities for the method of discretisation of (1.3), we will use a time discretisation scheme that appeared in [3], but will not present theoretical results on the time discretised dynamics; this is beyond the scope of this article. We refer instead the interested reader to [70] for a study on discretisation schemes for the system (1.3), [16] for a recent consideration on (1.2) and its time-discretisation and [28,29] for linking discrete time Markov chains with the overdamped Langevin system in (1.1).

¹ To the best of the authors' knowledge, there is no known direct translation between (1.4) and (1.3) for a non-constant T_t ; such a translation quite possibly exists and at the very least the intuition here is useful.

1.1 Contributions and organisation of the paper

Here we summarise the main contributions of the paper.

- We provide a complete theoretical analysis of the simulated annealing algorithm for the generalised Langevin equation (1.3). The main theoretical contribution consists of Theorem 5 that establishes convergence in probability of X_t in the higher order Markovian dynamics (1.3) to a global minimiser of U. For the optimal cooling schedule T_t , the rate of convergence is as the known rate for the Langevin system (1.2) presented in [55].
- The initially non-Markovian property and pronounced degeneracy in the sense of requiring a second commutator bracket for hypoellipticity by way of Hörmander introduces additional difficulties that are overcome using techniques from [55]. As such, we use a different form of the distorted entropy, stated formally in (4.39). Additional technical improvements include a different truncation argument and a limiting sequence of nondegenerate SDEs for establishing dissipation of this distorted entropy. These extensions also address certain technical issues in [55]; see Remarks 1, 3 and 6 for more details. Also we make an effort to emphasise the role of the critical factor of the cooling schedule in the rate of convergence in Theorem 5. This can be seen in our assumptions for T_t and U below.
- As a byproduct, we prove exponential convergence to equilibrium for the constant temperature $T_t = T > 0$ case in Proposition 6, which is relevant for sampling problems. See [60] and [64] for similar results.
- Detailed numerical experiments are provided to illustrate the performance of our approach. We also discuss thoroughly tuning issues. In particular, we investigate numerically the role of matrix A and how it can be chosen to increase exploration of the state space. As regards to time discretisation of (1.3) we use the leapfrog scheme of [3]. We compare this with a similar time discretisation of (1.2) and observe that exploration of the state space is increased considerably.

The paper is organised as follows. Section 2 will present the assumptions and main theoretical results. Detailed proofs can be found in Section 4. Section 3 presents numerical results demonstrating the effectiveness of our approach both in terms of reaching the global minimum and the exploration of the state space. In Section 5, we provide some concluding remarks.

2 Main Result

Let L_t denote the infinitesimal generator of the associated semigroup to (1.3) at t > 0 and temperature T_t . This is formally given by

$$L_t = (y \cdot \nabla_x - \nabla_x U(x) \cdot \nabla_y) + (z^\top \lambda \nabla_y - y^\top \lambda^\top \nabla_z) - T_t^{-1} z^\top A \nabla_z + A : D_z^2,$$
(2.1)

where we denote the gradient vector as $\nabla_x = (\partial_{x_1}, \ldots, \partial_{x_n})^{\top}$, the Hessian with D_x^2 and similarly for the y and z variables. For matrices $M, N \in \mathbb{R}^{r \times r}$ we denote $M : N = \sum_{i,j} M_{ij} N_{ij}$ for all $1 \le i, j \le r$ and the operator norm as $|M| = \sup \left\{ \frac{|Mv|}{|v|} : v \in \mathbb{R}^r$ with $x \ne 0 \right\}$. We will also use |v| to denote Euclidean distance for a vector v. Let m_t be the law of (X_t, Y_t, Z_t) in (1.3) and, with slight abuse of notation, we will also denote as m_t the corresponding Lebesgue density. Similarly we define μ_{T_t} be the instantaneous invariant law of the process

$$\mu_{T_t}(dx, dy, dz) = \frac{1}{Z_{T_t}} \exp\left(-\frac{1}{T_t} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2}\right)\right) dx \, dy \, dz \tag{2.2}$$

with $Z_{T_t} = \int \exp\left(-\frac{1}{T_t}\left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2}\right)\right) dx \, dy \, dz$. Finally, denote the density between the two laws:

$$h_t = \frac{dm_t}{d\mu_{T_t}}.$$
(2.3)

We proceed by stating our assumptions on the potential U.

Assumption 1

There exists $0 < \theta < 1$ such that U is smooth (belongs in $\mathcal{C}^{\infty}(\mathbb{R}^n)$) with bounded second derivatives

$$|D_x^2 U|_{\infty} := \sup_{x \in \mathbb{R}^n} \max\left(\sup_{ij} |\partial_i \partial_j U(x)|, |D_x^2 U(x)|\right) < \infty,$$
(2.4)

satisfies

$$\nabla_x U(x) \cdot x \ge r_1 |x|^2 - U_g \tag{2.5}$$

$$|\nabla_x U(x)|^2 \le r_2 |x|^2 + U_g \tag{2.6}$$

for some constants $r_1, r_2 \in \mathbb{R}$, $U_q > 0$ and either

(a)

 $\left|\bar{a} \circ x\right|^{2} + U_{m} \leq U(x) \leq \left|\bar{a} \circ x\right|^{2} + U_{M}$ (2.7)

for some $U_m, U_M \in \mathbb{R}, \ \bar{a} \in \mathbb{R}^n_+$, where \circ denotes the Hadamard product, or

(b) - U is a nonnegative Morse function, in the sense that there exists $1 \le C_H < \infty$ such that if $x \in \mathbb{R}^n$ satisfies $\nabla_x U(x) = 0$, then

$$\frac{\left|\xi\right|^{2}}{C_{H}} \leq \left\langle\xi, D_{x}^{2}U(x)\xi\right\rangle \leq C_{H}\left|\xi\right|^{2} \qquad \forall \xi \in \mathbb{R}^{n},$$

- U is nondegenerate in the sense that:

- For any two local minima $m_i, m_j \in \mathbb{R}^n$, there exists a unique (communicating saddle) point $s_{i,j} \in \mathbb{R}^n$ such that
 - $\nabla_x U(s_{i,j}) = 0$,
 - $U(s_{i,j}) = \inf\{\max_{s \in [0,1]} U(\gamma(s)) : \gamma \in C([0,1], \mathbb{R}^n), \gamma(0) = m_i, \gamma(1) = m_j\},\$
 - the dimension of the unstable subspace of $D_x^2 U(s_{i,j})$ is equal to 1.
- Setting m_1 to be the global minimum of U, there exists $\delta > 0$ and an ordering of the local minima $\{m_2, m_3, \ldots\}$ such that $U(s_{1,2}) U(m_2) \ge U(s_{1,i}) U(m_i) + \delta$ for all $i \ge 3$.

Note that (2.5) and (2.6) imply

$$a_m |x|^2 + U_m \leq U(x) \leq a_M |x|^2 + U_M$$
 (2.8)

for some $a_m, a_M > 0, U_m, U_M \in \mathbb{R}$. In the rest of the paper, if (2.7) holds then the smallest and largest element of \bar{a} is denoted with

$$a_m = \min_i \bar{a}_i, \quad a_M = \max_i \bar{a}_i,$$

where $\bar{a} = (\bar{a}_1, \ldots, \bar{a}_n)$.

Assumption 2 The temperature T_t satisfies

$$\lim_{t \to \infty} T_t = 0.$$

Before we proceed with further assumptions on the annealing schedule T_t and on the initial distribution, note that under Assumption 1 and 2, a log-Sobolev inequaity holds.

Proposition 1 Under Assumption 1 and Assumption 2, there exists constants $t_{ls}^{(0)}, \hat{E}, A_*^{(0)} > 0$ and a finite order polynomial $r^{(0)} : \mathbb{R}_+ \to \mathbb{R}_+$ with coefficients depending on U such that for all $0 < h \in C^{\infty}(\mathbb{R}^{2n+m})$,

$$\int h \ln h d\mu_{T_t} \le C_t^{(0)} \int \frac{|\nabla h|^2}{h} d\mu_{T_t},$$
(2.9)

where for $t > t_{ls}^{(0)}$,

$$C_t^{(0)} = r^{(0)} \left(T_t^{-\frac{1}{2}} \right) e^{\hat{E}T_t^{-1}}.$$
(2.10)

The proof is deferred and the constant \hat{E} from the above proposition will be used in stating the following assumption about T_t , as well as what follows. In the case of (2.7), \hat{E} can be taken as $U_M - U_m$, otherwise it is the critical depth [52] of U.

Assumption 3

The temperature $T_{\cdot}: [0, \infty) \to (0, \infty)$ is continuously differentiable, bounded above and there exists some constant $t_0 > 1$ such that T_t satisfies for all $t > t_0$:

(i) $T_t \ge E(\ln t)^{-1}$ for some constant $E > \hat{E} \ge 0$, where \hat{E} is the constant in Proposition 1, (ii) $|T'_t| \le \tilde{T}t^{-1}$ for some constant $\tilde{T} > 0$.

Assumption 4

The initial law m_0 admits a bounded density with respect to the Lebesgue measure on \mathbb{R}^{2n+m} , also denoted m_0 , satisfying:

(i) $m_0 \in \mathcal{C}^{\infty}(\mathbb{R}^{2n+m}),$ (ii) $\int \frac{|\nabla m_0|^2}{m_0} dx dy dz < \infty,$ (iii) $\int (|x|^2 + |y|^2 + |z|^2) m_0 dx dy dz < \infty,$

Remark 1 Note that (2.6) and (2.7) deviate from [55]. (2.7) is useful for a more self-contained exposition for the log-Sobolev constant in (4.52), but the alternative that U is a nonnegative nondegenerate Morse function is optimal in the sense that \hat{E} is in this case given as the critical depth of U. Condition (2.7) is satisfied for instance by a multivariate Gaussian after a rotation of the x coordinates.

We present two key propositions.

Proposition 2 Under Assumptions 1 and 3, for all t > 0, denote by $(X^{T_t}, Y^{T_t}, Z^{T_t})$ a r.v. with distribution μ_{T_t} . For any $\delta, \alpha > 0$, there exists a constant $\hat{A} > 0$ such that

$$\mathbb{P}(U(X^{T_t}) > \min U + \delta) \le \hat{A}e^{-\frac{\delta - \alpha}{T_t}}$$

holds for all t > 0.

Proof The result follows exactly as in Lemma 3 in [55].

Proposition 3 Under Assumptions 1, 3 and 4, for all t > 0, (X_t, Y_t, Z_t) are well defined as the unique strong solution to (1.3), $\mathbb{E}[|X_t|^2 + |Y_t|^2 + |Z_t|^2] < \infty$ and the law m_t admits an everywhere positive density with respect to the Lebesgue measure on \mathbb{R}^{2n+m} .

For the proof of Proposition 3, see Proposition 7 in Section 4.

Proposition 2 can be thought of as a Laplace principle; Proposition 3 asserts that the process (1.3) does not blow up in finite time and the noise in the dynamics (1.3c) for Z_t spreads throughout the system, that is to X_t and Y_t .

Proposition 4 Under Assumption 1, 3 and 4, for any $\alpha > 0$, there exists some constant B > 0 and $t_h > 0$, such that for all $t > t_h$,

$$\int h_t \ln h_t d\mu_{T_t} \le B\left(\frac{1}{t}\right)^{1-\frac{E}{E}-2\alpha}.$$
(2.11)

The full proof is the contained in Section 4 and follows from Proposition 10. Therein a similar statement is proved for the *distorted entropy* that has the following form:

$$H(t) := \int \left(\frac{\langle S \nabla h_t, \nabla h_t \rangle}{h_t} + \beta(T_t^{-1}) h_t \ln(h_t) \right) d\mu_{T_t},$$

where S being a well chosen matrix (so that (4.46) holds) and $\beta(\cdot)$ is a polynomial (see (4.39) for the precise form of H(t) and (4.44) for $\beta(\cdot)$). This construction of H compared to a standard definition of entropy compensates for the fact that the diffusion is degenerate (see [76] for a general discussion). The proof uses an approximating sequence of SDE's, in which all of the elements have nondegenerate noise. The problem is split into the partial time and partial temperature derivatives where, amongst other tools, (4.46) and a log-Sobolev inequality are used as in [55] to arrive at a bound that allows a Grönwall-type argument.

Remark 2 Proposition 10 is a statement about the distorted entropy H(t), which bounds the entropy $\int h_t \ln h_t d\mu_{T_t}$. In fact this is achieved in such a way that the bound becomes less sharp as t becomes large but without consequences for our main Theorem 5 below.

We proceed with the statement of our main result, using t_h from Proposition 4.

Theorem 5 Under Assumptions 1, 2, 3 and 4, for any $\delta > 0$, as $t \to \infty$,

$$\mathbb{P}(U(X_t) \le \min U + \delta) \to 1.$$

If in addition $T_t = E(\ln t)^{-1}$, then for any $\alpha > 0$, there exists a constant C > 0 such that for all $t > t_h$,

$$\mathbb{P}(U(X_t) \le \min U + \delta) \le C\left(\frac{1}{t}\right)^{r(E)}$$

where the exponential rate $r^e: (\hat{E}, \infty) \to \mathbb{R}$ is defined by

$$r^{e}(E) := \min\left(\frac{1 - \frac{\hat{E}}{E} - 2\alpha}{2}, \frac{\delta - \alpha}{E}\right)$$
$$= \begin{cases} \frac{1}{2} \left(1 - \frac{\hat{E}}{E} - 2\alpha\right) & \text{if } E < \frac{\hat{E} + 2(\delta - 2\alpha)}{1 - 2\alpha} \\ \frac{\delta - 2\alpha}{E} & \text{otherwise.} \end{cases}$$

Proof For all t > 0, denote by $(X^{T_t}, Y^{T_t}, Z^{T_t})$ a random variable with distribution μ_{T_t} . For all $\delta > 0$, with the definition (2.3) of h_t and triangle inequality,

$$\mathbb{P}(U(X_t) > \min U + \delta) \le \mathbb{P}(U(X^{T_t}) > \min U + \delta) + \int |h_t - 1| d\mu_{T_t}.$$

Pinsker's inequality gives

$$\int |h_t - 1| d\mu_{T_t} \le \left(2 \int h_t \ln h_t d\mu_{T_t} \right)^{\frac{1}{2}}, \tag{2.12}$$

which, by Proposition 4, together with Proposition 2 gives the result.

The cooling schedule $T_t = E(\ln t)^{-1}$ is optimal with respect to the method of proof for Proposition 10; see Proposition 11. This is a consistent with works in simulated annealing, e.g. [17,30,31,33,34,38,39,43].

The 'mountain-like' shape of r^e indicates the bottleneck for the rate of convergence at low and high values of E: a small E means convergence to the instantaneous equilibrium μ_{T_t} is slow and a large E means the convergence of μ_{T_t} to the global minima of U is slow.

Although the focus in Theorem 5 is for decaying T_t , it is only for convergence to the global minimum where Assumption 2 is used. In particular, the convergence result in Proposition 4 is valid for temperature schedules that are not converging to zero. This includes the instance of using a variable temperature in order to tackle the problem of metastability in the sampling problem.

We proceed below to show exponential convergence to equilibrium for the generalised Langevin equation (1.3) with constant temperature. Part of the analysis used in the proof of Proposition 10 can be used for the sampling case and $T_t = T$, i.e. working only with the partial time derivatives mentioned above for the invariant distribution.

Proposition 6 Let Assumption 1 and 4 hold and let $T_t = T$ for all t for some constant T > 0. There exist constants $C^c, C_* > 0$ such that

$$\int |h_t - 1| d\mu_T \le C^c e^{-\frac{C_*^{-1}}{2}t},$$

for all t > 0.

Proof See Appendix A.

3 Numerical results

Here we investigate the numerical performance of (1.3) in terms of convergence to a global optimum and exploration capabilities and compare with (1.2). In Section 3.1, we will present the discretisation we use for both sets of dynamics and some details related to the annealing schedule and parameters. In Section 3.2 and 3.3, for different parameters and cost functions, we present results for the probability of convergence to the global minimum and rates of transition between different regions of the state space. We will investigate thoroughly the effect of E appearing in the annealing schedule as well as the parameters in the dynamics (1.2) and (1.3).

3.1 Time discretisation

In order to simulate from (1.3), we will use the following time discretisation. For $k \in \mathbb{N}$,

$$Y_{k+\frac{1}{2}} = Y_k - \frac{\Delta t}{2} \gamma \nabla U(X_k) + \frac{\Delta t}{2} \lambda^\top Z_k, \qquad (3.1a)$$

$$X_{k+1} = X_k + \Delta t \gamma Y_{k+\frac{1}{2}},\tag{3.1b}$$

$$Z_{k+1} = Z_k - \theta \lambda Y_{k+\frac{1}{2}} - \theta A Z_k + \alpha \sqrt{T_k} \ \Sigma \xi_k, \qquad (3.1c)$$

$$Y_{k+1} = Y_{k+\frac{1}{2}} - \frac{\Delta t}{2} \gamma \nabla U(X_{k+1}) + \frac{\Delta t}{2} \lambda^{\top} Z_{k+1}, \qquad (3.1d)$$

where Δt denotes the time incremements in the discretisation, ξ_k are i.i.d. standard *m*-dimensional normal random variables with unit variance and $\theta = 1 - \exp(-\Delta t)$, and $\alpha = \sqrt{1 - \theta^2}$. Specifically this is method 2 of [3] applied on a slight modification of (1.3), where $\gamma Y_t dt$ and $\gamma \nabla U dt$ is used instead in the r.h.s. of (1.3a) and (1.3b). Tuning γ can improve numerical performance especially in high dimensional problems, but we note that this has no effect in terms of the instantaneous invariant density in (2.2); similar to λ and A, γ will not appear in (2.2). Unless stated otherwise, in the remainder we will use $\gamma = 1$.

As we will see below the choices for A make a difference in terms of performance. To illustrate this we will use different choices of the form

 $A = \mu A_i;$

i here is an index for different forms of A. The first choice will be to set m = n and set $A_1 = I_n$ where I_n is $n \times n$ identity matrix. For the rest, we will use m = 2n and set

$$A_{2} = \begin{pmatrix} 1.9I_{n} \ 0.4I_{n} \\ 0.1I_{n} \ 0.1I_{n} \end{pmatrix}, \quad A_{3} = \begin{pmatrix} I_{n} \ 0.5I_{n} \\ 0.5I_{n} \ I_{n} \end{pmatrix}, \quad (A_{4})_{ij} = \begin{cases} 1 & \text{if } i = j \\ \frac{1}{mn} & \text{otherwise} \end{cases}$$

Doubling the state space of Z_t relative to X_t , Y_t allows investigating the effect of injecting more noise in the dynamics has to the overall performance and the state space exploration. As per [36] (following [25]), the constraint that the trace of A is uniformly bounded has been used in selecting the above matrices. Note that A_2 does not satisfy the symmetry assumption for the results, but figures for A_2 are displayed in spite of this because there is an interesting improvement in performance for one of the cases below (see Figure 3.2 and also others for the sake of comparison). Similarly we will use in each case $\lambda = \bar{\lambda}\lambda_i$ with $\bar{\lambda} > 0$, $\lambda_1 = I_n$ and

$$\lambda_i = \begin{pmatrix} I_n \\ 0 \end{pmatrix}$$

for i = 2, 3, 4. As a result $\overline{\lambda}, \mu > 0$ are the main tuning constants for (3.1) that do not involve the annealing schedule. The Langevin system (1.2) will be approximated with a similar leapfrog scheme,

$$Y_{k+\frac{1}{2}} = Y_k - \hat{\theta}\gamma\nabla U(X_k) - \hat{\theta}\mu Y_k + \hat{\alpha}\sqrt{\mu T_k}\xi_k, \qquad (3.2a)$$

$$X_{k+1} = X_k + \Delta t \gamma Y_k, \tag{3.2b}$$

$$Y_{k+1} = Y_{k+\frac{1}{2}} - \hat{\theta}\gamma\nabla U(X_{k+1}) - \hat{\theta}\mu Y_{k+\frac{1}{2}} + \hat{\alpha}\sqrt{\mu T_{k+1}}\xi_{k+\frac{1}{2}}, \qquad (3.2c)$$

for $\hat{\theta} = 1 - \exp(-\frac{\Delta t}{2})$, and $\hat{\alpha} = \sqrt{1 - \hat{\theta}^2}$, where in the implementation, (3.2a) and (3.2c) are combined (aside from the first iteration) and only integer-indexed ξ are used. To make valid comparisons, both (3.1) and (3.2) will use $\gamma = 1$ and the same noise realisation ξ_k (or the first common *n* elements) and the same step size Δt .

Finally for both cases we will use following annealing schedule:

$$T_k = \left(\frac{1}{5} + \frac{\ln(1+k\Delta t)}{E}\right)^{-1},$$

where E is an additional tuning parameter (since \hat{E} is unknown in general).

3.2 Sample path properties

Our first set of simulations focus on illustrating some properties of the sample paths generated by (3.1) and (3.2). We will use the following bivariate potential function

$$U(x_1, x_2) = \frac{x_1^2}{5} + \frac{x_2^2}{10} + 5e^{-x_1^2} - 7e^{-(x_1+5)^2 - (x_2-3)^2} - 6e^{-(x_1-5)^2 - (x_2+2)^2} + \frac{\frac{2}{3}x_1^2 e^{-\frac{x_1^2}{9}}\cos(x_1+2x_2)\cos(2x_1-x_2)}{1+\frac{x_2^2}{9}}.$$
(3.3)

The global minimum is located at (-5,3), but there are plenty of local minima where the process can get trapped. In addition, there is a barrier along the vertical line $\{x_1 = 0\}$ that makes crossing from each half plane less likely. Here we set $\Delta t = 0.1$, E = 5 and each sample is initialised at (4,2). As a result, it is harder to cross $\{x_1 = 0\}$ to reach the global minimum and it is quite common to get stuck in other local minima such as near (5,-2). We use the number of crossings on $\{x_1 = 0\}$ as a scale for how stuck the process is in Table 3.1. Note that the asymmetric $A = A_2$ case displays the smallest number of crossings.

To illustrate this, in Figure 3.1 we present contour plots of U together with a typical realisation of sample paths (in the left panels) for (3.2) and (3.1) for the different choices of A_i . As expected, (3.1) generates smoother paths than those of (3.2). We also employ independent runs of each stochastic process for the same initialisation. The results are presented in the right panels of Figure 3.1, where we show heat maps for two dimensional histograms representing the frequency of visiting each (x_1, x_2) location over 20 independent realisations of each process. The heat maps in Figure 3.1 do not directly depict time dependence in the paths and only illustrate which areas are visited more frequently. Of course converging at the global minumum or the local one at (5, -2) will result in more visits at these areas. The aim here is to investigate the exploration of the state space.

Method equation	Number of transitions across $x = 0$
(3.2)	11295
(3.1) with $A = A_1$	11893
(3.1) with $A = A_2$	10915
(3.1) with $A = A_3$	11728
(3.1) with $A = A_4$	11771

Table 3.1: Number of crossings across the vertical line $\{x_1 = 0\}$ for U defined in (3.3). The results are summed from $k = 10^5$ iterations of 10^4 independent runs.

3.3 Performance and tuning

As expected, the tuning parameters, E, $\overline{\lambda}$ and μ play significant roles in the performance of (3.1) and (3.2). As E is common to both, we wish to demonstrate that the additional tuning variable for (3.1) will improve performance.

We first comment on relative scaling of $\bar{\lambda}$ and μ based on earlier work for quadratic U and $T_t = T$ being constant. A quadratic U satisfies the bounds in Assumption 1 and is of particular interest because analytical calculations are possible for the spectral gap of L_t , which in turn gives the (exponential) rate of convergence to the equilibrium distribution. It is observed numerically in [61] that in this case, (1.3) has a spectral gap that is approximately a function of $\frac{\bar{\lambda}^2}{\mu}$. On the other hand, the spectral gap of (1.2) with quadratic U is a function of μ thanks to Theorem 3.1 in [53]. For the rest of the comparison, we will use $\frac{\bar{\lambda}^2}{\mu}$ and μ as variables for (3.1) and (3.2) respectively as these quantities appear to have a distinct effect on the mixing in each case.

We will consider three different cost functions U and set $\Delta t = 0.02$. As before we will initialise at a point well separated from the global minimum and consider each method to be successful if it convergences at a particular tolerance region near the global minimum. The details are presented in Table 3.2. We choose the popular Alpine function in 12 dimensions (∇U_1 here is a subgradient) and two variants of (3.3). U_2 is modified to have the same quadratic confinement in x_1 and x_2 direction and there are several additional local minima due to the last term in the sum. More importantly, compared to (3.3) (and U_3) it has a narrow region near the origin that allows easier passage through { $x_1 = 0$ }. On the other hand U_3 similar to (3.3) except that the well near the global minimum (and the dominant local minimum at (5, -2)) are elongated in the direction of x_2 (and x_1 respectively).

Cost function	Initial condition	Tolerance sets
$U_1(x) = \frac{1}{2} \sum_{i=1}^{12} x_i \sin(x_i) + 0.1x_i $	$x_j = 6 \forall j$	$x_j \in [-2,2] \; \forall j$
$U_{2}(x_{1}, x_{2}) = \frac{x_{1}^{2}}{7} + \frac{x_{2}^{2}}{7} + 5\left(1 - e^{-9x_{2}^{2}}\right)e^{-x_{1}^{2}} - 7e^{-(x_{1}+5)^{2} - (x_{2}-3)^{2}} - 6e^{-(x_{1}-5)^{2} - (x_{2}+2)^{2}} + \frac{\frac{2}{3}x_{1}^{2}e^{-\frac{x_{1}^{2}}{9}}\cos(x_{1}+2x_{2})\cos(2x_{1}-x_{2})}{1 + \frac{x_{2}^{2}}{9}}$	$\begin{aligned} x_1 &= 4, \\ x_2 &= 2 \end{aligned}$	$x_1 \in [-6.5, -4.5], \\ x_2 \in [1.5, 4.5]$
$U_3(x_1, x_2) = \frac{x_1^2}{5} + \frac{x_2^2}{10} + 5e^{-x_1^2} - 7e^{-2(x_1+5)^2 - \frac{(x_2-3)^2}{5}} - 6e^{-\frac{(x_1-5)^2}{5} - 2(x_2+2)^2}$	$\begin{aligned} x_1 &= 4, \\ x_2 &= 2 \end{aligned}$	$x_1 \in [-6.5, -4.5], \\ x_2 \in [1.5, 4.5]$

Table 3.2: Details of three different cost functions, initialisation and tolerance regions corresponding to regions of attraction of the global minimum.

In Figure 3.2 we present proportions of simulations converging at the region near the global minimum for $U = U_1$ depending on E and μ for (3.2) and on E and $\frac{\bar{\lambda}^2}{\mu}$ for (3.1) based on discussion above. To produce the figures related to (3.1) after setting E, $\frac{\bar{\lambda}^2}{\mu}$ we pick a random value of μ from a grid. The aim of this procedure is to ease visualisation, reduce computational cost and to emphasise that it is $\frac{\bar{\lambda}^2}{\mu}$ that is crucial for mixing and the performance here is not a product of a tedious tuning for μ . The left panels of Figure 3.2 are based on final state and the right on an average of the positions (of X) over the last 5000 iterations. In this example it is clear empirically that the generalised Langevin dynamics (3.1) result in a higher probability of reaching the global minumum. Another interesting observation is that for the generalised Langevin dynamics good performance is more robust to the chosen value of E. In this example, this means that adding an additional tuning variable and scaling μ proportional to $\bar{\lambda}^2$, makes it easier to find a configuration of the parameters $E, \mu, \bar{\lambda}$ that leads to good performance, compared to using (3.2) and tuning E, μ . It's also worth noting the cases of small E where the generalised Langevin dynamics and larger E. This is an improvement that is not completely encapsulated by the analytic results here; it indicates that the deterministic dynamics (E = 0) can be inherently much more successful at climbing out of local minima, which translates to better convergence rates in the E > 0 cases.

In Figures 3.3 and 3.4 we present results for U_2 and U_3 . A notable difference to Figure 3.2 here is that the panels on the left show proportions of the position average of the last 5000 iterations being near the correct global minimum and the panels on the right present the number of jumps across $\{x_1 = 0\}$ demonstrated by a position

average at each iteration of the previous 5000 iterations. More precisely, the panels on the right show the number of jumps shown by the trajectory

$$\tilde{X}_k = \frac{1}{5000} \sum_{k'=1}^{5000} X_{k-k'+1}$$

for all k > 5000. All results are averaged over 20 independent runs. The aim here is to measure the extent of exploration of each process similar to Table 3.1. We observe that in both cases using (3.1) leads to a similar number of jumps. We believe the benefit of the higher order dynamics here are the robustness of performance for different values of E and $\frac{\bar{\lambda}^2}{\mu}$. This is especially for using A_3 and A_4 . Finally we note that despite similarities between U_2 and U_3 there are significant features that are different: the sharpness in the confinement, the shape and number of attracting wells and the shape of barriers that obstruct crossing regions in the state space. This will have a direct effect in performance, which can explain the difference in performance when comparing Figures 3.3 and 3.4; U_3 is a harder cost function to minimise.

The selection $A = A_2$, shown as the middle row in each of Figures 3.2, 3.3 and 3.4, does not satisfy the probably superfluous symmetry assumption as stated in the introduction, but it is noteworthy that the performance varies to such a large extent for different U and that any optimality of A, left as future work, could change depending on whether the symmetry assumption is in place.

4 Proofs

4.1 Notation and preliminaries

Unless stated otherwise, ∂_t is used to denote the partial derivative with respect to t with T_t fixed (whenever its operand depends on T_t), whereas $\frac{d}{dt}$ denotes the full derivative in t. In addition, ∇ denotes the gradient in \mathbb{R}^{2n+m} space and $d\zeta$ will be used for the Lebesgue measure on \mathbb{R}^{2n+m} . The notation $\mathbb{1}_S$ will be used for the indicator function on the set S.

Recall the standard mollifier $\varphi : \mathbb{R} \to \mathbb{R}$ to be:

$$\varphi(x) := \begin{cases} e^{\frac{1}{x^2 - 1}} \left(\int_{-1}^{1} e^{\frac{1}{y^2 - 1}} dy \right)^{-1} & \text{if } -1 < x \le 1 \\ 0 & \text{otherwise,} \end{cases}$$
$$\varphi_k(x) := \frac{1}{k} \varphi\left(\frac{x}{k}\right) \quad \forall k > 0. \tag{4.1}$$

Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a complete probability space and \mathcal{F}_t , $t \in [0, \infty)$ be a normal filtration² with $(W_t)_{t\geq 0}$ a standard Wiener process on \mathbb{R}^m with respect to \mathcal{F}_t , $t \in [0, \infty)$ and $\zeta_0 = (X_0, Y_0, Z_0) : \Omega \to \mathbb{R}^{2n+m}$ an \mathcal{F}_0 -measurable map admitting Lebesgue density m_0 satisfying Assumption 4.

The formal³ $L^2(\mu_{T_t})$ -adjoint L_t^* of L_t is given by

$$L_t^* = -\left(y \cdot \nabla_x - \nabla_x U(x) \cdot \nabla_y\right) - \left(z^\top \lambda \nabla_y - y^\top \lambda^\top \nabla_z\right) - T_t^{-1} z^\top A \nabla_z + A : D_z^2.$$

$$\tag{4.2}$$

Let $\mathcal{C}^{\infty}_{+} = \{ f \in \mathcal{C}^{\infty} : f > 0 \}$. For $\Phi : \mathcal{C}^{\infty}_{+} \to \mathcal{C}^{\infty}$ differentiable in the sense that for any $f \in \mathcal{C}^{\infty}_{+}, g \in \mathcal{C}^{\infty}$,

$$(d\Phi(f).g)(\zeta) \quad := \quad \lim_{s \to 0} \frac{(\Phi(f+sg))(\zeta) - (\Phi(f))(\zeta)}{s}$$

exists for all $\zeta \in \mathbb{R}^{2n+m}$, the Γ_{Φ} operator for $L_t^{\epsilon*}$ is defined by

$$\Gamma_{L_t^{\epsilon*}, \Phi}(h) := \frac{1}{2} (L_t^{\epsilon*} \Phi(h) - d\Phi(h) . (L_t^{\epsilon*} h)).$$

$$(4.3)$$

 $^{^2\,}$ In other words, satisfying the usual conditions.

 $^{^{3}}$ See for instance Appendix B in [23]. In the present paper the infinitesimal generators and their adjoints are considered as honest differential operators acting on smooth functions.

It will be helpful to keep in mind that $L_t^{\epsilon*}$ does not satisfy the standard chain and product rules, due to the additional term from the second derivatives in $L_t^{\epsilon*}$; straightforward calculations give:

$$L_t^{\epsilon*}(\psi(f)) = \psi'(f)L_t^{\epsilon*}f + \psi''(f)\nabla f \cdot (A^{\epsilon}\nabla f)$$

$$(4.4)$$

$$L_t^{\epsilon*}(fg) = fL_t^{\epsilon*}(g) + gL_t^{\epsilon*}(f) + \nabla f \cdot (2A^{\epsilon}\nabla g)$$

$$(4.5)$$

for all $f, g \in C^{\infty}$ and $\psi \in C^{\infty}$. Note $\nabla f \cdot (A^{\epsilon} \nabla f)$ and $\nabla f \cdot (2A^{\epsilon} \nabla g)$ are respectively the *carré du champ* and its symmetric bilinear operator via polarisation for $L_t^{\epsilon*}$.

In addition, for a scalar-valued D_1 and a vector-valued operator D_2 both acting on scalar-valued functions, denote the commutator bracket as follows:

$$[D_1, D_2]h = (D_1(D_2h)_1 - (D_2D_1h)_1, \dots, D_1(D_2h)_{d_{D_2}} - (D_2D_1h)_{d_{D_2}})$$
(4.6)

for $h \in \mathcal{C}^{\infty}$, where $d_{D_2} \in \mathbb{N}$ is the number of elements in the output of D_2 .

Let $\epsilon \geq 0$ and consider the perturbed system

$$dX_t^{\epsilon} = Y_t^{\epsilon} dt + \epsilon (-T_t^{-1} \nabla_x U(X_t^{\epsilon}) dt + dW_t^1), \qquad (4.7a)$$

$$dY_t^{\epsilon} = -\nabla_x U(X_t^{\epsilon}) dt + \lambda^{\top} Z_t^{\epsilon} dt + \epsilon (-T_t^{-1} Y_t^{\epsilon} dt + dW_t^2), \tag{4.7b}$$

$$dZ_t^{\epsilon} = -\lambda Y_t^{\epsilon} dt - T_t^{-1} A Z_t^{\epsilon} dt + \Sigma dW_t^3, \qquad (4.7c)$$

with $(X_0^{\epsilon}, Y_0^{\epsilon}, Z_0^{\epsilon}) = (X_0, Y_0, Z_0)$ restricted as in Assumption 4, where W_t^1, W_t^2, W_t^3 are independent *n*-dimensional and *m*-dimensional Wiener processes. As before, the law and density of (4.7) will be denoted by m_t^{ϵ} along with

$$h_t^{\epsilon} = \frac{dm_t^{\epsilon}}{d\mu_{T_t}}.$$

Let the linear differential operators S_t^x , S_t^y and their respective formal L^2 -adjoints $S_t^{x\top}$ and $S_t^{y\top}$ be given by

$$\begin{split} S_t^x &= -T_t^{-1} \nabla_x U \cdot \nabla_x + \Delta_x, \\ S_t^{x\top} &= T_t^{-1} \nabla_x U \cdot \nabla_x + T_t^{-1} \Delta_x U + \Delta_x, \end{split} \qquad \qquad S_t^{y\top} &= -T_t^{-1} y \cdot \nabla_y + \Delta_y, \\ S_t^{x\top} &= T_t^{-1} \nabla_x U \cdot \nabla_x + T_t^{-1} \Delta_x U + \Delta_x, \end{split}$$

so that the generator, denoted L_t^{ϵ} , associated to (4.7) is given by the formal operator

$$L_t^{\epsilon} = L_t + \epsilon (S_t^x + S_t^y).$$

Note that the formal $L^2(\mu_{T_t})$ -adjoints of S_t^x and S_t^y coincide with S_t^x and S_t^y , so that the formal $L^2(\mu_{T_t})$ -adjoint of L_t^{ϵ} , denoted $L_t^{\epsilon*}$, is

$$L_t^{\epsilon*} = L_t^* + \epsilon (S_t^x + S_t^y)$$

For any $\phi \in \mathcal{C}^{\infty}$ and $f : \mathbb{R}^{2n+m} \to \mathbb{R}$ smooth enough,

$$L_t^{\epsilon}(\phi(f)) = \phi'(f)L_t^{\epsilon}(f) + \phi''(f)\Gamma_t^{\epsilon}(f), \qquad (4.8)$$

where Γ_t^{ϵ} is the carré du champ operator for L_t^{ϵ} given by

$$\Gamma_t^{\epsilon}(f) = \frac{1}{2} L_t^{\epsilon}(f^2) - f L_t^{\epsilon}(f) = \nabla f \cdot (A^{\epsilon} \nabla f),$$
(4.9)

 $A^{\epsilon} \in \mathbb{R}^{(2n+m) \times (2n+m)}$ denotes the matrix with entries

$$A_{ij}^{\epsilon} := \begin{cases} \epsilon & \text{if } 1 \leq i = j \leq 2n, \\ A_{i-2n,j-2n} & \text{if } 2n+1 \leq i, j \leq 2n+m \\ 0 & \text{otherwise} \end{cases}$$

and $A_{i,j}$ denotes the $(i,j)^{\text{th}}$ entry of A.

4.2 Auxiliary results

For the next result, the space of smooth functions that will be used is from [15]: let $\mathcal{C}_{b,c}^{\infty} = \mathcal{C}_{b,c}^{\infty}(\mathbb{R}_+ \times \mathbb{R}^{2n+m})$ be the space of real-valued functions $f : \mathbb{R}_+ \times \mathbb{R}^{2n+m} \to \mathbb{R}$ such that

1. f is measurable with respect to $\mathcal{B}(\mathbb{R}_+) \otimes \mathcal{B}(\mathbb{R}^{2n+m})$,

2. for all t > 0, $f(t, \cdot)$ is smooth and f is bounded on compact subsets of $\mathbb{R}_{>0} \times \mathbb{R}^{2n+m}$.

Proposition 7 Under Assumption 1, 3 and 4, for all t > 0 and $\epsilon \ge 0$, the unique strong solution $(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon})$ to (4.7) is well-defined and there exists some constant $\kappa > 0$ such that

$$\mathbb{E}\left[|X_t^{\epsilon}|^2 + |Y_t^{\epsilon}|^2 + |Z_t^{\epsilon}|^2\right] \le e^{\kappa t} \mathbb{E}\left[|X_0|^2 + |Y_0|^2 + |Z_0|^2\right] < \infty.$$
(4.10)

Furthermore, for all time t > 0, the law of the $(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon})$

- admits an almost-everywhere finite strictly positive density, also denoted m_t^{ϵ} , w.r.t. the Lebesgue measure on \mathbb{R}^{2n+m} ,
- is the unique integrable distributional solution to

$$\begin{cases} \partial_t m_t^{\epsilon} = (L_t^{\top} + \epsilon (S_t^{x^{\top}} + S_t^{y^{\top}})) m_t^{\epsilon} \\ m_0^{\epsilon} = m_0, \end{cases}$$

$$\tag{4.11}$$

where L_t^{\top} is the formal L^2 -adjoint of L_t .

Finally when $\epsilon > 0$, m_{\bullet} and its partial derivative in time belongs in $C_{b.c}^{\infty}$.

For the notion of integrable distributional solutions, see p.338 in [7].

Proof Existence and uniqueness of an almost surely continuous \mathcal{F}_t -adapted processes follows by conditions (2.4) and (2.6) using Theorem 3.1.1 in [67]; in addition, (4.10) holds by the same theorem. For the claim that the law admits a density, we will apply Theorem 1 in [40] for the case of an arbitrary deterministic starting point. First, condition (H1) in the same article is verified. Take the sets ' K_n ' to be

$$K_p = \prod_{i=1}^{2n+m} [-p, p]$$

for all $p \in \mathbb{N}$. The unique solution to (4.7) with a deterministic starting point $(X_0, Y_0, Z_0) = (x_0, y_0, z_0) \in \mathbb{R}^{2n+m}$ satisfies the same bound (4.10) as before when initialising from m_0 . Moreover, for the random sets

$$\Xi_p = \{s > 0 : (X_u^{\epsilon}, X_u^{\epsilon}, X_u^{\epsilon}) \in K_p, 0 \le u \le s\},\$$

for $p \in \mathbb{N}$, the solution $(\hat{X}_t^{\epsilon}, \hat{Y}_t^{\epsilon}, \hat{Z}_t^{\epsilon})$ to the stopped stochastic differential equation

$$d\hat{X}_t^{\epsilon,p} = \mathbb{1}_{\Xi_p}(t)(\hat{Y}_t^{\epsilon,p} dt + \epsilon(-T_t^{-1}\nabla_x U(\hat{X}_t^{\epsilon,p}) dt + dW_t^1)),$$
(4.12a)

$$d\hat{Y}_t^{\epsilon,p} = \mathbb{1}_{\Xi_p}(t)(-\nabla_x U(\hat{X}_t^{\epsilon,p})\,dt + \lambda^\top \hat{Z}_t^{\epsilon,p}\,dt + \epsilon(-T_t^{-1}\hat{Y}_t^{\epsilon,p}\,dt + dW_t^2)),\tag{4.12b}$$

$$d\hat{Z}_t^{\epsilon,p} = \mathbb{1}_{\mathcal{Z}_p}(t)(-\lambda \hat{Y}_t^{\epsilon,p} dt - T_t^{-1} A \hat{Z}_t^{\epsilon,p} dt + \Sigma dW_t^3),$$
(4.12c)

is well-defined by the same Theorem 3.1.1 in [67] and the corresponding bound

$$\mathbb{E}\left[|\hat{X}_{t}^{\epsilon,p}|^{2} + |\hat{Y}_{t}^{\epsilon,p}|^{2} + |\hat{Z}_{t}^{\epsilon,p}|^{2}\right] \le e^{\kappa t} \left(|x_{0}|^{2} + |y_{0}|^{2} + |z_{0}|^{2}\right) < \infty$$

holds. Identifying $(\hat{X}_t^{\epsilon,p}, \hat{Y}_t^{\epsilon,p}, \hat{Z}_t^{\epsilon,p}) = (X_{t \land \sup \Xi_p}^{\epsilon}, Y_{t \land \sup \Xi_p}^{\epsilon}, Z_{t \land \sup \Xi_p}^{\epsilon})$ a.s. yields that⁴ for any $\tau > 0$

$$\mathbb{P}(\inf\{t \ge 0 : (X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}) \notin K_p\} \le \tau) \le \frac{1}{p^2} \mathbb{E}\left[|X_{\tau \land \sup \Xi_p}^{\epsilon}|^2 + |Y_{\tau \land \sup \Xi_p}^{\epsilon}|^2 + |Z_{\tau \land \sup \Xi_p}^{\epsilon}|^2\right]$$
$$\le \frac{e^{\kappa \tau}}{p^2} \left(|x_0|^2 + |y_0|^2 + |z_0|^2\right)$$

 $^{^4\,}$ Alternatively Corollary 1.2 of Section 5 in [24] can be used.

and in particular that for any $\tau > 0$,

$$\mathbb{P}(\inf\{t \ge 0 : (X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}) \notin K_p\} \le \tau) \to 0 \quad \text{as } p \to \infty.$$
(4.13)

Suppose for contradiction that with nonzero probability, the increasing-in-p random variable $\inf\{t \ge 0 : (X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}) \notin K_p\}$ converges to a real value as $p \to \infty$. Then there exists a time $\hat{\tau} > 0$ such that with nonzero probability,

$$\inf\{t \ge 0 : (X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}) \notin K_p\} \le \hat{\tau} \quad \forall p \in \mathbb{N},$$

which contradicts (4.13). Therefore condition (H1) in [40] holds for (4.7). Condition (H2) in the same article holds due the K_p being compact and the smoothness assumption on U. It can be readily checked that the local weak Hörmander condition (LWH) in [40] also holds at any (t, y_0) for any $r \in (0, t)$ and R > 0. Therefore by Theorem 1 in [40], due to our Assumptions 1 and 3, the solution to (4.7) with a deterministic starting point $\zeta_0 \in \mathbb{R}^{2n+m}$ admits a smooth density $p_t^{\zeta_0} \in \mathcal{C}^{\infty}(\mathbb{R}^{2n+m})$ for all t > 0. Moreover by Theorem 2 in [40], for any fixed $\zeta \in \mathbb{R}^{2n+m}$, $\mathbb{R}^{2n+m} \ni \zeta_0 \mapsto p_t^{\zeta_0}(\zeta)$ is lower semi continuous and hence measurable, so that the $\mathbb{R} \cup \{\pm\infty\}$ -valued function on \mathbb{R}^{2n+m} ,

$$\int_{\mathbb{R}^{2n+m}} p_t^{\zeta_0} m_0(d\zeta_0), \tag{4.14}$$

is integrable by Fubini's theorem and so is almost everywhere \mathbb{R} -valued on \mathbb{R}^{2n+m} . By Itô's rule, (4.14) solves (4.11) in the distributional sense. In addition, (4.11) is the unique integrable solution by Theorem 9.6.3 in [7], which requires for any T > 0 that there exists $V \in C^2(\mathbb{R}^{2n+m})$ such that

- 1. $V(x) \to \infty$ as $|x| \to \infty$ and
- 2. for some constant $C_V > 0$ and all $(x,t) \in \mathbb{R}^{2n+m} \times (0,T)$, it holds that $L_t^{\epsilon} V \ge -C_V V$ and $|\nabla V| \le C_V V$.

Setting $V(x,y,z) = 1 + U(x) - U_m + \frac{|y|^2}{2} + \frac{|z|^2}{2}$ and calculating

$$L_t^{\epsilon} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right) = \epsilon \left(-\frac{1}{T_t} |\nabla_x U|^2 + \Delta_x U - \frac{1}{T_t} |y|^2 + n \right) - \frac{1}{T_t} z^\top A z + \text{Tr}A$$
(4.15)

it is clear from assumptions (2.4), (2.6) and either (2.7) or (2.8) on U that these conditions are satisfied since T is finite; therefore there is a unique integrable solution to (4.11) in the sense of p.338 in [7]. The expression in (4.14) is thus the density for the law of the solution to (4.7) with initial law m_0 at time t.

For $\epsilon > 0$, the time-depending law of $(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon})$ and its partial derivative with respect to time belongs in $\mathcal{C}_{b,c}^{\infty}$ by Theorem 1.1 in [15] because (4.14) satisfies (4.11).

For positivity of the density where $\epsilon = 0$, the steps in Lemma 3.4 of [51] can be followed; the associated control problem has the expression

$$\frac{d}{dt} \begin{pmatrix} Q_t \\ P_t \\ V_t \end{pmatrix} = \begin{pmatrix} P_t \\ -\nabla U(Q_t) + \lambda^\top V_t \\ -\lambda P_t - T_t A V_t + \Sigma \frac{d\tilde{U}}{dt} \end{pmatrix}.$$
(4.16)

It suffices to show that given any S > 0 and any pair $(Q_0, P_0, V_0) \in \mathbb{R}^{2n+m}$ and $(Q^*, P^*, V^*) \in \mathbb{R}^{2n+m}$, there exists a control $\tilde{U} : [0, \infty) \to \mathbb{R}^m$ such that the solution (Q_t, P_t, V_t) to (4.16) starting at (Q_0, P_0, V_0) satisfies $(Q_S, P_S, V_S) = (Q^*, P^*, V^*)$. Fix $S > 0, \epsilon > 0, (Q_0, P_0, V_0) \in \mathbb{R}^{2n+m}, (Q^*, P^*, V^*) \in \mathbb{R}^{2n+m}$. Using the mollifier (4.1), let

$$\nu := \varphi_{\frac{1}{2}} * \mathbb{1}_{\left(-\infty, \frac{1}{2}\right]},$$

where * denotes convolution. Define a smooth function $\hat{Q}_{\cdot} : [0, S] \to \mathbb{R}^n$ by

$$\hat{Q}_t = \left(\left(-\nabla U(Q_0) + \lambda^\top V_0 \right) \frac{t^2}{2} + P_0 t + Q_0 \right) \nu \left(\frac{t}{S} \right) + \left(\left(-\nabla U(Q^*) + \lambda^\top V^* \right) \frac{t^2}{2} + P^* t + Q^* \right) \nu \left(1 - \frac{t}{S} \right)$$
(4.17)

which satisfies

$$\hat{Q}_0 = Q_0, \qquad \qquad \hat{Q}_S = Q^*,$$

$$\frac{d\hat{Q}_t}{dt}(0) = P_0, \qquad \qquad \frac{d\hat{Q}_t}{dt}(S) = P^*.$$

Define $\hat{P} : [0, S] \to \mathbb{R}^n$ through

$$\hat{P}_t = \frac{d\hat{Q}_t}{dt}.\tag{4.18}$$

For $\hat{V} : [0, S] \to \mathbb{R}^m$, $\hat{V} : [0, S] \to \mathbb{R}^m$ is defined with

$$\hat{V}_{t} = \lambda (\lambda^{\top} \lambda)^{-1} \left(\nabla U(\hat{Q}_{t}) + \partial_{t}^{2} \left[\left(-\nabla U(Q_{0}) \frac{t^{2}}{2} + P_{0}t + Q_{0} \right) \nu \left(\frac{t}{S} \right) + \left(-\nabla U(Q^{*}) \frac{t^{2}}{2} + P^{*}t + Q^{*} \right) \nu \left(1 - \frac{t}{S} \right) \right] \right) + \partial_{t}^{2} \left[V_{0} \frac{t^{2}}{2} \nu \left(\frac{t}{S} \right) + V^{*} \frac{t^{2}}{2} \nu \left(1 - \frac{t}{S} \right) \right]$$

$$(4.19)$$

where $(\lambda^{\top}\lambda)^{-1}$ exists by λ having rank n. Note that \hat{V}_t satisfies $\hat{V}_0 = V_0$ and $\hat{V}_S = V^*$. Let the smooth function $\tilde{U}: [0, \infty) \to \mathbb{R}^m$ be given by

$$\frac{d\tilde{U}}{dt} = \Sigma^{-1} \left(\frac{d\hat{V}_t}{dt} + \lambda \hat{P}_t + T_t A \hat{V}_t \right), \quad \tilde{U}(0) = 0.$$
(4.20)

For this \tilde{U} , the solution to (4.16) with initial condition (Q_0, P_0, V_0) is $(\hat{Q}_t, \hat{P}_t, \hat{V}_t)$ by construction; its uniqueness is guaranteed by considering the system satisfied by the difference between two supposedly different solutions (Q_t^1, P_t^1, V_t^1) and (Q_t^2, P_t^2, V_t^2)

$$\frac{d}{dt} \begin{pmatrix} Q_t^1 - Q_t^2 \\ P_t^1 - P_t^2 \\ V_t^1 - V_t^2 \end{pmatrix} = \begin{pmatrix} P_t^1 - P_t^2 \\ -\nabla U(Q_t^1) - \nabla U(Q_t^2) + \lambda^\top (V_t^1 - V_t^2) \\ -\lambda (P_t^1 - P_t^2) - T_t A(V_t^1 - V_t^2) \end{pmatrix}$$

and the time derivative of $|Q_t^1 - Q_t^2|^2 + |P_t^1 - P_t^2|^2 + |V_t^1 - V_t^2|^2$, using (2.4) and the mean value theorem on $|\nabla U(Q_t^1) - \nabla U(Q_t^2)|^2$.

With non-zero probability, the path of Brownian motion stays within an ϵ -neighbourhood of any continuously differentiable path, in particular of \tilde{U} . Positivity of m_t follows by the support theorem of Stroock and Varadhan (Theorem 5.2 in [72]). The above construction for the $\epsilon > 0$ case follows with a simple modification; equation (4.16) becomes

$$\frac{d}{dt} \begin{pmatrix} Q_t \\ P_t \\ V_t \end{pmatrix} = \begin{pmatrix} P_t - \epsilon \nabla U(Q_t) + \epsilon \frac{d\tilde{U}_1}{dt} \\ -\nabla U(Q_t) + \lambda^\top V_t - \epsilon P_t + \epsilon \frac{d\tilde{U}_2}{dt} \\ -\lambda P_t - T_t A V_t + \Sigma \frac{d\tilde{U}}{dt} \end{pmatrix},$$
(4.21)

so setting $\frac{d\tilde{U}_1}{dt} = \nabla U(\hat{Q}_t)$ and $\frac{d\tilde{U}_2}{dt} = \hat{P}_t$ together with (4.20) gives the solution (4.17), (4.18) and (4.19) to equation (4.21) and concludes the proof.

Remark 3 For smoothness of the density, the results in [75] can also be considered, but there the assumptions are slightly mismatched. Firstly, the statement assumes boundedness of $\partial^{\alpha} V$ for any multiindex α where V would in the case here be any of the coefficients appearing in (1.3), which fails for $|\alpha| = 0$. Secondly, in case of (A.1), condition (i) fails and in case of (A.2), condition (i) fails due to V_0 . Both of these pedantries seem possibly unneeded in the proofs but we avoid this in favour of the more recent work [40].

The results below up to Proposition 10 are directed towards showing dissipation of a distorted entropy as required in the proof of Theorem 5.

4.3 Lyapunov function

Lemma 1 Under Assumption 1, 3 and 4, there exist constants $a, b, c, d, \delta > 0$ independent of ϵ such that R: $\mathbb{R}^{2n+m+1} \to \mathbb{R}$ defined as

$$R(x, y, z, T_t) := U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} + \delta T_t \left(y^\top \lambda^{-1} z + \frac{1}{2} x \cdot y \right)$$
(4.22)

satisfies

$$a(|x|^{2} + |y|^{2} + |z|^{2}) - d \leq R(x, y, z, T_{t}) \leq b(|x|^{2} + |y|^{2} + |z|^{2}) + d,$$

$$(4.23)$$

and there exists $0 < \epsilon' \leq 1$ for which $\epsilon \leq \epsilon'$ implies

$$L_t^{\epsilon} R \le -cT_t R + \frac{d}{T_t}.$$
(4.24)

Proof By the quadratic assumption (2.8) on U and boundedness Assumption 3 on T_t , it is clear that there exists $\hat{\delta} > 0$ such that the first statement (4.23) holds with $d = \max(|U_m|, |U_M|)$ for all $\delta \in (0, \hat{\delta}]$. For the second statement in (4.24), fix $\delta > 0$ to be

$$\delta \leq \min\left(\hat{\delta}, 1, \frac{4r_1^2}{(r_2+1)\sup_{s\geq 0} T_s}, 2\left(\sup_{s\geq 0} T_s\right)^{-1}, \frac{A_c}{2} \left[\left(\frac{|\lambda|^2}{2r_1} + 1 + \frac{r_2}{r_1}|\lambda^{-1}|^2\right)\left(\sup_{s\geq 0} T_s\right)^2 + 2(|A|^2 + 1)|\lambda^{-1}|^2\right]^{-1}\right), \tag{4.25}$$

where $|\cdot|$ is the operator norm here and $A_c > 0$ is the coercivity constant of the positive definite matrix A. Consider each of the terms of $L_t^{\epsilon}(R)$ separately.

$$L_{t}^{\epsilon}\left(U(x) + \frac{|y|^{2}}{2} + \frac{|z|^{2}}{2}\right) = \epsilon \left(-\frac{1}{T_{t}}|\nabla_{x}U|^{2} + \Delta_{x}U - \frac{1}{T_{t}}|y|^{2} + n\right) - \frac{1}{T_{t}}z^{\top}Az + \text{Tr}A.$$

$$\leq \epsilon \left(-\frac{1}{T_{t}}(r_{1}^{2}|x|^{2} - 2r_{1}U_{g}) + n|D_{x}^{2}U|_{\infty} - \frac{1}{T_{t}}|y|^{2} + n\right) - \frac{1}{T_{t}}z^{\top}Az + \text{Tr}A.$$

$$(4.26)$$

$$\leq \epsilon \left(-\frac{1}{T_t} (r_1^2 |x|^2 - 2r_1 U_g) + n |D_x^2 U|_{\infty} - \frac{1}{T_t} |y|^2 + n \right) - \frac{1}{T_t} z^\top A z + \text{Tr}A, \qquad (4.27)$$

where the last inequality follows from (2.5) and $\nabla_x U \cdot x \leq \frac{1}{2r_1} |\nabla_x U|^2 + \frac{r_1}{2} |x|^2$. Using the quadratic bound (2.6) on $\nabla_{x}U$, we get

$$L_{t}^{\epsilon}(y^{\top}\lambda^{-1}z) = -\epsilon T_{t}^{-1}y^{\top}\lambda^{-1}z - \nabla_{x}U\lambda^{-1}z + |z|^{2} - |y|^{2} - T_{t}^{-1}z^{\top}A(\lambda^{-1})^{\top}y$$

$$\leq \frac{|y|^{2}}{4} + 2T_{t}^{-2}(|A|^{2} + \epsilon^{2})|\lambda^{-1}|^{2}|z|^{2} + \frac{r_{1}}{4r_{2}}|\nabla_{x}U|^{2} + \frac{r_{2}}{r_{1}}|\lambda^{-1}|^{2}|z|^{2} + |z|^{2} - |y|^{2}$$

$$(4.28)$$

$$\leq \frac{r_1}{4} |x|^2 + \frac{r_1}{4r_2} U_g - \frac{3}{4} |y|^2 + \left(1 + \frac{r_2}{r_1} |\lambda^{-1}|^2 + 2T_t^{-2} (|A|^2 + 1) |\lambda^{-1}|^2\right) |z|^2.$$
(4.29)

Then using also (2.5) for $\nabla_x U \cdot x$, we get

$$L_t^{\epsilon}(x \cdot y) = -\epsilon T_t^{-1} y \cdot \nabla_x U - \epsilon T_t^{-1} x \cdot y + |y|^2 - \nabla_x U \cdot x + z^\top \lambda x$$

$$(4.30)$$

$$\leq \epsilon T_t^{-1} \left(\left(\frac{r_2}{2} + \frac{1}{2} \right) |x|^2 + |y|^2 + \frac{U_g}{2} \right) + |y|^2 - r_1 |x|^2 + U_g + \frac{|\lambda^+|^2}{r_1} |z|^2 + \frac{r_1}{4} |x|^2.$$

$$\tag{4.31}$$

Combining (4.22), (4.27), (4.29), (4.31) and taking $\epsilon \leq 1$,

$$\begin{split} L_{t}^{\epsilon}(R(x,y,z,T_{t})) &= L_{t}^{\epsilon} \bigg(U(x) + \frac{|y|^{2}}{2} + \frac{|z|^{2}}{2} \bigg) + \delta T_{t} L_{t}(y^{\top} \lambda^{-1} z) + \frac{\delta T_{t}}{2} L_{t}(x \cdot y) \\ &\leq -\delta T_{t} \frac{r_{1}}{8} |x|^{2} - \delta T_{t} \frac{1}{4} |y|^{2} - \frac{1}{T_{t}} z^{\top} A z + C + \frac{2\epsilon r_{1} U_{g}}{T_{t}} \\ &+ \delta T_{t} \bigg[\frac{|\lambda^{\top}|^{2}}{2r_{1}} + \bigg(1 + \frac{r_{2}}{r_{1}} |\lambda^{-1}|^{2} + 2T_{t}^{-2} (|A|^{2} + 1) |\lambda^{-1}|^{2} \bigg) \bigg] |z|^{2} . \\ &+ \epsilon T_{t}^{-1} \bigg[\bigg(\frac{\delta T_{t}}{4} (r_{2} + 1) - r_{1}^{2} \bigg) |x|^{2} + \bigg(\frac{\delta T_{t}}{2} - 1 \bigg) |y|^{2} \bigg], \end{split}$$

$$(4.32)$$

where $0 < C = n(|D_x^2 U|_{\infty} + 1) + \text{Tr}A + \delta \frac{r_1 U_g}{4r_2} \sup_{s \ge 0} T_s + \delta U_g(\frac{1}{4} + \frac{\sup_{s \ge 0} T_s}{2})$. Therefore for δ satisfying the bound (4.25), the first square bracket term satisfies

$$\delta T_t \left[\frac{\left| \lambda^{\top} \right|^2}{2r_1} + \left(1 + \frac{r_2}{r_1} \left| \lambda^{-1} \right|^2 + 2T_t^{-2} (\left| A \right|^2 + 1) \left| \lambda^{-1} \right|^2 \right) \right] \le \frac{1}{2} \left(\sup_{s \ge 0} T_s \right)^{-1} A_c |z|^2$$

and the second square bracket term is negative, where the assumption that T_t is bounded above for all time has been used. Rearranging,

$$\begin{split} L_t^{\epsilon}(R(x,y,z,T_t)) &\leq -\delta T_t \frac{r_1}{8} |x|^2 - \delta T_t \frac{1}{4} |y|^2 - \frac{A_c}{2 \sup_s T_s} |z|^2 + C + \frac{2\epsilon r_1 U_g}{T_t} \\ &\leq -c T_t R + C' T_t^{-1}, \end{split}$$

where c > 0 is small enough, C' > 0 is large enough and the right inequality of (4.23) has been used. The result follows using $d = \max(C', |U_m|, |U_M|)$.

Lemma 2 Under Assumption 1, 3, 4 and for $0 \le \epsilon \le \epsilon'$, the solution $(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon})$ to (4.7) is such that $\frac{\mathbb{E}[R(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}, T_t)]}{(\ln(e+t))^2}$ is bounded uniformly in time t and in ϵ .

Proof It is equivalent to prove the result for R + d > 0 in place of R. Let $R_t := R(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon}, T_t)$. Consider the following terms separately for $t > t_0$,

$$\frac{d}{dt}\mathbb{E}[(R_t+d)] = \partial_t \mathbb{E}[(R_t+d)] + T'_t \partial_{T_t} \mathbb{E}[(R_t+d)].$$
(4.34)

Firstly, by (4.22), the left hand bound in (4.23) and the Assumption 3,

$$T_{t}^{\prime}\partial_{T_{t}}\mathbb{E}[R_{t}+d] = T_{t}^{\prime}\mathbb{E}\left[\delta\left((Y_{t}^{\epsilon})^{\top}\lambda^{-1}Z_{t} + \frac{1}{2}X_{t}^{\epsilon}\cdot Y_{t}^{\epsilon}\right)\right]$$

$$\leq |T_{t}^{\prime}|\mathbb{E}\left[\delta\left|(Y_{t}^{\epsilon})^{\top}\lambda^{-1}Z_{t}^{\epsilon} + \frac{1}{2}X_{t}^{\epsilon}\cdot Y_{t}^{\epsilon}\right|\right]$$

$$\leq \frac{B}{t}\mathbb{E}[R_{t}+d]$$

$$(4.35)$$

for a constant $B \ge 0$ independent of ϵ . The exchange in the order of differentiation and integration is justified by the right hand bound of (4.23) together with the mean value theorem and the fact that for any T > 0 the inequality

$$\mathbb{E}\left[\sup_{0\leq t\leq T}|X_t^{\epsilon}|^2\right] = \mathbb{E}\left[\left(\sup_{0\leq t\leq T}|X_t^{\epsilon}|\right)^2\right] = \mathbb{E}\left[\left(\sup_{0\leq t\leq T}\left|X_0 + \int_0^t (Y_s^{\epsilon} + \epsilon(-T_s^{-1}\nabla_x U(X_s^{\epsilon})))\,ds + \epsilon\int_0^t dW_s^1\right|\right)^2\right] \\
\leq K_T^1 \mathbb{E}\int_0^T (1 + |X_s^{\epsilon}|^2 + |Y_s^{\epsilon}|^2)ds < \infty$$
(4.36)

holds for some constant $K_T^1 > 0$ depending on T but independent of ϵ (using $\epsilon \leq \epsilon'$), where (2.6), (4.10), Jensen's inequality and Doob's maximal inequality have been used. Similar expressions for $\mathbb{E}[\sup_{0 \leq t \leq T} |Y_t^{\epsilon}|^2]$ and $\mathbb{E}[\sup_{0 < t < T} |Z_t^{\epsilon}|^2]$ hold.

Considering together with the other term in (4.34), by Itô's rule and for $t_0 < s < t$,

$$\mathbb{E}R_t - \mathbb{E}R_s = \mathbb{E}\int_s^t (T'_u \partial_{T_t} R + L^{\epsilon}_u R)(X^{\epsilon}_u, Y^{\epsilon}_u, Z^{\epsilon}_u, T_u) du = \int_s^t \mathbb{E}(T'_u \partial_{T_t} R + L^{\epsilon}_u R)(X^{\epsilon}_u, Y^{\epsilon}_u, Z^{\epsilon}_u, T_u) du,$$

where the last equality follows by Fubini, (4.35) and (4.32) together with (4.26), (4.28), (4.30), (2.4), (2.6), (4.36). Property (4.24) from Lemma 1 and (4.35) give

$$\mathbb{E}[R_t + d] - \mathbb{E}[R_s + d] \leq \int_s^t \left(\frac{B}{u} \mathbb{E}[R_u + d] + \mathbb{E}[-cT_uR_u + dT_u^{-1}]\right) du$$
$$\leq \int_s^t \left(\left(\frac{B}{u} - cT_u\right) \mathbb{E}[R_u + d] + B'T_u^{-1}\right) du$$
(4.37)

for a constant $B' \ge 0$ independent of ϵ . In order to obtain a differential inequality for all t as opposed to almost all t from Lebesgue differentiation theorem, the above expression can be divided by t - s, mollified in time with (4.1) for 0 < k < 1 and have $s \to t$ taken as follows. For $t > t_0 + 1$,

$$\begin{split} \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{t-1}^{t+1} \varphi_k(t-u) (\mathbb{E}[R_{u+\hat{\epsilon}}+d] - \mathbb{E}[R_{u-\hat{\epsilon}}+d]) du \\ &\leq \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{t-1}^{t+1} \varphi_k(t-u) \int_{u-\hat{\epsilon}}^{u+\hat{\epsilon}} \left(\left(\frac{B}{u'} - cT_{u'}\right) \mathbb{E}[R_{u'}+d] + B'T_{u'}^{-1} \right) du' du \\ &\leq \int_{t-1}^{t+1} \varphi_k(t-u) \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{u-\hat{\epsilon}}^{u+\hat{\epsilon}} \left(\left(\frac{B}{u'} - cT_{u'}\right) \mathbb{E}[R_{u'}+d] + B'T_{u'}^{-1} \right) du' du \\ &= \int_{t-1}^{t+1} \varphi_k(t-u) (\left(\left(\frac{B}{u} - cT_u\right) \mathbb{E}[R_u+d] + B'T_u^{-1} \right) du, \end{split}$$

where the second-to-last inequality follows by Fatou's lemma and dominated convergence; the last line follows from the Lebesgue differentiation theorem. In other words, for $\hat{g}: \mathbb{R}_+ \to \mathbb{R}$ given by $\hat{g}(t) := Bt^{-1} - cT_t$, it holds that

$$\begin{aligned} \frac{d}{dt}(\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) &\leq (\varphi_k * (\hat{g}\mathbb{E}[R_{\bullet} + d] + B'T_{\bullet}^{-1}))(t) \\ &\leq \left(\frac{B}{t-1} - c\inf_{t-1 \leq s \leq t+1} T_s\right)(\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) + B'\left(\inf_{t-1 \leq s \leq t+1} T_s\right)^{-1}. \end{aligned}$$

Using Assumption 3, we get

$$\frac{d}{dt}(\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) \le -\frac{cE}{2}(\ln(t+1))^{-1}(\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) + \frac{B'}{E}\ln(t+1)$$

for $t > t_0^*$, where $t_0^* > t_0$ is such that $\frac{B}{t-1} \le \frac{cE}{2\ln(t+1)}$ for $t > t_0^*$. Then, for $t > t_0^*$,

$$\begin{aligned} \frac{d}{dt} \left(e^{\frac{cE}{2} \int_{t_0}^t (\ln(s+1))^{-1} ds} (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) \right) &\leq \frac{B'}{E} \ln(t+1) e^{\frac{cE}{2} \int_{t_0}^t (\ln(s+1))^{-1} ds}, \\ (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t) &\leq (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) e^{-\frac{cE}{2} \int_{t_0}^t (\ln(s+1))^{-1} ds} \\ &+ \int_{t_0}^t \frac{B'}{E} \ln(s+1) e^{-\frac{cE}{2} \int_{s}^t (\ln(u+1))^{-1} du} ds \\ &\leq (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) + \frac{B'}{E} \int_{t_0}^t \ln(s+1) e^{-\frac{cE}{2} \int_{s}^t (\ln(u+1))^{-1} du} ds \\ &\leq (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) + \frac{B'}{E} \ln(t+1) \int_{t_0}^t e^{-\frac{cE}{2\ln(t+1)}(t-s)} ds \\ &\leq (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) + B' \frac{2(\ln(t+1))^2}{cE^2} \left(1 - e^{-\frac{cE}{2}(\ln(t+1))^{-1}(t-t_0^*)}\right) \\ &\leq (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) + B' \frac{2(\ln(t+1))^2}{cE^2}. \end{aligned}$$

Using (4.37),

$$\mathbb{E}[R_t+d] = \mathbb{E}[R_t+d] \int_{t-2k}^t \varphi_k(t-k-s)ds \le \int_{t-2k}^t \varphi_k(t-k-s)\mathbb{E}[R_s+d]ds + \bar{g}(2k)$$
(4.38)

for some $\bar{g}: \mathbb{R} \to \mathbb{R}$ satisfying $\bar{g}'(k') \to 0$ as $k' \to 0$, so that for $t > t_0^* + 2$,

$$\mathbb{E}[R_t + d] \le (\varphi_k * \mathbb{E}[R_{\bullet} + d])(t_0^*) + B' \frac{2(\ln(t - k + 1))^2}{cE^2} + \bar{g}(2k),$$

where the first term on the right can be bounded independently of k via Proposition 7 and (4.23) in a similar spirit to (4.38). The result follows by taking $k \to 0$.

Corollary 1 Under Assumption 1, 3, 4 and for $0 \le \epsilon \le \epsilon'$, the solution $(X_t^{\epsilon}, Y_t^{\epsilon}, Z_t^{\epsilon})$ to (4.7) is such that $\frac{\mathbb{E}[|X_t^{\epsilon}|^2 + |Y_t^{\epsilon}|^2 + |Z_t^{\epsilon}|^2]}{(\ln(e+t))^2}$ is bounded uniformly in time and in ϵ .

Proof By the lower bound on R in (4.23),

$$\mathbb{E}\left[\left|X_{t}^{\epsilon}\right|^{2}+\left|Y_{t}^{\epsilon}\right|^{2}+\left|Z_{t}^{\epsilon}\right|^{2}\right] \leq \mathbb{E}\left[\frac{R(X_{t}^{\epsilon},Y_{t}^{\epsilon},Z_{t}^{\epsilon},T_{t})+d}{a}\right]$$

which concludes by Lemma 2.

4.4 Form of Distorted Entropy

For $\epsilon \geq 0$, let $H^{\epsilon}(t)$ be the distorted entropy

$$H^{\epsilon}(t) = \int \left(\frac{\left| 2\nabla_{x} h_{t}^{\epsilon} + 8S_{0}(\nabla_{y} h_{t}^{\epsilon} + \lambda^{-1} \nabla_{z} h_{t}^{\epsilon}) \right|^{2}}{h_{t}^{\epsilon}} + \frac{\left| \nabla_{y} h_{t}^{\epsilon} + S_{1} \lambda^{-1} \nabla_{z} h_{t}^{\epsilon} \right|^{2}}{h_{t}^{\epsilon}} + \beta(T_{t}^{-1}) h_{t}^{\epsilon} \ln(h_{t}^{\epsilon}) \right) d\mu_{T_{t}}, \quad (4.39)$$

where $S_0, S_1 > 0$ are the constants

$$S_0 := (1 + |D_x^2 U|_{\infty}^2)^{\frac{1}{2}}, \tag{4.40}$$

$$S_1 := 2 + 28S_0^2 + 1024S_0^4 \tag{4.41}$$

and β is a second order polynomial (see (4.44) and (4.50)) to be determined by Proposition 8 and independent of ϵ .

Remark 4 This particular expression for H is not necessarily the best possible choice. However the above is a working expression and optimality is left as future work; see also [64].

We now present an auxiliary result which can be found as Lemma 12 of [55]. We state this along with its proofs from [55].

Lemma 3 For

$$\Phi^*(h) = \frac{|M\nabla h|^2}{h},$$

where M is matrix-valued,

$$\Gamma_{L_t^{\epsilon*}, \Phi^*}(h) > \frac{(M\nabla h) \cdot [L_t^{\epsilon*}, M\nabla]h}{h}$$

holds for all $h \in \mathcal{C}^{\infty}_+$.

Notice the Φ^* appears in the first two terms of $H^{\epsilon}(t)$.

Proof The second term in definition (4.3) of $\Gamma_{L_t^{\epsilon*}, \Phi^*}(h)$ can be calculated to be

$$-d\Phi^*(h).L_t^{\epsilon*}h = -\frac{2}{h}(M\nabla h) \cdot (M\nabla L_t^{\epsilon*}h) + \frac{L_t^{\epsilon*}h}{h^2}|M\nabla h|^2.$$

$$(4.42)$$

Using (4.5) and (4.4) for $L_t^{\epsilon*}$, the first term in the definition of $\Gamma_{L_t^{\epsilon*},\Phi}$ in (4.3) can be calculated to be

$$\begin{split} L_t^{\epsilon*}(\varPhi^*(h)) &= \frac{1}{h} L_t^{\epsilon*}(|M\nabla h|^2) + |M\nabla h|^2 L_t^{\epsilon*}\left(\frac{1}{h}\right) - \sum_i \frac{4}{h^2} (M\nabla h)_i \nabla h \cdot (A^{\epsilon} \nabla (M\nabla h)_i) \\ &= \frac{2}{h} \bigg((M\nabla h) \cdot L_t^{\epsilon*} M \nabla h + \sum_i \nabla (M\nabla h)_i \cdot (A^{\epsilon} \nabla (M\nabla h)_i) \bigg) \\ &+ |M\nabla h|^2 L_t^{\epsilon*}\left(\frac{1}{h}\right) - \sum_i \frac{4}{h^2} (M\nabla h)_i \nabla h \cdot (A^{\epsilon} \nabla (M\nabla h)_i), \end{split}$$

where the last summands can be bounded below because A and A^{ϵ} are positive definite, that is, for $v, w \in \mathbb{R}^{2n+m}$ and $c \in \mathbb{R}$, we have

$$(cv - c^{-1}w)^{\top} A^{\epsilon} (cv - c^{-1}w) = c^2 v^{\top} A^{\epsilon} v + c^{-2} w^{\top} A^{\epsilon} w - 2v^{\top} A^{\epsilon} w > 0.$$

Therefore, for all i,

$$-\frac{4}{h^2}(M\nabla h)_i\nabla h\cdot (A^{\epsilon}\nabla(M\nabla h)_i) > -\frac{2}{h^3}(M\nabla h)_i^2(\nabla h)\cdot A^{\epsilon}\nabla h - \frac{2}{h}(\nabla(M\nabla h)_i)\cdot A^{\epsilon}\nabla(M\nabla h)_i,$$

which produces the bound

$$L_t^{\epsilon*}(\varPhi^*(h)) > \frac{2}{h}(M\nabla h) \cdot L_t^{\epsilon*}M\nabla h + |M\nabla h|^2 L_t^{\epsilon*}\left(\frac{1}{h}\right) - \frac{2}{h^3}|M\nabla h|^2 \nabla h \cdot (A^{\epsilon}\nabla h).$$

Combining this with (4.42) then using (4.4) and noting

$$[L_t^{\epsilon*}, M\nabla]h = (L_t^{\epsilon*}(M\nabla h)_1 - (M\nabla L_t^{\epsilon*}h)_1, \dots, L_t^{\epsilon*}(M\nabla h)_{2n+m} - (M\nabla L_t^{\epsilon*}h)_{2n+m}),$$
(4.43)

we get

$$\begin{split} \Gamma_{L_t^{\epsilon*}, \varPhi^*}(h) &> \frac{1}{h} (M \nabla h) \cdot [L_t^{\epsilon*}, M \nabla] h + \frac{1}{2} |M \nabla h|^2 \left(L_t^{\epsilon*} \left(\frac{1}{h} \right) + \frac{L_t^{\epsilon*} h}{h^2} \right) - \frac{1}{h^3} |M \nabla h|^2 \nabla h \cdot (A^{\epsilon} \nabla h) \\ &= \frac{1}{h} (M \nabla h) \cdot [L_t^{\epsilon*}, M \nabla] h. \end{split}$$

Using Lemma 3, the following proposition shows the distorted entropy (4.39) is a useful one.

Proposition 8 There exist $\beta_0, \beta_1, \beta_2 > 0$ independent of ϵ such that for $\beta : \mathbb{R} \to \mathbb{R}$ given by

$$\beta(x) := 1 + \beta_0 + \beta_1 x + \beta_2 x^2, \tag{4.44}$$

the operator Ψ_{T_t} ,

$$\Psi_{T_t}(h) := \frac{\left|2\nabla_x h + 8S_0(\nabla_y h + \lambda^{-1}\nabla_z h)\right|^2}{h} + \frac{\left|\nabla_y h + S_1 \lambda^{-1}\nabla_z h\right|^2}{h} + \beta(T_t^{-1})h\ln(h)$$
(4.45)

for $h \in \mathcal{C}^{\infty}_+$, satisfies

$$\Gamma_{L_t^{\epsilon*},\Psi_{T_t}}(h) \ge \frac{|\nabla h|^2}{h} \tag{4.46}$$

for all $0 \leq \epsilon \leq 1$.

Remark 5 $\beta_0, \beta_1, \beta_2$ depend on $|D_x^2 U|_{\infty}, |A|$ and

$$\hat{\lambda}^2 := \max\left(\left|\lambda\right|^2, \left|\lambda^{\top}\right|^2, \left|\lambda^{-1}\right|^2, \left|\lambda^{-1}\right| \left|\lambda^{\top}\right|\right).$$
(4.47)

H satisfying property (4.46) is crucial for proving dissipation in Proposition 10. *Proof* Let Φ_1, Φ_2, Φ_3 be the terms in Ψ_{T_t} ,

$$\Phi_1(h) := \frac{\left| 2\nabla_x h + 8S_0(\nabla_y h + \lambda^{-1} \nabla_z h) \right|^2}{h},$$
(4.48a)

$$\Phi_2(h) := \frac{\left|\nabla_y h + S_1 \lambda^{-1} \nabla_z h\right|^2}{h},\tag{4.48b}$$

$$\Phi_2(h) := h \ln(h). \tag{4.48c}$$

Note that the Γ_{Φ} operator is linear in the Φ argument by linearity of $L_t^{\epsilon*}$, so that (4.46) can be written as

$$\Gamma_{L_t^{\epsilon*},\Phi_1}(h) + \Gamma_{L_t^{\epsilon*},\Phi_2}(h) + \beta(T_t^{-1})\Gamma_{L_t^{\epsilon*},\Phi_3}(h) \ge \frac{|\nabla h|^2}{h}.$$

Consider $\Gamma_{L_t^{\epsilon_*}, \Phi_3}$ first. Using the definition (4.3) of $\Gamma_{L_t^{\epsilon_*}, \Phi}$, the product and chain rule (4.5) and (4.4) for $L_t^{\epsilon_*}$, and the coercivity property of A, we get

$$\Gamma_{L_{t}^{\epsilon*},\Phi_{3}}(h) = \frac{1}{2} \left((\ln h + 1) L_{t}^{\epsilon*} h + \frac{1}{h} \nabla h \cdot (A^{\epsilon} \nabla h) - (1 + \ln h) L_{t}^{\epsilon*} h \right) \\
= \frac{1}{2h} \nabla h \cdot (A^{\epsilon} \nabla h) \\
\geq \frac{1}{2h} (\epsilon |\nabla_{x} h|^{2} + \epsilon |\nabla_{y} h|^{2} + A_{c} |\nabla_{z} h|^{2}).$$
(4.49)

Since the goal is to show (4.46), the availability of (4.49) counteracts any negative contributions in the zderivative term, and any order ϵ contributions in the x- and y-derivatives, from $\Gamma_{L_t^{\epsilon_*}, \Phi_1}$ and $\Gamma_{L_t^{\epsilon_*}, \Phi_2}$; this counterweight materialises as β .

For $\Gamma_{L_t^{\epsilon*},\Phi_1}$ and $\Gamma_{L_t^{\epsilon*},\Phi_2}$, $S_0 > 0$ and $S_1 > 0$ as in (4.40)-(4.41) are used. Lemma 3 gives

$$\begin{split} h\Gamma_{L_t^*,\varPhi_2}(h) &> (\nabla_y + S_1\lambda^{-1}\nabla_z)h \cdot [L_t^{**}, \nabla_y + S_1\lambda^{-1}\nabla_z]h \\ &= (\nabla_y + S_1\lambda^{-1}\nabla_z)h \cdot (\nabla_x - \lambda^{\top}\nabla_z + \epsilon T_t^{-1}\nabla_y + S_1\nabla_y + S_1T_t^{-1}\lambda^{-1}A\nabla_z)h \\ &= \nabla_x h \cdot \nabla_y h - \nabla_y h \cdot (\lambda^{\top}\nabla_z h) + \epsilon T_t^{-1}|\nabla_y h|^2 + S_1|\nabla_y h|^2 + S_1T_t^{-1}\nabla_y h \cdot (\lambda^{-1}A\nabla_z h) \\ &+ S_1\nabla_x h \cdot (\lambda^{-1}\nabla_z h) - S_1(\lambda^{-1}\nabla_z h) \cdot (\lambda^{\top}\nabla_z h) + \epsilon T_t^{-1}S_1\nabla_y h \cdot (\lambda^{-1}\nabla_z h) \\ &+ S_1^2\nabla_y h \cdot (\lambda^{-1}\nabla_z h) + S_1^2T_t^{-1}(\lambda^{-1}\nabla_z h) \cdot (\lambda^{-1}A\nabla_z h) \end{split}$$

In order to get a bound in terms of $(\partial_i h)^2$ terms rather than $\partial_i h \partial_j h$ terms, we bound the $\partial_i h \partial_j h$ terms in the following ways,

$$\begin{split} \nabla_{x}h\cdot\nabla_{y}h &\geq -\frac{1}{2}|\nabla_{x}h|^{2} - \frac{1}{2}|\nabla_{y}h|^{2},\\ -\nabla_{y}h\cdot(\lambda^{\top}\nabla_{z}h) &\geq -\frac{1}{6}|\nabla_{y}h|^{2} - \frac{3}{2}|\lambda^{\top}|^{2}|\nabla_{z}h|^{2},\\ S_{1}T_{t}^{-1}\nabla_{y}h\cdot(\lambda^{-1}A\nabla_{z}h) &\geq -\frac{1}{6}|\nabla_{y}h|^{2} - \frac{3}{2}S_{1}^{2}T_{t}^{-2}|\lambda^{-1}|^{2}|A|^{2}|\nabla_{z}h|^{2},\\ S_{1}\nabla_{x}h\cdot(\lambda^{-1}\nabla_{z}h) &\geq -\frac{1}{2}|\nabla_{x}h|^{2} - \frac{1}{2}S_{1}^{2}|\lambda^{-1}|^{2}|\nabla_{z}h|^{2},\\ \epsilon T_{t}^{-1}S_{1}\nabla_{y}h\cdot(\lambda^{-1}\nabla_{z}h) &\geq -\epsilon T_{t}^{-1}|\nabla_{y}h|^{2} - \frac{\epsilon}{4}S_{1}^{2}T_{t}^{-1}|\lambda^{-1}|^{2}|\nabla_{z}h|^{2},\\ S_{1}^{2}\nabla_{y}h\cdot(\lambda^{-1}\nabla_{z}h) &\geq -\frac{1}{6}|\nabla_{y}h|^{2} - \frac{3}{2}S_{1}^{4}|\lambda^{-1}|^{2}|\nabla_{z}h|^{2} \end{split}$$

and using (4.47) gives

$$\begin{split} h\Gamma_{L_t^*, \varPhi_2}(h) &> -|\nabla_x h|^2 + (1+28S_0^2+1024S_0^4)|\nabla_y h|^2 \\ &\quad -\frac{1}{2}\hat{\lambda}^2 \bigg(3+2S_1+S_1^2+3S_1^4+S_1^2T_t^{-1}\bigg(|A|+\frac{\epsilon}{2}\bigg)+3S_1^2T_t^{-2}|A|^2\bigg)|\nabla_z h|^2. \end{split}$$

Lastly, $\varGamma_{L_t^{\epsilon*}, \varPhi_1}$ compensates for the negative x-derivative:

$$\begin{split} h\Gamma_{L_{t}^{\epsilon*},\varPhi_{1}}(h) &> (2\nabla_{x} + 8S_{0}(\nabla_{y} + \lambda^{-1}\nabla_{z}))h \cdot [L_{t}^{\epsilon*}, 2\nabla_{x} + 8S_{0}(\nabla_{y} + \lambda^{-1}\nabla_{z})]h \\ &= (2\nabla_{x} + 8S_{0}(\nabla_{y} + \lambda^{-1}\nabla_{z}))h \cdot (-2(D_{x}^{2}U)(\nabla_{y} - \epsilon T_{t}^{-1}\nabla_{x}) \\ &+ 8S_{0}(\nabla_{x} + \epsilon T_{t}^{-1}\nabla_{y} - \lambda^{\top}\nabla_{z} + \nabla_{y} + T_{t}^{-1}\lambda^{-1}A\nabla_{z}))h \\ &= ((16S_{0}I_{n} + 4\epsilon T_{t}^{-1}D_{x}^{2}U)\nabla_{x}h) \cdot \nabla_{x}h + 2\nabla_{x}h \cdot ((-2D_{x}^{2}U + 8S_{0}(1 + \epsilon T_{t}^{-1})I_{n})\nabla_{y}h) \\ &+ 2\nabla_{x}h \cdot (8S_{0}(-\lambda^{\top} + T_{t}^{-1}\lambda^{-1}A)\nabla_{z}h) + ((64S_{0}^{2}I_{n} + 16S_{0}\epsilon T_{t}^{-1}D_{x}^{2}U)\nabla_{x}h) \cdot \nabla_{y}h \\ &+ 8S_{0}\nabla_{y}h \cdot ((-2D_{x}^{2}U + 8S_{0})\nabla_{y}h) + 8S_{0}\nabla_{y}h \cdot (8S_{0}(-\lambda^{\top} + T_{t}^{-1}\lambda^{-1}A)\nabla_{z}h) \\ &+ ((64S_{0}^{2}I_{n} + 16S_{0}\epsilon T_{t}^{-1}D_{x}^{2}U)\nabla_{x}h) \cdot (\lambda^{-1}\nabla_{z}h) \\ &+ ((-16S_{0}D_{x}^{2}U + 64S_{0}^{2}(1 + \epsilon T_{t}^{-1})I_{n})\nabla_{y}h) \cdot (\lambda^{-1}\nabla_{z}h) \\ &+ 64S_{0}^{2}(\lambda^{-1}\nabla_{z}h) \cdot ((-\lambda^{\top} + T_{t}^{-1}\lambda^{-1}A)\nabla_{z}h). \end{split}$$

Bounding the $\partial_i h \partial_j h$ terms as for Φ_2 , using (4.47) and (2.4) yields

$$\begin{split} h\Gamma_{L_{t}^{*},\varPhi_{1}}(h) &> (16S_{0} - 4\epsilon T_{t}^{-1}|D_{x}^{2}U|_{\infty})|\nabla_{x}h|^{2} \\ &- \left(2|\nabla_{x}h|^{2} + 2|D_{x}^{2}U|_{\infty}^{2}|\nabla_{y}h|^{2} + 8(1 + \epsilon T_{t}^{-1})|\nabla_{x}h|^{2} + 8S_{0}^{2}(1 + \epsilon T_{t}^{-1})|\nabla_{y}h|^{2}\right) \\ &- \left(2|\nabla_{x}h|^{2} + 32S_{0}^{2}\hat{\lambda}^{2}\left(1 + T_{t}^{-2}|A|^{2}\right)|\nabla_{z}h|^{2}\right) \\ &- \left((1 + 8S_{0}\epsilon T_{t}^{-1}|D_{x}^{2}U|_{\infty}^{2})|\nabla_{x}h|^{2} + (1024S_{0}^{4} + 8S_{0}\epsilon T_{t}^{-1})|\nabla_{y}h|^{2}\right) \\ &- \left(16S_{0}|D_{x}^{2}U|_{\infty}|\nabla_{y}h|^{2} - 64S_{0}^{2}|\nabla_{y}h|^{2}\right) - \left(32S_{0}^{2}|\nabla_{y}h|^{2} + 32S_{0}^{2}\hat{\lambda}^{2}\left(1 + T_{t}^{-2}|A|^{2}\right)|\nabla_{z}h|^{2}\right) \\ &- \left((1 + 8S_{0}\epsilon T_{t}^{-1}|D_{x}^{2}U|_{\infty}^{2})|\nabla_{x}h|^{2} + (1024S_{0}^{4} + 8S_{0}\epsilon T_{t}^{-1})\hat{\lambda}^{2}|\nabla_{z}h|^{2}\right) \\ &- \left(\left(2|D_{x}^{2}U|_{\infty}^{2} + 32S_{0}^{2}(1 + \epsilon T_{t}^{-1})\right)|\nabla_{y}h|^{2} + (32S_{0}^{2} + 32\epsilon T_{t}^{-1}S_{0}^{2})\hat{\lambda}^{2}|\nabla_{z}h|^{2}\right) \\ &- 64S_{0}^{2}\hat{\lambda}^{2}\left(1 + T_{t}^{-2}|A|^{2}\right)|\nabla_{z}h|^{2} \\ &\geq \left(2 - 4(2 + (1 + 4S_{0}^{2})S_{0})\epsilon T_{t}^{-1}\right)|\nabla_{x}h|^{2} + \left(S_{0}^{2}(-28 - 1024S_{0}^{2}) - 8S_{0}(1 + 5S_{0})\epsilon T_{t}^{-1}\right)|\nabla_{y}h|^{2} \\ &- \left(S_{0}^{2}\hat{\lambda}^{2}(160 + 128T_{t}^{-2}|A|^{2} + 1024S_{0}^{2}) + 8S_{0}\hat{\lambda}^{2}(1 + 4S_{0})\epsilon T_{t}^{-1}\right)|\nabla_{z}h|^{2}. \end{split}$$

Matching powers in T_t^{-1} to take

$$\beta_0 = \frac{1}{A_c} \left(S_0^2 \hat{\lambda}^2 (160 + 1024S_0^2) + \frac{1}{2} \hat{\lambda}^2 (3 + 2S_1 + S_1^2 + 3S_1^4) \right)$$
(4.50a)

$$\beta_1 = \frac{1}{A_c} \left(4(2 + (1 + 4S_0^2)S_0) + 8S_0(1 + 5S_0) + 8S_0\hat{\lambda}^2(1 + 4S_0) + \frac{1}{2}\hat{\lambda}^2 \left(S_1^2 \left(|A| + \frac{1}{2} \right) \right) \right)$$
(4.50b)

$$\beta_2 = \frac{1}{A_c} \left(128S_0^2 \hat{\lambda}^2 |A|^2 + \frac{3}{2} \hat{\lambda}^2 S_1^2 |A|^2 \right), \tag{4.50c}$$

using $\epsilon \leq 1$ and putting together the bounds for $\Gamma_{L_t^{\epsilon*}, \Phi_3}, \Gamma_{L_t^{\epsilon*}, \Phi_2}, \Gamma_{L_t^{\epsilon*}, \Phi_1}$ gives (4.46).

4.5 Log-Sobolev Inequality

Proof of Proposition 1 Firstly, the case that U satisfies (2.7) is dealt with. The standard log-Sobolev inequality for a Gaussian measure [35] alongside the properties that log-Sobolev inequalities tensorises and are stable under perturbations, which can be found as Theorem 4.4 and Property 4.6 in [37] respectively, yields the result. In particular,

$$\begin{split} \int h \ln h d\mu_{T_t} &= \int (h \ln h - h + 1) d\mu_{T_t} \\ &\leq \int (h \ln h - h + 1) Z_{T_t}^{-1} e^{-\frac{U_m}{T_t}} e^{-\frac{1}{T_t} \left(|\bar{a} \circ x|^2 + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)} dx dy dz \\ &= e^{-\frac{U_m}{T_t}} Z_{T_t}^{-1} \int h \ln h e^{-\frac{1}{T_t} \left(|\bar{a} \circ x|^2 + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)} dx dy dz \\ &\leq e^{-\frac{U_m}{T_t}} \max \left(\frac{T_t}{2}, \max_i \frac{T_t}{4\bar{a}_i^2} \right) Z_{T_t}^{-1} \int \frac{|\nabla h|^2}{h_t} e^{-\frac{1}{T_t} \left(|\bar{a} \circ x|^2 + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)} dx dy dz \\ &\leq e^{\frac{U_M - U_m}{T_t}} \max \left(\frac{T_t}{2}, \frac{T_t}{4\bar{a}_m^2} \right) \int \frac{|\nabla h|^2}{h} d\mu_{T_t}, \end{split}$$

where the first inequality follows by (2.7) since $x \ln x - x + 1 \ge 0$ for all $x \ge 0$, so that

$$C_t^{(0)} = \max\left(2, a_m^{-2}\right) \frac{T_t}{4} e^{(U_M - U_m)T_t^{-1}}$$

For the case where U is a nonnegative nondegenerate Morse function satisfying (2.8), the inequality in the xmarginals is taken as a consequence of Corollary 2.17 in [52]; for the announced form (2.10) of $C_t^{(0)}$, equation (2.18) in [52] can be used by taking $t_{ls}^{(0)}$ large enough such that for $t > t_{ls}^{(0)}$, T_t is small enough. As before, tensorisation with the inequality for Gaussian measures concludes.

Proposition 9 Under Assumption 1, 2 and for $\epsilon \geq 0$, there exists constants t_{ls} , $A_* > 0$ and a finite order polynomial $r : \mathbb{R}_+ \to \mathbb{R}_+$ with coefficients depending on U and λ but independent of ϵ such that the distorted entropy (4.39) satisfies

$$H^{\epsilon}(t) \le C_t \int \frac{|\nabla h_t^{\epsilon}|^2}{h_t^{\epsilon}} d\mu_{T_t}, \qquad (4.51)$$

where for $t > t_{ls}$,

$$C_t = A_* + r \left(T_t^{-\frac{1}{2}} \right) e^{\hat{E}T_t^{-1}}.$$
(4.52)

Proof Given Proposition 1, only the first two terms in the integrand of $H^{\epsilon}(t)$ are left, which lead directly to the inequality corresponding to A_* .

4.6 Proof of Dissipation

Lemma 4 below constructs a sequence of compactly supported functions that are multiplied with the integrand in H(t). It gives sufficient properties for retrieving a bound on $\partial_t H(t)$ after passing the derivative under the integral sign and passing the limit in the sequence of approximating initial densities. The key sufficient property turns out to be (4.53) below.

Let φ_k be given as in (4.1),

$$\nu_k := \varphi_k * \mathbb{1}_{(-\infty,k^2]} \le 1$$

for k > 0.

Lemma 4 For k > 0, define the smooth functions $\eta_k : \mathbb{R}^{2n+m+1} \to \mathbb{R}$

$$\eta_k = \nu_k (-\ln(R+2d)),$$

where d > 0 is the same as in (4.23). The following properties hold:

1. η_k is compactly supported;

2. η_k converges to 1 pointwise as $k \to \infty$;

3. for some constant C > 0 independent of k, t and $0 \le \epsilon \le \min(1, \epsilon')$

$$L_t^{\epsilon} \eta_k \le \frac{CT_t^{-1}}{k}.\tag{4.53}$$

Proof By the quadratic assumption (2.8) on U and the bound (4.23) on R, R grows quadratically and in particular for an arbitrarily large constant $R_{(0)} > 0$, a compact set K can be chosen such that $R > R_{(0)}$ in $\mathbb{R}^{2n+m} \setminus K$; along with the support of ν_m being bounded below, the first statement is clear. The second statement is also trivial to check.

For the third statement, using the chain rule (4.8) and (4.9) for L_t ,

$$L_t^{\epsilon} \eta_m = -\nu'_m (-\ln(R+2d)) L_t^{\epsilon} \ln(R+2d) + \nu''_m (-\ln(R+2d)) (\nabla \ln(R+2d))^{\top} A^{\epsilon} \nabla \ln(R+2d).$$

It can be seen that ν'_m and ν''_m are estimated by terms at most of order m^{-1} ; to see this, for all $x \in \mathbb{R}$,

$$\nu_m(x) = \int_{-\infty}^{m^2} \varphi_m(x-y) dy = \int_{x-m^2}^{\infty} \varphi_m(z) dz$$

so that

$$0 \ge \nu'_m(x) = -\varphi_m(x - m^2) \ge -m^{-1} \max \varphi$$

and

$$|\nu_m''(x)| = \left|\varphi_m'(x - m^2)\right| \le m^{-2} \max \varphi'$$

Therefore there exists a constant $\bar{C} > 0$ such that

$$\begin{split} L_t^{\epsilon} \eta_m &\leq -\nu'_m (-\ln(R+2d)) \max(0, L_t^{\epsilon} \ln(R+2d)) + m^{-2} \max \varphi' \big| (\nabla \ln(R+2d))^\top A^{\epsilon} \nabla \ln(R+2d) \big| \\ &\leq \bar{C} \Big(m^{-1} \max(0, L_t^{\epsilon} \ln(R+2d)) + m^{-2} \big| (\nabla \ln(R+2d))^\top A^{\epsilon} \nabla \ln(R+2d) \big| \Big). \end{split}$$

A calculation using property (4.24) with (4.8) and (4.9) for L^{ϵ}_t reveals

$$\begin{split} L_t^{\epsilon} \ln(R+2d) &= \frac{L_t^{\epsilon} R}{R+2d} - \frac{(\nabla R)^{\top} A^{\epsilon} \nabla R}{(R+2d)^2} \\ &\leq \frac{-cT_t R + dT_t^{-1}}{R+2d} - \frac{\epsilon(|\nabla_x R|^2 + |\nabla_y R|^2) + A_c |\nabla_z R|^2}{(R+2d)^2} \\ &\leq \frac{-cT_t (R+d) + cT_t d + dT_t^{-1}}{R+2d} - \frac{\epsilon(|\nabla_x R|^2 + |\nabla_y R|^2) + A_c |\nabla_z R|^2}{(R+2d)^2} \\ (\nabla \ln(R+2d))^{\top} A^{\epsilon} \nabla \ln(R+2d) &\leq (|A|+2) |\nabla \ln(R+2d)|^2 \\ &= (|A|+2) \bigg| \frac{\nabla R}{R+2d} \bigg|^2, \end{split}$$

which are bounded above as claimed considering (4.23) and that ∇R grows linearly in space and is uniformly bounded in time.

Remark 6 Lemma 4 is different to Lemma 16 in [55]. We believe the first few equations in the proof of Lemma 16 in [55] contain a sign error; as a consequence the proofs in [55] beyond that point require significant modifications. Here we address this by modifying the truncation arguments we require proving (4.53) instead of Lemma 17 of [55]. In addition, the finiteness of the distorted entropy is required, which is the reason for using the perturbed dynamics in (4.7) and then later taking $\epsilon \to 0$.

The proof of Proposition 10 follows in the direction of Lemma 19 of [55].

Proposition 10 Under Assumption 1, 2, 3 and 4 and for $0 < \epsilon \le \min(1, \epsilon')$, it holds that for any $0 < \alpha \le \frac{1}{2}(1-\frac{E}{E})$, there exists some constant B > 0 and some $t_H > 0$ both independent of ϵ , such that for all $t > t_H$,

$$H^{\epsilon}(t) \le B\left(\frac{1}{t}\right)^{1-\frac{\hat{E}}{E}-2\alpha}.$$
(4.54)

Proof Consider for $t \ge 0$ the auxiliary distorted entropies

$$H_{k}^{\epsilon}(t) = \int \eta_{k} \left(\frac{\left| 2\nabla_{x} h_{t}^{\epsilon} + 8S_{0}(\nabla_{y} h_{t}^{\epsilon} + \lambda^{-1} \nabla_{z} h_{t}^{\epsilon}) \right|^{2}}{h_{t}^{\epsilon}} + \frac{\left| \nabla_{y} h_{t}^{\epsilon} + S_{1} \lambda^{-1} \nabla_{z} h_{t}^{\epsilon} \right|^{2}}{h_{t}^{\epsilon}} + \beta(T_{t}^{-1}) h_{t}^{\epsilon} \ln(h_{t}^{\epsilon}) \right) d\mu_{T_{t}}$$

$$= \int \eta_{k} (\Phi_{1}(h_{t}^{\epsilon}) + \Phi_{2}(h_{t}^{\epsilon}) + \beta(T_{t}^{-1}) \Phi_{3}(h_{t}^{\epsilon})) d\mu_{T_{t}}$$

$$= \int \eta_{k} \Psi_{T_{t}}(h_{t}^{\epsilon}) d\mu_{T_{t}}, \qquad (4.55)$$

where $h_t^{\epsilon} = m_t^{\epsilon} \mu_{T_t}^{-1}$ is as defined (2.3), Φ_1 , Φ_2 , Φ_3 is as in (4.48) and η_k are as in Lemma 4. Due to η_k , the order between the time derivative and the integral can be exchanged:

$$\frac{d}{dt}H_k^{\epsilon}(t) = \int \eta_k \partial_t (\Psi_{T_t}(h_t^{\epsilon})) d\mu_{T_t} + T_t' \int \eta_k \partial_{T_t} (\Psi_{T_t}(h_t^{\epsilon})\mu_{T_t}) dx dy dz.$$
(4.56)

The terms will be considered separately. Since m_t^{ϵ} is the density of the law of (4.7) and $L_t^{\epsilon*}$ is the $L^2(\mu_{T_t})$ adjoint of L_t^{ϵ} , by Itô's rule for smooth compactly supported f on \mathbb{R}^{2n+m} ,

$$\int f\partial_t m_t^{\epsilon} = \partial_t \int fm_t^{\epsilon} = \int L_t^{\epsilon} fm_t^{\epsilon} = \int L_t^{\epsilon} f\frac{m_t^{\epsilon}}{\mu_{T_t}} \mu_{T_t} = \int fL_t^{\epsilon*} \left(\frac{m_t^{\epsilon}}{\mu_{T_t}}\right) \mu_{T_t}.$$
(4.57)

The first term in (4.56) is then bounded as follows.

$$\int \eta_k \partial_t (\Psi_{T_t}(h_t^{\epsilon})) d\mu_{T_t} = \int \eta_k d\Psi_{T_t}(h_t^{\epsilon}) \partial_t h_t^{\epsilon} d\mu_{T_t}
= \int \eta_k d\Psi_{T_t}(h_t^{\epsilon}) \frac{\partial_t m_t^{\epsilon}}{\mu_{T_t}} d\mu_{T_t}
= \int \eta_k d\Psi_{T_t}(h_t^{\epsilon}) L_t^{\epsilon*} h_t^{\epsilon} d\mu_{T_t}
= -\int 2\eta_k \Gamma_{L_t^{\epsilon*},\Psi_{T_t}}(h_t^{\epsilon}) d\mu_{T_t} + \int \eta_k L_t^{\epsilon*} (\Psi_{T_t}(h_t^{\epsilon})) d\mu_{T_t}
= -\int 2\eta_k \Gamma_{L_t^{\epsilon*},\Psi_{T_t}}(h_t^{\epsilon}) d\mu_{T_t} + \int L_t^{\epsilon} \eta_k \Big(\Psi_{T_t}(h_t^{\epsilon}) + \beta(T_t^{-1})e^{-1} \Big) d\mu_{T_t}
\leq -2 \int \eta_k \frac{|\nabla h_t^{\epsilon}|^2}{h_t^{\epsilon}} d\mu_{T_t} + \frac{CT_t^{-1}}{k} \int \Big(\Psi_{T_t}(h_t^{\epsilon}) + \beta(T_t^{-1})e^{-1} \Big) d\mu_{T_t},$$
(4.58)

using Proposition 8 and Lemma 4, where $\beta(T_t^{-1})e^{-1}\int L_t^{\epsilon*}\eta_k d\mu_{T_t} = 0$ is added to force

$$\beta(T_t^{-1})(h_t^{\epsilon} \ln h_t^{\epsilon} + e^{-1}) \ge 0$$
, so that $\Psi_{T_t}(h_t^{\epsilon}) + \beta(T_t^{-1})e^{-1} \ge 0$.

For the second term in (4.56), consider the Φ_1 and Φ_2 terms in the integrand $\eta_k \partial_{T_t}(\Psi_{T_t}\mu_{T_t}) = \eta_k \partial_{T_t}((\Phi_1 + \Phi_2 + \beta(T_t^{-1})\Phi_3)\mu_{T_t}))$ of $H_k(t)$ with the forms

$$\partial_{T_t}(\Phi_i(h_t^{\epsilon})\mu_{T_t}) = \partial_{T_t} \left| M_i \nabla \ln \left(\frac{m_t^{\epsilon}}{\mu_{T_t}} \right) \right|^2 m_t^{\epsilon}, \qquad i = 1, 2$$

for the corresponding matrices M_1 and M_2 depending on S_0 , S_1 and λ . Applying the partial derivative in T_t ,

$$\partial_{T_t}(\Phi_i(h_t^{\epsilon})\mu_{T_t}) = -2(M_i \nabla \ln h_t^{\epsilon} \cdot M_i \nabla \partial_{T_t} \ln \mu_{T_t}) m_t^{\epsilon}, \qquad (4.59)$$

and using definition (2.2) for μ_{T_t} and $Z_{T_t} = \int_{\mathbb{R}^{2n+m}} e^{-\frac{1}{T_t} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)} dx dy dz$, gives

$$\partial_{T_t} \ln \mu_{T_t} = \mu_{T_t}^{-1} \partial_{T_t} \left(Z_{T_t}^{-1} e^{-\frac{1}{T_t} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)} \right)$$

$$= \mu_{T_t}^{-1} \left(-Z_{T_t}^{-2} \partial_{T_t} Z_{T_t} + \frac{Z_{T_t}^{-1}}{T_t^2} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right) \right) e^{-\frac{1}{T_t} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right)}$$

$$= \mu_{T_t}^{-1} \left(-\mu_{T_t} Z_{T_t}^{-1} \partial_{T_t} Z_{T_t} + \frac{\mu_{T_t}}{T_t^2} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right) \right)$$

$$= -\int \frac{1}{T_t^2} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right) d\mu_{T_t} + \frac{1}{T_t^2} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right). \tag{4.60}$$

Note the exchange in differentiation and integration is justified by the quadratic bounds (2.8) on U. Integrating by parts in y and z (or simply using formulae for second moments) gives $\frac{n+m}{2T_t}$ for the $|y|^2$ and $|z|^2$ terms in the first integral. The integral over U can be dealt with using assumptions (2.5) and (2.6), to be specific:

$$\begin{split} \int U d\mu_{T_t} &\leq \int (a_M^2 |x|^2 + U_M) d\mu_{T_t} \leq \int \left(\frac{a_M^2}{r_1} (\nabla U \cdot x + U_g) + U_M \right) d\mu_{T_t} = \frac{a_M^2}{r_1} (nT_t + U_g) + U_M \\ \int U d\mu_{T_t} &\geq \int (a_m^2 |x|^2 + U_m) d\mu_{T_t} \\ &\geq \int \left(\frac{a_m^2}{r_2 + 1} (|\nabla U|^2 - U_g + |x|^2) + U_m \right) d\mu_{T_t} \\ &\geq \int \left(\frac{a_m^2}{r_2 + 1} (2\nabla U \cdot x - U_g) + U_m \right) d\mu_{T_t} = \frac{a_m^2}{r_2 + 1} (2nT_t - U_g) + U_m. \end{split}$$

Plugging into (4.60) gives

$$p_1\left(T_t^{-1}\right) \le \partial_{T_t} \ln \mu_{T_t} - \frac{1}{T_t^2} \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} - \frac{n+m}{2} T_t \right) \le p_2\left(T_t^{-1}\right).$$
(4.61)

where $p_1(x) = -\frac{a_M^2 n}{r_1} x - \left(\frac{a_M^2 U_g}{r_1} + U_M\right) x^2$ and $p_2(x) = -\frac{2a_m^2 n}{r_2 + 1} x + \left(\frac{a_m^2 U_g}{r_2 + 1} - U_m\right) x^2$. Substituting (4.60) back into (4.59),

$$\partial_{T_t}(\Phi_i(h_t^{\epsilon})\mu_{T_t}) \le \left(|M_i \nabla \ln h_t^{\epsilon}|^2 + T_t^{-4} \left| M_i \nabla \left(U(x) + \frac{|y|^2}{2} + \frac{|z|^2}{2} \right) \right|^2 \right) m_t^{\epsilon} \\ \le \Phi_i(h_t^{\epsilon})\mu_{T_t} + \widetilde{C}T_t^{-4} \left(1 + |x|^2 + |y|^2 + |z|^2 \right) m_t^{\epsilon}$$
(4.62)

for a constant $\widetilde{C} \geq 0$ independent of k and ϵ by the quadratic assumption (2.6) on $|\nabla_x U|^2$ and $\eta_m \leq 1$. For the last integrand in the last term of the right hand side of (4.56), namely the derivative over $\Phi_3(h_t^{\epsilon})\mu_{T_t} = \frac{m_t^{\epsilon}}{\mu_{T_t}} \ln \frac{m_t^{\epsilon}}{\mu_{T_t}} \mu_{T_t}$, the left inequality of (4.61) gives

$$\begin{aligned} \partial_{T_t}(\beta(T_t^{-1})\Phi_3(h_t^{\epsilon})\mu_{T_t}) &= -T_t^{-2}\beta'(T_t^{-1})\Phi_3(h_t^{\epsilon})\mu_{T_t} + \beta(T_t^{-1})\partial_{T_t}\ln\frac{m_t^{\epsilon}}{\mu_{T_t}}m_t^{\epsilon} \\ &= -T_t^{-2}\beta'(T_t^{-1})(\Phi_3(h_t^{\epsilon}) + e^{-1})\mu_{T_t} + T_t^{-2}\beta'(T_t^{-1})e^{-1}\mu_{T_t} - \beta(T_t^{-1})\partial_{T_t}\ln\mu_{T_t}m_t^{\epsilon} \\ &\leq T_t^{-2}\beta'(T_t^{-1})e^{-1}\mu_{T_t} + \beta(T_t^{-1})\left|p_1\left(T_t^{-1}\right) + \frac{1}{T_t^2}\left(-\frac{n+m}{2}T_t + U_M + a_M|x|^2 + \frac{|y|^2}{2} + \frac{|z|^2}{2}\right)\right|m_t^{\epsilon}, \end{aligned}$$
(4.63)

where in the last step $\Phi_3 + e^{-1} \ge 0$, $\beta_1, \beta_2 > 0$ and (2.8) have been used. Putting together the bounds (4.62) and (4.63) and applying Corollary 1 yields

$$\int \eta_k \partial_{T_t} (\Psi_{T_t}(h_t^{\epsilon}) \mu_{T_t}) d\zeta \leq q \left(T_t^{-1} \right) \left(H_k^{\epsilon}(t) + \mathbb{E} \left[1 + |X_t^{\epsilon}|^2 + |Y_t^{\epsilon}|^2 + |Z_t^{\epsilon}|^2 \right] \right)$$
$$\leq p \left(T_t^{-1} \right) \left(H_k^{\epsilon}(t) + \hat{C} \right), \tag{4.64}$$

where p and q are some finite order polynomials with nonnegative coefficients, $\hat{C} > 0$, both independent of k and ϵ . Returning to (4.56), collecting (4.58) and (4.64) then integrating from any $s \ge 0$ to t > s gives

$$H_{k}^{\epsilon}(t) - H_{k}^{\epsilon}(s) \leq 2 \int_{s}^{t} \left(-\int \eta_{k} \frac{|\nabla h_{u}^{\epsilon}|^{2}}{h_{u}} d\mu_{T_{u}} + \frac{CT_{u}^{-1}}{k} (H^{\epsilon}(u) + \beta(T_{u}^{-1})e^{-1}) + |T_{u}'|p\Big(T_{u}^{-1}\Big)\Big(H_{k}^{\epsilon}(u) + \hat{C}\Big) \right) du.$$

$$(4.65)$$

Fix an arbitrary S > 0. By the square integrability Theorem 7.4.1 in [7], the log-Sobolev inequality (4.51), (2.6) and the finiteness of second moments (4.10), it holds that

$$\int_{0}^{S} H^{\epsilon}(u) du \leq \int_{0}^{S} C_{u} \int \frac{\left|\nabla h_{u}^{\epsilon}\right|^{2}}{h_{u}^{\epsilon}} d\mu_{T_{u}} du$$
$$= \int_{0}^{S} C_{u} \int \frac{\left|\nabla m_{u}^{\epsilon} + T_{u}^{-1} m_{u}^{\epsilon} (\nabla_{x} U + y + z)\right|^{2}}{m_{u}^{\epsilon}} dx dy dz du < \infty.$$
(4.66)

Then in (4.65) the $k \to \infty$ limit can be taken. Due to (4.66), the term denominated by k goes to zero. Applying Fatou's lemma (adding and subtracting $\beta(T_t^{-1})e^{-1}\int \eta_m d\mu_{T_t}$ wherever necessary for positivity) and using $\eta_m \leq 1$, it holds that for s < t,

$$H^{\epsilon}(t) - H^{\epsilon}(s) \leq -2 \int_{s}^{t} \int \frac{|\nabla h_{u}^{\epsilon}|^{2}}{h_{u}^{\epsilon}} d\mu_{T_{u}} du + \int_{s}^{t} |T_{u}'| p\left(T_{u}^{-1}\right) \left(H^{\epsilon}(u) + \hat{C}\right) du$$

$$(4.67)$$

and for⁵ $t_{ls} < s < t$,

$$H^{\epsilon}(t) - H^{\epsilon}(s) \leq \int_{s}^{t} \left(\left(|T_{u}'| p\left(T_{u}^{-1}\right) - 2C_{u}^{-1} \right) H^{\epsilon}(u) + \hat{C} |T_{u}'| p\left(T_{u}^{-1}\right) \right) du.$$

$$(4.68)$$

Since $t^{\alpha} \gg (\ln t)^{\frac{\rho}{2}}$ for any $\rho, \alpha > 0$ and large enough t > 0, for any $\alpha > 0$, there exists $t_1 > \max(t_{ls}, t_0)$, where t_0 is as in Assumption 3, and $c_1, c_2 > 0$ independent of k, ϵ such that for all $t \ge t_1$,

$$|T_t'|p\left(T_t^{-1}\right) \le c_1\left(\frac{1}{t}\right)^{1-\alpha},\tag{4.69}$$

$$-2C_t^{-1} \le -c_2 \left(\frac{1}{t}\right)^{\frac{\nu}{E}+\alpha},\tag{4.70}$$

where the assumption $T_t \geq \frac{E}{\ln t}$ and (4.52) have been used. Using further that $E > \hat{E}$ by Assumption 3, then taking $\alpha < \frac{1}{2}(1 - \frac{\hat{E}}{E})$, there exists $t_2 \geq t_1$ independent of ϵ such that for $t \geq t_2$,

$$|T_t'| p\left(T_t^{-1}\right) - 2C_t^{-1} \le -c_3 \left(\frac{1}{t}\right)^{\frac{E}{E} + \alpha}$$
(4.71)

and from (4.68), for $t_2 < s < t$,

$$H^{\epsilon}(t) - H^{\epsilon}(s) \leq \int_{s}^{t} \left(-c_{3}\left(\frac{1}{u}\right)^{\frac{E}{E}+\alpha} H^{\epsilon}(u) + \hat{C}c_{1}\left(\frac{1}{u}\right)^{1-\alpha} \right) du.$$

$$(4.72)$$

 $^{^5 \} t_{ls}$ from Proposition 9

To obtain the corresponding differential inequality for all time, (4.72) can be divided by t - s, mollified with (4.1) for 0 < k < 1 and the limit $s \to t$ can be taken:

$$\begin{split} \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{t-1}^{t+1} \varphi_k(t-u) (H^{\epsilon}(u+\hat{\epsilon}) - H^{\epsilon}(u-\hat{\epsilon})) du \\ &\leq \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{t-1}^{t+1} \varphi_k(t-u) \int_{u-\hat{\epsilon}}^{u+\hat{\epsilon}} \left(-c_3 \left(\frac{1}{u'}\right)^{\frac{\hat{E}}{E}+\alpha} H^{\epsilon}(u') + \hat{C}c_1 \left(\frac{1}{u'}\right)^{1-\alpha} \right) du' du \\ &\leq \int_{t-1}^{t+1} \varphi_k(t-u) \lim_{\hat{\epsilon} \to 0} \frac{1}{2\hat{\epsilon}} \int_{u-\hat{\epsilon}}^{u+\hat{\epsilon}} \left(-c_3 \left(\frac{1}{u'}\right)^{\frac{\hat{E}}{E}+\alpha} H^{\epsilon}(u') + \hat{C}c_1 \left(\frac{1}{u'}\right)^{1-\alpha} \right) du' du \\ &= \int_{t-1}^{t+1} \varphi_k(t-u) \left(-c_3 \left(\frac{1}{u}\right)^{\frac{\hat{E}}{E}+\alpha} H^{\epsilon}(u) + \hat{C}c_1 \left(\frac{1}{u}\right)^{1-\alpha} \right) du \end{split}$$

for $t \ge t_2 + 2$, where the second-to-last line follows from Fatou's lemma and dominated convergence (adding and subtracting $\beta(T_{u'}^{-1})e^{-1}$ to H^{ϵ} for Fatou); the last equality follows by the Lebesgue differentiation theorem. Therefore

$$\frac{d}{dt}(\varphi_k * H^{\epsilon})(t) \le -c_3 \left(\frac{1}{t+1}\right)^{\frac{\hat{E}}{E}+\alpha} (\varphi_k * H^{\epsilon})(t) + \hat{C}' \left(\frac{1}{t-1}\right)^{1-\alpha}$$

for some constant $\hat{C}' > 0$ independent of k, ϵ . Setting

$$\gamma_1(t) := c_3 \left(\frac{1}{t+1}\right)^{\frac{E}{E}+\alpha}, \qquad \gamma_2(t) := \hat{C}' \left(\frac{1}{t-1}\right)^{1-\alpha}$$

and following the argument as per [55] from Lemma 6 in [54], there exists $t_3 \ge t_2 + 2$, $c_4, c_5, c_6 > 0$ independent of k and ϵ such that for $t \ge t_3$,

$$\frac{d}{dt} \left(\frac{\gamma_2}{\gamma_1}\right)(t) = \frac{(t+1)^{\frac{E}{E}+\alpha}}{(t-1)^{1-\alpha}} \left(\frac{c_4}{t+1} - \frac{c_5}{t-1}\right) \ge -c_6 t^{-1},$$

so that there exists $t_4 \ge t_3$ independent of k and ϵ such that for $t \ge t_4$,

$$\frac{d}{dt}\left(\varphi_k * H^{\epsilon} - \frac{2\gamma_2}{\gamma_1}\right)(t) \le -\gamma_1(t)\left(\varphi_k * H^{\epsilon}(t) - \frac{2\gamma_2(t)}{\gamma_1(t)}\right)$$

and consequently

$$\varphi_k * H^{\epsilon}(t) \le \frac{2\gamma_2(t)}{\gamma_1(t)} + \varphi_k * H^{\epsilon}(t_4) e^{-\int_{t_4}^t \gamma_1(u) du}.$$
(4.73)

Finally, from (4.72) (adding and subtracting $\beta(T_{u'}^{-1})e^{-1}$ to H^{ϵ}), it holds that for $t \ge t_4 + 2$,

$$H^{\epsilon}(t) = \int_{t-2k}^{t} \varphi_k(t-k-s) ds H^{\epsilon}(t) \le \int_{t-2k}^{t} \varphi_k(t-k-s) H^{\epsilon}(s) ds + \tilde{g}(2k)$$

$$(4.74)$$

for some $\tilde{g}: \mathbb{R} \to \mathbb{R}$ satisfying $\tilde{g}(k') \to 0$ as $k' \to 0$, so that (4.73) yields

$$H^{\epsilon}(t) \leq \frac{2\gamma_2(t-k)}{\gamma_1(t-k)} + \varphi_k * H^{\epsilon}(t_4) e^{-\int_{t_4}^{t-k} \gamma_1(u) du} + \tilde{g}(2k),$$

where $\varphi_k * H^{\epsilon}(t_4)$ can be bounded independently of k in a similar spirit to (4.74), and taking $k \to 0$ concludes the proof.

Remark 7 The annealing schedule T_t is chosen to satisfy the relationship (4.71) between C_t^{-1} and $|T_t'| p(T_t^{-1})$.

4.7 Degenerate noise limit

After taking advantage of the square integrability Theorem 7.4.1 in [7] for the case with a nondegenerate diffusion term in the proof of Proposition 10, the $\epsilon \to 0$ limit is taken to obtain the same dissipation inequality in this section.

Proof (of Proposition 4) From (4.67), for any $0 \le s < t$ and $0 < \epsilon \le \min(1, \epsilon')$, it holds that

$$H^{\epsilon}(t) - H^{\epsilon}(s) \leq \int_{s}^{t} |T'_{u}| p\Big(T_{u}^{-1}\Big) \Big(H^{\epsilon}(u) + \hat{C}\Big) du,$$

where p is a finite order polynomial with nonnegative coefficients and $\hat{C} > 0$ is a constant both independent of ϵ . Therefore, mollifying in time and taking $s \to t$ as in the end of the proof by Proposition 10, it is straightforward that H^{ϵ} is uniformly bounded in⁶ $0 \le t \le t_H$ and $0 < \epsilon \le \min(1, \epsilon')$. Moreover by Proposition 10, the entropy $\int h_t^{\epsilon} \ln h_t^{\epsilon} d\mu_{T_t}$ is bounded uniformly in $t > t_H$ and $0 < \epsilon \le \min(1, \epsilon')$. Therefore for any $t \ge 0$ by the de la Vallée-Poussin criterion (see for example [18]), the subset $\{h_t^{\epsilon} : 0 < \epsilon \le \min(1, \epsilon')\} \subset L^1(\mu_{T_t})$ is uniformly integrable and consequently the Dunford-Pettis theorem imposes the existence of a weak limit $g_t \in L^1(\mu_{T_t})$ for a (sub)sequence $(\epsilon_i)_{i\in\mathbb{N}}$ such that $\epsilon_i \to 0$,

$$h_t^{\epsilon_i} \rightharpoonup g_t$$
, in $L^1(\mu_{T_t})$ as $i \to \infty$.

For any S > 0, any compactly supported smooth test function $\phi : [0, S) \times \mathbb{R}^{2n+m} \to \mathbb{R}$, omitting the dependence on the space variable $\zeta = (x, y, z)$ wherever convenient and using Itô's rule,

$$0 = \lim_{i \to \infty} \int_{(0,S) \times \mathbb{R}^{2n+m}} (m_t^{\epsilon_i} - g_t \mu_{T_t}) (-\partial_t - L_t) \phi dt d\zeta$$

$$= \lim_{i \to \infty} \int_{(0,S) \times \mathbb{R}^{2n+m}} \epsilon_i m_t^{\epsilon_i} (S_t^x + S_t^y) \phi dt d\zeta + \int_{(0,T) \times \mathbb{R}^{2n+m}} g_t \mu_{T_t} (\partial_t + L_t) \phi dt d\zeta + \int_{\mathbb{R}^{2n+m}} m_0 \phi(0,\zeta) dt d\zeta,$$

$$= \int_{(0,S) \times \mathbb{R}^{2n+m}} g_t \mu_{T_t} (\partial_t + L_t) \phi dt d\zeta + \int_{\mathbb{R}^{2n+m}} m_0 \phi(0,\zeta) dt d\zeta, \qquad (4.75)$$

so that in the distributional sense of [7],

$$\begin{cases} \partial_t (g_t \mu_{T_t}) = L_t^\top (g_t \mu_{T_t}) & \text{on } \mathbb{R}^{2n+m} \quad \forall t > 0, \\ (g_0 \mu_{T_0}) = m_0. \end{cases}$$

$$(4.76)$$

By Proposition 7, the solution to (4.76) is unique in the class of integrable solutions and since m_t belongs in this same class, it holds that

$$g_t \mu_{T_t} = m_t$$

for all $t \in [0, S]$, which is that

$$m_t^{\epsilon_i} \rightharpoonup m_t$$
, in $L^1(\mu_{T_t})$ as $i \to \infty$.

for all $0 \le t < S$. By Corollary 3.8 in [9], there exists a sequence $(\hat{m}_t^i)_{i \in \mathbb{N}}$ made up of convex combinations of $m_t^{\epsilon_i}$ that converge strongly to m_t in L^1 , hence a subsequence $(\hat{m}_t^{i_j})_{j \in \mathbb{N}}$ that convergences pointwise almost everywhere. By Fatou's lemma, convexity of $f(x) = x \ln x \ge e^{-1}$ for x > 0 and Proposition 10, for $t > t_H$, we get

$$\int h_t \ln h_t d\mu_{T_t} = \int m_t \ln \left(\frac{m_t}{\mu_{T_t}}\right)$$
$$\leq \liminf_{j \to \infty} \int \hat{m}_t^{i_j} \ln \left(\frac{\hat{m}_t^{i_j}}{\mu_{T_t}}\right)$$
$$\leq B\left(\frac{1}{t}\right)^{1-\frac{\hat{E}}{E}-2\alpha}.$$

 $^{^{6}}$ t_{H} from Proposition 10

5 Conclusions

We explored the possibility of using the generalised Langevin equations in the context of simulated annealing. Our main purpose was to establish convergence as for the underdamped Langevin equation and provide a proof of concept in terms of performance improvement. Although the theoretical results hold for any scaling matrix A given the stated restrictions, we saw in our numerical results that its choice has great impact on the performance. In Section 3, A_2 , A_3 or A_4 seemed to improve the exploration on the state space and/or the success proportion of the algorithm. There is plenty of work still required in terms of providing a more complete methodology for choosing A. This is left as future work and is also closely linked with time discretisation issues as a poor choice for A could lead to numerical integration stiffness. This motivates the development and study of improved numerical integration schemes, in particular, the extension of the conception and analysis on numerical schemes such as BAOAB [45] for the Langevin equation for (1.3) and the extension of the work in [57] for non-identity matrices λ and A. See [46] for work in this direction.

In addition, the system in (1.3) is not the only way to add an auxiliary variable to the underdamped Langevin equations in (1.2) whilst retaining the appropriate equilibrium distribution. Our choice was motivated by a clear connection to the generalised Langevin equation (1.4) and link with accelerated gradient descent, but it could be the case that a different third or higher order equations could be used with possibly improved performance. Along these lines, one could consider adding skew-symmetric terms as in [20]. As regards to theory, an interesting extension could involve establishing how the results here can be extended to establish a comparison of optimisation and sampling in a nonconvex setting for an arbitrary number of dimensions similar to [49]. We leave for future work finding optimal constants in the convergence results, investigating dependence on parameters and how the limits of these parameters and constants relate to existing results for the Langevin equation in (1.2) in [55,64]. Finally, one could also aim to extend large deviation results in [42,50,68] for the overdamped Langevin dynamics to the underdamped and generalised case.

Acknowledgements

The authors would like to thank Tony Lelievre, Gabriel Stoltz and Urbain Vaes for their helpful remarks. M.C. was funded under a EPSRC studentship. G.A.P. was partially supported by the EPSRC through grants EP/P031587/1, EP/L024926/1, and EP/L020564/1. N.K. and G.A.P. were funded in part by JPMorgan Chase & Co under a J.P. Morgan A.I. Research Awards 2019. Any views or opinions expressed herein are solely those of the authors listed, and may differ from the views and opinions expressed by JPMorgan Chase & Co. or its affiliates. This material is not a product of the Research Department of J.P. Morgan Securities LLC. This material does not constitute a solicitation or offer in any jurisdiction.

References

- S. A. Adelman and B. J. Garrison. Generalized Langevin theory for gas/solid processes: Dynamical solid models. The Journal of Chemical Physics, 65(9):3751–3761, 1976.
- H. AlRachid, L. Mones, and C. Ortner. Some remarks on preconditioning molecular dynamics. SMAI J. Comput. Math., 4:57–80, 2018.
- 3. A. D. Baczewski and S. D. Bond. Numerical integration of the extended variable generalized Langevin equation with a positive Prony representable memory kernel. *Journal of Chemical Physics*, 139(4):044107–044107, Jul 2013.
- 4. C. H. Bennett. Mass tensor molecular dynamics. Journal of Computational Physics, 19(3):267 279, 1975.
- 5. R. Biswas and D. R. Hamann. Simulated annealing of silicon atom clusters in Langevin molecular dynamics. *Phys. Rev. B*, 34:895–901, Jul 1986.
- V. I. Bogachev, N. V. Krylov, M. Röckner, and S. V. Shaposhnikov. Fokker-Planck-Kolmogorov equations, volume 207 of Mathematical Surveys and Monographs. American Mathematical Society, Providence, RI, 2015.
- 8. L. Bottou, F. E. Curtis, and J. Nocedal. Optimization methods for large-scale machine learning. SIAM Rev., 60(2):223–311, 2018.
- H. Brezis. Functional analysis, Sobolev spaces and partial differential equations. Universitext. Springer, New York, 2011.
 J. Carrillo, S. Jin, L. Li, and Y. Zhu. A consensus-based global optimization method for high dimensional machine learning problems.
- 09 2019. 11 J. A. Carrillo, Y.-P. Choi, C. Totzeck, and O. Tse. An analytical framework for consensus-based global optimization method. *Math.*
- J. A. Carrillo, Y.-P. Choi, C. Totzeck, and O. Tse. An analytical framework for consensus-based global optimization method. *Math. Models Methods Appl. Sci.*, 28(6):1037–1066, 2018.

- 12. M. Ceriotti. Generalized Langevin equation thermostats for ab initio molecular dynamics, 2014.
- M. Ceriotti, G. Bussi, and M. Parrinello. Langevin equation with colored noise for constant-temperature molecular dynamics simulations. *Phys. Rev. Lett.*, 102:020601, Jan 2009.
- M. Ceriotti, G. Bussi, and M. Parrinello. Colored-noise thermostats à la carte. Journal of Chemical Theory and Computation, 6(4):1170–1180, 2010.
- M. Chaleyat-Maurel and D. Michel. Hypoellipticity theorems and conditional laws. Z. Wahrsch. Verw. Gebiete, 65(4):573–597, 1984.
- X. Cheng, N. S. Chatterji, P. L. Bartlett, and M. I. Jordan. Underdamped Langevin MCMC: A non-asymptotic analysis. In S. Bubeck, V. Perchet, and P. Rigollet, editors, *Proceedings of the 31st Conference On Learning Theory*, volume 75 of *Proceedings of Machine Learning Research*, pages 300–323. PMLR, 06–09 Jul 2018.
- 17. T.-S. Chiang, C.-R. Hwang, and S. J. Sheu. Diffusion for global optimization in Rⁿ. SIAM J. Control Optim., 25(3):737–753, 1987.
- J. Diestel. Uniform integrability: an introduction. volume 23, pages 41–80 (1993). 1991. School on Measure Theory and Real Analysis (Grado, 1991).
- A. B. Duncan, T. Lelièvre, and G. A. Pavliotis. Variance reduction using nonreversible Langevin samplers. J. Stat. Phys., 163(3):457–491, 2016.
- A. B. Duncan, N. Nüsken, and G. A. Pavliotis. Using perturbed underdamped Langevin dynamics to efficiently sample from probability distributions. J. Stat. Phys., 169(6):1098–1131, 2017.
- A. Durmus and E. Moulines. High-dimensional Bayesian inference via the unadjusted Langevin algorithm. Bernoulli, 25(4A):2854– 2882, 2019.
- A. Eberle, A. Guillin, and R. Zimmer. Couplings and quantitative contraction rates for Langevin dynamics. Ann. Probab., 47(4):1982–2010, 2019.
- J.-P. Eckmann and M. Hairer. Non-equilibrium statistical mechanics of strongly anharmonic chains of oscillators. Comm. Math. Phys., 212(1):105–164, 2000.
- A. Friedman. Stochastic differential equations and applications. Vol. 1. Academic Press [Harcourt Brace Jovanovich, Publishers], New York-London, 1975. Probability and Mathematical Statistics, Vol. 28.
- S. Gadat and L. Miclo. Spectral decompositions and L²-operator norms of toy hypocoercive semi-groups. *Kinet. Relat. Models*, 6(2):317–372, 2013.
- S. Gadat and F. Panloup. Long time behaviour and stationary regime of memory gradient diffusions. Ann. Inst. Henri Poincaré Probab. Stat., 50(2):564–601, 2014.
- X. Gao, M. Gurbuzbalaban, and L. Zhu. Breaking reversibility accelerates langevin dynamics for global non-convex optimization. arXiv e-prints, 12 2018. arXiv:1812.07725.
- S. B. Gelfand and S. K. Mitter. Recursive stochastic algorithms for global optimization in R^d. SIAM J. Control Optim., 29(5):999– 1018, 1991.
- S. B. Gelfand and S. K. Mitter. Weak convergence of Markov chain sampling methods and annealing algorithms to diffusions. J. Optim. Theory Appl., 68(3):483–498, 1991.
- S. Geman and D. Geman. Stochastic relaxation, Gibbs distributions and the Bayesian restoration of images. IEEE Transactions on Pattern Analysis and Machine Intelligence - PAMI, PAMI-6:721–741, 1984.
- 31. S. Geman and C.-R. Hwang. Diffusions for global optimization. SIAM J. Control Optim., 24(5):1031–1043, 1986.
- 32. S. Ghadimi and G. Lan. Accelerated gradient methods for nonconvex nonlinear and stochastic programming. *Mathematical Programming*, 156(1):59–99, 2016.
- B. Gidas. Global optimization via the Langevin equation. In 1985 24th IEEE Conference on Decision and Control, pages 774 778, Dec 1985.
- 34. B. Gidas. Nonstationary Markov chains and convergence of the annealing algorithm. J. Statist. Phys., 39(1-2):73-131, 1985.
- 35. L. Gross. Logarithmic Sobolev inequalities. Amer. J. Math., 97(4):1061-1083, 1975.
- A. Guillin and P. Monmarché. Optimal linear drift for the speed of convergence of an hypoelliptic diffusion. *Electron. Commun. Probab.*, 21:Paper No. 74, 14, 2016.
- A. Guionnet and B. Zegarlinski. Lectures on logarithmic Sobolev inequalities. In Séminaire de Probabilités, XXXVI, volume 1801 of Lecture Notes in Math., pages 1–134. Springer, Berlin, 2003.
- 38. R. Holley and D. Stroock. Simulated annealing via Sobolev inequalities. Comm. Math. Phys., 115(4):553-569, 1988.
- R. A. Holley, S. Kusuoka, and D. W. Stroock. Asymptotics of the spectral gap with applications to the theory of simulated annealing. J. Funct. Anal., 83(2):333–347, 1989.
- R. Höpfner, E. Löcherbach, and M. Thieullen. Strongly degenerate time inhomogeneous SDEs: densities and support properties. Application to Hodgkin-Huxley type systems. *Bernoulli*, 23(4A):2587–2616, 2017.
- 41. C.-R. Hwang. Laplace's method revisited: weak convergence of probability measures. Ann. Probab., 8(6):1177-1182, 1980.
- 42. C.-R. Hwang and S. J. Sheu. Large-time behavior of perturbed diffusion Markov processes with applications to the second eigenvalue problem for Fokker-Planck operators and simulated annealing. *Acta Appl. Math.*, 19(3):253–295, 1990.
- H. J. Kushner. Asymptotic global behavior for stochastic approximation and diffusions with slowly decreasing noise effects: global minimization via Monte Carlo. SIAM J. Appl. Math., 47(1):169–185, 1987.
- 44. H. Lei, N. A. Baker, and X. Li. Data-driven parameterization of the generalized Langevin equation. Proc. Natl. Acad. Sci. USA, 113(50):14183–14188, 2016.
- 45. B. Leimkuhler and C. Matthews. *Molecular dynamics*, volume 39 of *Interdisciplinary Applied Mathematics*. Springer, Cham, 2015. With deterministic and stochastic numerical methods.
- 46. B. Leimkuhler and M. Sachs. Efficient Numerical Algorithms for the Generalized Langevin Equation. arXiv e-prints, page arXiv:2012.04245, Dec. 2020.
- 47. T. Lelièvre, F. Nier, and G. A. Pavliotis. Optimal non-reversible linear drift for the convergence to equilibrium of a diffusion. J. Stat. Phys., 152(2):237–274, 2013.

- 48. C. Li, C. Chen, D. Carlson, and L. Carin. Preconditioned stochastic gradient langevin dynamics for deep neural networks. In Proceedings of the Thirtieth AAAI Conference on Artificial Intelligence, AAAI'16, pages 1788–1794. AAAI Press, 2016.
- Y.-A. Ma, Y. Chen, C. Jin, N. Flammarion, and M. I. Jordan. Sampling can be faster than optimization. Proc. Natl. Acad. Sci. USA, 116(42):20881–20885, 2019.
- 50. D. Márquez. Convergence rates for annealing diffusion processes. Ann. Appl. Probab., 7(4):1118–1139, 1997.
- J. C. Mattingly and A. M. Stuart. Geometric ergodicity of some hypo-elliptic diffusions for particle motions. volume 8, pages 199–214. 2002. Inhomogeneous random systems (Cergy-Pontoise, 2001).
- G. Menz and A. Schlichting. Poincaré and logarithmic Sobolev inequalities by decomposition of the energy landscape. Ann. Probab., 42(5):1809–1884, 2014.
- G. Metafune, D. Pallara, and E. Priola. Spectrum of Ornstein-Uhlenbeck operators in L^p spaces with respect to invariant measures. J. Funct. Anal., 196(1):40–60, 2002.
- L. Miclo. Recuit simulé sur Rⁿ. Étude de l'évolution de l'énergie libre. Ann. Inst. H. Poincaré Probab. Statist., 28(2):235–266, 1992.
- P. Monmarché. Hypocoercivity in metastable settings and kinetic simulated annealing. Probab. Theory Related Fields, 172(3-4):1215–1248, 2018.
- 56. P. Monmarché. Generalized Γ calculus and application to interacting particles on a graph. Potential Anal., 50(3):439–466, 2019.
- W. Mou, Y.-A. Ma, M. J. Wainwright, P. L. Bartlett, and M. I. Jordan. High-order langevin diffusion yields an accelerated mcmc algorithm. Journal of Machine Learning Research, 22(42):1–41, 2021.
- M. Nava, M. Ceriotti, C. Dryzun, and M. Parrinello. Evaluating functions of positive-definite matrices using colored-noise thermostats. *Phys. Rev. E*, 89:023302, Feb 2014.
- Y. Nesterov. Lectures on convex optimization, volume 137 of Springer Optimization and Its Applications. Springer, Cham, 2018. Second edition of [MR2142598].
- 60. M. Ottobre and G. A. Pavliotis. Asymptotic analysis for the generalized Langevin equation. Nonlinearity, 24(5):1629–1653, 2011.
- M. Ottobre, G. A. Pavliotis, and K. Pravda-Starov. Exponential return to equilibrium for hypoelliptic quadratic systems. J. Funct. Anal., 262(9):4000–4039, 2012.
- S. Patterson and Y. W. Teh. Stochastic gradient Riemannian Langevin dynamics on the probability simplex. In C. J. C. Burges, L. Bottou, M. Welling, Z. Ghahramani, and K. Q. Weinberger, editors, Advances in Neural Information Processing Systems 26, pages 3102–3110. Curran Associates, Inc., 2013.
- 63. G. A. Pavliotis. *Stochastic processes and applications*, volume 60 of *Texts in Applied Mathematics*. Springer, New York, 2014. Diffusion processes, the Fokker-Planck and Langevin equations.
- 64. G. A. Pavliotis, G. Stoltz, and U. Vaes. Scaling limits for the generalized Langevin equation. J. Nonlinear Sci., 31(1):Paper No. 8, 58, 2021.
- M. Pelletier. Weak convergence rates for stochastic approximation with application to multiple targets and simulated annealing. Ann. Appl. Probab., 8(1):10–44, 1998.
- R. Pinnau, C. Totzeck, O. Tse, and S. Martin. A consensus-based model for global optimization and its mean-field limit. Math. Models Methods Appl. Sci., 27(1):183–204, 2017.
- 67. C. Prévôt and M. Röckner. A concise course on stochastic partial differential equations, volume 1905 of Lecture Notes in Mathematics. Springer, Berlin, 2007.
- 68. G. Royer. A remark on simulated annealing of diffusion processes. SIAM J. Control Optim., 27(6):1403–1408, 1989.
- 69. S. Ruder. An overview of gradient descent optimization algorithms. CoRR, abs/1609.04747, 2016.
- 70. M. Sachs. The generalised Langevin equation: asymptotic properties and numerical analysis. PhD thesis, The University of Edinburgh, 2017.
- H. Song, I. Triguero, and E. Özcan. A review on the self and dual interactions between machine learning and optimisation. Progress in Artificial Intelligence, 8(2):143–165, 2019.
- 72. D. W. Stroock and S. R. S. Varadhan. On the support of diffusion processes with applications to the strong maximum principle. In Proceedings of the Sixth Berkeley Symposium on Mathematical Statistics and Probability (Univ. California, Berkeley, Calif., 1970/1971), Vol. III: Probability theory, pages 333–359, 1972.
- W. Su, S. Boyd, and E. J. Candès. A differential equation for modeling Nesterov's accelerated gradient method: theory and insights. J. Mach. Learn. Res., 17:Paper No. 153, 43, 2016.
- 74. Y. Sun and A. Garcia. Interactive diffusions for global optimization. J. Optim. Theory Appl., 163(2):491-509, 2014.
- S. Taniguchi. Applications of Malliavin's calculus to time-dependent systems of heat equations. Osaka J. Math., 22(2):307–320, 1985.
- 76. C. Villani. Hypocoercivity. Mem. Amer. Math. Soc., 202(950):iv+141, 2009.
- X. Wu, B. R. Brooks, and E. Vanden-Eijnden. Self-guided Langevin dynamics via generalized Langevin equation. J Comput Chem, 37(6):595–601, Mar 2016.

Appendices

Appendix A Additional Results

We present the analog of Proposition 10 for the $T_t = T > 0$ sampling case and a result about the choice of the annealing schedule.

Proof (of Proposition 6) After Pinsker's inequality (2.12) and consideration of the definition (4.39) of H, what remains is the partial time derivative part of the proof of Proposition 10. The proof concludes by the same calculations as in Proposition 10, keeping in mind $T'_t = 0$, until (4.68) followed by the Grönwall argument. Note that (4.52) and (4.70) are not required and a log-Sobolev constant (in t also) works, in which case (4.51) and hence the current argument follow without requiring Assumption 2. The limiting ϵ argument as in Proposition 4 is the same.

Proposition 11 Under Assumption 1, 3 and 4, the schedule $T_t = \frac{E}{\ln(e+t)}$, $E > \hat{E}$ is optimal in the sense that for any differentiable $f : \mathbb{R}_+ \to \mathbb{R}_+$, if

$$T_t = \frac{1}{f(t)} \left(\frac{\hat{E}}{\ln(e+t)} \right),\tag{A.1}$$

 C_t is the log-Sobolev factor (4.52) and p is the finite order polynomial with nonnegative coefficients from the proof of Proposition 10, then the relation

$$2C_t^{-1} \gg |T_t'| p\left(T_t^{-1}\right) \tag{A.2}$$

holds for large times only if $\limsup_{t\to\infty} f(t) \leq 1$.

Proof Suppose there exists a constant $\delta > 0$ and times $(t_i)_{i \in \mathbb{N}}$ such that $0 < t_i \to \infty$ and

$$f(t_i) \ge 1 + \delta \quad \forall i.$$

From (4.52),

$$C_t^{-1}\sim \mathcal{O}(e^{-\hat{E}T_t^{-1}}T_t^{-1}),$$

which after substituting in (A.1) gives

$$e^{-\hat{E}T_t^{-1}}T_t^{-1} = (e+t)^{-f(t)}\frac{f(t)\ln(e+t)}{\hat{E}} \sim \mathcal{O}(t^{-f(t)}f(t)\ln t).$$
(A.3)

Compare this to

$$|T_t'| p\left(T_t^{-1}\right) \propto \frac{p(f(t)\ln(e+t))}{(f(t)\ln(e+t))^2} \left(\frac{f(t)}{e+t} + |f'(t)|\ln(e+t)\right),\tag{A.4}$$

which has order at least $(tf(t))^{-1}(\ln t)^{-2}$. For $t = t_i$, *i* large enough, $f(t) \ge 1 + \delta$ and so

$$t^{-f(t)}f(t)\ln t \ll (tf(t))^{-1}(\ln t)^{-2},$$
(A.5)

which violates (A.2).

Remark 8 One can strengthen the proposition by making precise the form of p from Proposition 10, which will determine how slowly f(t) is allowed to converge to 1; in fact p should be at least sixth order. This seems inconsequential with respect to optimality and so is omitted.



Fig. 3.1: Dynamics in order from top: (3.2), (3.1) with $A = A_1, \ldots, A_4$. Left: One instance of noise realisation. Right: Log histogram of 20 independent runs.



Fig. 3.2: Proportion of simulations satisfying optimality tolerance for $U = U_1$. Panels from top to bottom: (3.2), (3.1) with $A = A_1, A_2, A_3$. Left: Final position. Right: time-average of last 5000 iterations. We use $\gamma = 3$ for improving visualisation, the results and improvement in using (3.1) are similar for the case of $\gamma = 1$. Results here are for 20 independent runs and $k \leq 5 \cdot 10^4$ -iterations.



Fig. 3.3: Both proportion of success and numerical transition rates for $U = U_2$. Panels from top to bottom: (3.2), (3.1) with $A = A_1, A_2, A_3, A_4$. Left: Proportion satisfying the optimality tolerance for time-average of last 5000 iterations. Right: Average number of crossings of position averages over 5000 iterations across $\{x_1 = 0\}$ for each independent run. The remaining details are as in caption of Figure 3.2.



Fig. 3.4: Results for $U = U_3$. Details are as in caption of Figure 3.3.