ON THE SIMULATED ANNEALING IN $\mathbb{R}^d$

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Abstract. Using a localization procedure and the result of Holley-Kusuoka-Stroock [7] in the torus, we widely weaken the usual growth assumptions concerning the success of the continuous-time simulated annealing in $\mathbb{R}^d$. Our only assumption is the existence of an invariant probability measure for a sufficiently low temperature. We also prove, in an appendix, a non-explosion criterion for a class of time-inhomogeneous diffusions.

1. Introduction and results

1.1. Main results.

We work with the following setting.

Assumption (A). *Fix a dimension $d \geq 1$ and a function $U : \mathbb{R}^d \to \mathbb{R}_+$ of class C^∞ such that $\lim_{|x|\to\infty} U(x) = \infty$ and $\min_{x\in\mathbb{R}^d} U(x) = 0$. For $x, y \in \mathbb{R}^d$, we set*

$$E(x,y) = \inf\Big\{ \max_{t\in[0,1]} U(\gamma_t) - U(x) - U(y) \;:\; \gamma \in C([0,1],\mathbb{R}^d), \gamma_0 = x, \gamma_1 = y\Big\}$$

and we suppose that $c_* = \sup\{E(x,y) : x, y \in \mathbb{R}^d\} < \infty$.

Actually, $c_* = \sup\{E(x,y) : x$ local minimum of U, y global minimum of $U\}$ represents the maximum potential energy required to reach a global minimum y of U when starting from anywhere else.

We fix $x_0 \in \mathbb{R}^d$, $c > 0$ and $\beta_0 > 0$ and consider the time-inhomogeneous S.D.E.

$$X_t = x_0 + B_t - \frac{1}{2}\int_0^t \beta_s \nabla U(X_s)\mathrm{d}s \quad \text{where} \quad \beta_t = \frac{\log(e^{c\beta_0} + t)}{c} \tag{1}$$

and where $(B_t)_{t\geq0}$ is a d-dimensional Brownian motion. By Theorem 15 proved in the appendix, since $U \geq 0$ under (A), (1) has a pathwise unique non-exploding solution $(X_t)_{t\geq0}$. Here is our main result.

Theorem 1. *Assume (A) and that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$ for some $\alpha_0 > 0$. Fix $c > c_*$, $x_0 \in \mathbb{R}^d$ and $\beta_0 > 0$ and consider the unique solution $(X_t)_{t\geq0}$ to (1). Then $\lim_{t\to\infty} U(X_t) = 0$ in probability.*

One of the ingredients of the proof is the following proposition, which asserts that, in full generality, the simulated annealing is successful on the event where the process $(X_t)_{t\geq0}$ does not escape to infinity in large time.

Proposition 2. *Assume (A), fix $c > c_*$, $x_0 \in \mathbb{R}^d$ and $\beta_0 > 0$. For $(X_t)_{t\geq0}$ the solution to (1),*

$$\forall\, \varepsilon > 0, \quad \lim_{t\to\infty} \mathbb{P}\Big(\liminf_{s\to\infty} |X_s| < \infty \text{ and } U(X_t) > \varepsilon\Big) = 0.$$

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1.2. **Comments and references.** The simulated annealing has been introduced by Kirkpatrick-Gelatt-Vecchi [10] as a numerical procedure to find a (possibly non unique) global minimum of a function U on a given state space. We refer to Azencott [1] for an early review of the method and its links with the theory of Freidlin-Wentzell [3].

With our notation and in our context where the state space is $\mathbb{R}^d$, the main idea of the simulated annealing is the following. The solution to (1), with β constant, has $\mu_\beta(\mathrm{d}x) = \mathcal{Z}_\beta^{-1} e^{-\beta U(x)}\mathrm{d}x$ as invariant probability distribution, if $\mathcal{Z}_\beta = \int_{\mathbb{R}^d} e^{-\beta U(x)}\mathrm{d}x < \infty$.

Using that $\min U = 0$ and that ∇U is locally bounded, we deduce that there is $\kappa > 0$ such that $\mathcal{Z}_\beta \geq e^{-1}\int_{\{U\leq 1/\beta\}} \mathrm{d}x \geq \kappa\beta^{-d}$ for all $\beta \geq 1$. Hence under the condition that $\mathcal{Z}_{\alpha_0} < \infty$ for some $\alpha_0 > 0$, it holds that for all $\varepsilon > 0$,

$$\mu_\beta(U > \varepsilon) \leq \mathcal{Z}_\beta^{-1} \int_{\{U>\varepsilon\}} e^{-\beta U(x)}\mathrm{d}x \leq \frac{\beta^d}{\kappa}\mathcal{Z}_{\alpha_0} e^{-(\beta-\alpha_0)\varepsilon} \longrightarrow 0 \quad \text{as } \beta \to \infty. \tag{2}$$

Hence one hopes that the solution to (1), with $\lim_{t\to\infty}\beta_t = \infty$, satisfies $\lim_{t\to\infty} U(X_t) = 0$ in probability. However, it is necessary that β_t increases sufficiently slowly to infinity, so that $\mathrm{Law}(X_t)$ remains close, for all times, to μ_{β_t}. If β_t increases too fast to infinity, one may remain stuck near a local minimum of U, as in the classical deterministic gradient method.

A major contribution is due to Holley-Kusuoka-Stroock [7], see also Holley-Stroock [8]. Replacing $\mathbb{R}^d$ by a compact manifold M, they showed that when $\beta_t \simeq c^{-1}\log(1+t)$, the simulated annealing procedure is successful, i.e. $\lim_{t\to\infty} U(X_t) = 0$ in probability, if and only if $c > c_*$. Their proof is almost purely analytic and very elegant. It relies on precise spectral gap estimates providing an asymptotically optimal Poincaré inequality. They use at many places the compactness of the state space.

This kind of proof involving functional inequalities has been extended to the non-compact case of $\mathbb{R}^d$ by Royer [14] and Miclo [11], at the price of many growth conditions on U, like

$$\lim_{|x|\to\infty} U(x) = \lim_{|x|\to\infty} |\nabla U(x)| = \infty \quad \text{and} \quad \forall\, x \in \mathbb{R}^d, \quad \Delta U(x) \leq C + |\nabla U(x)|^2. \tag{3}$$

Zitt [15], taking advantage of some weak Poincaré inequalities, worked under another set of rather stringent conditions, still implying that all the local minima of U are lying in a compact set. He in particular assumes that $|\nabla U|$ is bounded and that there is $\varepsilon > 0$ such that, for all x outside a compact, $U(x) \geq \log^{1+\varepsilon}|x|$ and $\Delta U(x) \leq 0$.

Here we only assume that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$ for some $\alpha_0 > 0$, which seems very natural in view of (2). This covers and consequently extends the previously cited works in $\mathbb{R}^d$. In particular, nothing forbids U to oscillate, as strongly as it wants, and as far as it wants from compact sets, and thus in particular to have an unbounded set of local minima.

1.3. **Short heuristics.** Let us emphasis that our proof relies on the following two main points. An entropy computation, see Lemma 5, shows that the condition $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$ implies that $\liminf_{t\to\infty} |X_t| < \infty$ a.s. Now, recall that in the compact case, see Holley-Kusuoka-Stroock [7] or Miclo [12], its a.s. holds that $\limsup_{t\to\infty} U(X_t) = c$. Combining these two points, its seems rather clear from the Borel-Cantelli Lemma that, in the non compact setting, the process will also satisfy $\limsup_{t\to\infty} U(X_t) = c$ a.s. Hence it will eventually remain in a compact set and Theorem 1 will follow from the compact case.

Apart from Lemma 5, which seems new and efficient, there are a number of technical issues, that are detailed in the next subsection.

1.4. **Plan of the proof.** We denote by $(X_t)_{t\geq 0}$ the solution to (1). We assume (A) and the conditions that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$ for some $\alpha_0 > 0$ and $c > c_*$.

(a) In Section 2, we prove some auxiliary weak regularization property for the law of the solution to (1). This allows us, when applying P.D.E. techniques, to do as if the law of X_0 had a bounded density concentrated around x_0, with a precise bound as a function of β_0.

(b) In Section 3, we show that $\liminf_{t\to\infty} |X_t| < \infty$: the process cannot escape to infinity in large time. This does not use the condition $c > c_*$. The key argument is the following: under the additional assumptions that $\mathrm{Law}(X_0)$ is smooth and $\beta_0 > \alpha_0$, we prove the important *a priori* estimate $\sup_{t\geq 0} \mathbb{E}[U(X_t)] < \infty$, see Lemma 5, which *a priori* implies that $\liminf_{t\to\infty} |X_t| < \infty$ by the Fatou lemma and since $\lim_{|x|\to\infty} U(x) = \infty$. We then make all this rigorous and get rid of the additional assumptions using point (a) and that our process does not explode in finite time.

This central *a priori* estimate is derived from a rather original entropy computation. Let us mention that deducing that $\sup_{t\geq 0} \mathbb{E}[U(X_t)] < \infty$ directly from the Itô formula would necessarily require some stringent conditions on ∇U and ΔU.

(c) In Section 4, we verify in Lemma 7 that, with an abuse of language, $U(X_t) \to 0$ in probability as $t \to \infty$ on the event where $\sup_{t\geq 0} |X_t| < \infty$.

This is easy, by localization, in view of the results of Holley-Kusuoka-Stroock [7] applied to a large flat torus: the condition $\sup_{t\geq 0} |X_t| < \infty$ almost tells us that we are in a compact setting.

(d) Still in Section 4, we check, although stated in slightly different words, see Proposition 8, that for any $B \geq 1$, there are $C_B > B$ and $t_B > 0$ such that

$$\inf_{|x_0|\leq B, t_0\geq t_B} \mathbb{P}_{t_0,x_0}\Big(\sup_{t\geq 0} |X_t| \leq C_B\Big) \geq \frac{1}{2}.$$

This is rather natural: in the compact setting, it is well-known, see [7] or Miclo [12], that $\limsup_{t\to\infty} U(X_t) = c$ a.s. It would not be too difficult to deduce that in the non-compact case, there exists $C_{t_0,x_0} > 0$ such that $\mathbb{P}_{t_0,x_0}(\sup_{t\geq 0} |X_t| \leq C_{t_0,x_0}) \geq 1/2$. The main issue is to show that C_{t_0,x_0} does not depend too much on t_0 and x_0. This is tedious, and we have to revisit the proof of [7].

(e) In Section 5, we prove Proposition 2: by (d), on the event $\liminf_{s\to\infty} |X_s| < \infty$, our process will eventually be absorbed in a compact set, so that $\sup_{s\geq 0} |X_s| < \infty$, whence the success of the simulated annealing by point (c).

(f) Still in Section 5, we conclude the proof of Theorem 1: $\liminf_{t\to\infty} |X_t| < \infty$ a.s. by (b), whence the success of the simulated annealing by (e).

1.5. **More comments.** It is well-know that, even in the compact case, the condition $c > c_*$ is necessary, see Holley-Kusuoka-Stroock [7, Corollary 3.11].

Our proof completely breaks down for slower freezing schemes, i.e. if $\beta_t \ll \log t$ as $t \to \infty$: in such a case, point (d) above cannot hold true, even non uniformly in t_0 and x_0.

Observe that we do not assume any Lyapunov condition, which would involve ΔU and ∇U and would forbid U to oscillate too strongly.

As already mentioned and in view of (2), our only assumption, i.e. the existence of an invariant probability measure for some (low) temperature, is very natural and allows for potentials with a very general shape.

However, we have shown in a previous paper with Monmarché [2] that things may work even without this condition. In [2, Theorem 1 and Proposition 2], we see that if $d \geq 3$ and $U(x) = a \log\log|x|$ outside a compact, the simulated annealing works if $c > c_*$ and $c < 2a/(d-2)$ and fails if $c > 2a/(d-2)$. But it is not clear that a general growth condition exists. In particular, we deduce from [2, Proposition 2] and a comparison argument that if $U(x) = \log^{\circ 3}|x|$ outside a compact, then the simulated annealing fails for all $c > 0$. But in [2, Proposition 3], we built some (very oscillating) potential U such that $\log^{\circ 3}|x| \leq U(x) \leq 3\log^{\circ 3}|x|$ outside a compact for which the simulated annealing works for some values of c. Thus, without the condition that $\int_{\mathbb{R}^d} \exp(-\alpha_0 U(x))\mathrm{d}x < \infty$ for some $\alpha_0 > 0$, the situation may be very intricate and really depend on the shape of U.

1.6. **Non-explosion.** The non-explosion of the solution to (1), using only that $U \geq 0$, is checked in the appendix. Actually, we treat, without major complication, the more general case where $\beta : \mathbb{R}_+ \to (0,\infty)$ is any smooth function and where $U : \mathbb{R}^d \to \mathbb{R}$ is smooth and satisfies $U(x) \geq -L(1+|x|^2)$ for some constant $L > 0$. This is not so easy, since we do not want to assume any local condition on ∇U. We use purely deterministic techniques inspired by the seminal work of Grigor'yan [5], also exposed in [6, Section 9] and by the paper of Ichihara [9], both dealing with more general but *time-homogeneous* processes.

Let us mention that in the homogeneous case, Ichihara uses the P.D.E. satisfied by $v(x) = \mathbb{E}_x[e^{-\sigma_1}]$, where $\sigma_1 = \inf\{t \geq 0 : |X_t| \leq 1\}$, while Grigor'yan rather studies the P.D.E. satisfied by $w(t,x) = \mathbb{P}_x[\zeta < t]$, where ζ is the life-time of the solution. In the inhomogeneous setting, we study, roughly, the P.D.E. satisfied by $u(t,x) = \mathbb{E}_{t,x}[e^{-\zeta}]$, where ζ is the life-time of the solution. The situation is slightly more complicated, but we manage to take advantage of some computations found in [5] and [9] to show that $u \equiv 0$.

2. Weak regularization

We prove some weak regularization that will allow us, when using P.D.E. techniques, to replace the Dirac initial condition δ_{x_0} by some bounded function concentrated around x_0. One might invoke the Hörmander theorem, but since we need a precise bound as a function of β_0 (see Lemma 14 below), we will rather use the following weaker lemma based on stopping times.

Lemma 3. *Assume (A) and fix $c > 0$. For any $A > 1$, there is a constant $C_A^{(1)}$ such that for any $x_0 \in \{U \leq A\}$, any $\beta_0 > 0$, denoting by $(X_t)_{t\geq 0}$ the corresponding solution to (1), there exists a stopping time $\tau \in [0,1]$ such that $\sup_{t\in[0,\tau]} |X_t - x_0| \leq 1$ and such that the law of (τ, X_τ) has a density bounded by $\exp(C_A^{(1)}(\beta_0+1))\mathbf{1}_{\{[0,1]\times B(x_0,1)\}}$.*

Proof. We fix $x_0 \in \{U \leq A\}$ and $\beta_0 > 0$. We introduce some random variable R, uniformly distributed in $[1/2,1]$ and independent of $(X_t)_{t\geq 0}$. We claim that

$$\tau = \inf\{t \geq 0 : |X_t - x_0| = R\} \wedge R$$

satisfies the requirements of the statement.

First, $\tau \leq R \leq 1$ and $\sup_{t\in[0,\tau]} |X_t - x_0| \leq R \leq 1$.

Next, we consider a d-dimensional Brownian motion $(W_t)_{t\geq 0}$ independent of R and we set $\tilde\tau = \inf\{t \geq 0 : |W_t| = R\} \wedge R$. We introduce the martingale

$$L_t = -\frac{1}{2}\int_0^{t\wedge\tilde\tau} \beta_s \nabla U(x_0 + W_s)\cdot \mathrm{d}W_s,$$

as well as its exponential $\mathcal{E}_t = \exp(L_t - \frac{1}{2}\langle L\rangle_t)$, which is uniformly integrable by the Novikov criterion, see Revuz-Yor [13, Proposition 1.15 p 332], because $\langle L\rangle_\infty \le \frac{1}{4}(\sup_{B(x_0,1)} |\nabla U|^2)\int_0^1 \beta_s^2 \mathrm{d}s$ is bounded. The Girsanov theorem tells us that under $\mathcal{E}_\infty \cdot \mathbb{P}$, the process

$$B_{t\wedge\tilde\tau} = W_{t\wedge\tilde\tau} + \frac{1}{2}\int_0^{t\wedge\tilde\tau} \beta_s \nabla U(x_0+W_s)\mathrm{d}s, \quad t\ge 0$$

is a (stopped) Brownian motion, so that $x_0 + W_{t\wedge\tilde\tau}$ is a (stopped) solution to (1). Hence for all measurable $\phi : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}_+$, $\mathbb{E}[\phi(\tau, X_\tau)] = \mathbb{E}[\phi(\tilde\tau, x_0 + W_{\tilde\tau})\mathcal{E}_\infty]$.

By the Itô formula,

$$\beta_{t\wedge\tilde\tau} U(x_0+W_{t\wedge\tilde\tau}) = \beta_0 U(x_0) + \int_0^{t\wedge\tilde\tau} \beta_s' U(x_0+W_s)\mathrm{d}s - 2L_t + \frac{1}{2}\int_0^{t\wedge\tilde\tau} \beta_s \Delta U(x_0+W_s)\mathrm{d}s,$$

whence, since $U\ge 0$ and $\beta \ge 0$,

$$L_\infty \le \frac{1}{2}\Big(\beta_0 U(x_0) + \int_0^{\tilde\tau} \beta_s' U(x_0+W_s)\mathrm{d}s + \frac{1}{2}\int_0^{\tilde\tau} \beta_s \Delta U(x_0+W_s)\mathrm{d}s\Big).$$

Recalling that $\tilde\tau \le 1$, that $\sup_{[0,\tilde\tau]} |W_s| \le R \le 1$ that $x_0 \in \{U \le A\}$, that $\beta_s' \le 1/c$ and that $\sup_{[0,1]} \beta_s \le \beta_0 + 1/c$, we deduce that

$$L_\infty \le \frac{1}{2}\Big(\beta_0 + \frac{1}{c}\Big)\Big(A + \sup_{x\in\{U\le A\}} \sup_{y\in B(x,1)} \Big[U(y) + \frac{1}{2}|\Delta U(y)|\Big]\Big) \le C_A(1+\beta_0),$$

for some finite constant $C_A > 0$ depending on A and c. We used that $\cup_{x\in\{U\le A\}} B(x,1)$ is bounded because $\lim_{|x|\to\infty} U(x) = \infty$.

Hence $\mathcal{E}_\infty = \exp(L_\infty - \frac{1}{2}\langle L\rangle_\infty) \le \exp(L_\infty) \le e^{C_A(1+\beta_0)}$ and for all measurable $\phi : \mathbb{R}_+ \times \mathbb{R}^d \to \mathbb{R}_+$,

$$\mathbb{E}[\phi(\tau, X_\tau)] \le e^{C_A(1+\beta_0)} \mathbb{E}[\phi(\tilde\tau, x_0 + W_{\tilde\tau})]. \tag{4}$$

We now verify that $(\tilde\tau, W_{\tilde\tau})$ has a bounded density, necessarily supported in $[0,1]\times B(0,1)$. For $r>0$, we introduce $\tau_r = \inf\{t>0 : |W_t| = r\}$. We have $\tilde\tau = \tau_R \wedge R$, so that the density of $(\tilde\tau, W_{\tilde\tau})$ is bounded by the sum of the densities of (τ_R, W_{τ_R}) and (R, W_R). Recall that $R \sim \mathcal{U}([1/2,1])$.

The density of (R, W_R) is $2e^{-|x|^2/(2r)}/(2\pi r)^{d/2}\mathbf{1}_{\{r\in[1/2,1], x\in\mathbb{R}^d\}}$, which is bounded.

Next, denoting by $\mu_r(s)$ the density of τ_r, we have by scaling that $\mu_r(s) = r^{-2}\mu_1(r^{-2}s)$, because τ_r has the same law as $r^2\tau_1$. One may then check that the density of (τ_R, W_{τ_R}) is $|x|^{-d-1}\mu_1(|x|^{-2}r)\mathbf{1}_{\{r>0, |x|\in[1/2,1]\}}$, up to some normalization constant. Since μ_1 is bounded, so is the density of (τ_R, W_{τ_R}).

Denoting by C the bound of the density of $(\tilde\tau, W_{\tilde\tau})$, we conclude from (4) that (τ, X_τ) has a density bounded by $Ce^{C_A(1+\beta_0)}\mathbf{1}_{\{s\in[0,1], x\in B(x_0,1)\}}$. The conclusion follows. □

3. No escape in large time

In this section, we prove that $\liminf_{t\to\infty} |X_t| < \infty$.

Proposition 4. *Assume (A) and fix $c > 0$, $x_0 \in \mathbb{R}^d$ and $\beta_0 > 0$. Suppose that there is $\alpha_0 > 0$ such that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$. For $(X_t)_{t\ge 0}$ the solution to (1), $\liminf_{t\to\infty} |X_t| < \infty$ a.s.*

The crucial point is the following uniform in time *a priori* estimate.

Lemma 5. *Assume (A), fix $c > 0$, $\beta_0 > 0$ and assume that there is $\alpha_0 \in (0, \beta_0)$ such that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)} \mathrm{d}x < \infty$. Let f_0 be a probability density on $\mathbb{R}^d$. Let $(X_t)_{t\geq 0}$ be the solution to* (1) *starting from X_0 with law f_0. If*

$$\kappa(f_0) = \int_{\mathbb{R}^d} f_0(x) \log(1 + f_0(x) e^{\beta_0 U(x)}) \mathrm{d}x < \infty,$$

setting $a_0 = [\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)} \mathrm{d}x]^{-1}$, we informally have

$$\sup_{t\geq 0} \mathbb{E}[U(X_t)] \leq \frac{\kappa(f_0) - \log(a_0)}{\beta_0 - \alpha_0}.$$

This relies on a rather indirect entropy computation. As already mentioned, obtaining a uniform in time moment bound, using the Itô formula, would require much more stringent conditions involving ∇U and ΔU. Observe that the computation below is rather original, in that we do not differentiate the *true* relative entropy $\int_{\mathbb{R}^d} f_t(x) \log(f_t(x) \mathcal{Z}_{\beta_t} e^{\beta_t U(x)}) \mathrm{d}x$, where $\mathcal{Z}_\beta = \int_{\mathbb{R}^d} e^{-\beta U(x)} \mathrm{d}x$, but rather the relative entropy *without normalization constant* $\int_{\mathbb{R}^d} f_t(x) \log(f_t(x) e^{\beta_t U(x)}) \mathrm{d}x$. Strangely, using the true relative entropy functional does not seem to provide interesting results.

Proof. As mentioned in the statement, we give an informal proof. The law f_t of X_t weakly solves

$$\partial_t f_t(x) = \frac{1}{2} \mathrm{div}[\nabla f_t(x) + \beta_t f_t(x) \nabla U(x)] = \frac{1}{2} \mathrm{div}[e^{-\beta_t U(x)} \nabla (f_t(x) e^{\beta_t U(x)})]. \tag{5}$$

For any smooth $\phi : \mathbb{R}_+ \to \mathbb{R}$, we have, setting $\psi(u) = u\phi'(u) - \phi(u)$ for all $u \geq 0$,

(6)
$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^d} \phi(f_t(x) e^{\beta_t U(x)}) e^{-\beta_t U(x)} \mathrm{d}x \\
=& \int_{\mathbb{R}^d} \Big[\partial_t f_t(x) \phi'(f_t(x) e^{\beta_t U(x)}) + \beta_t' U(x) f_t(x) \phi'(f_t(x) e^{\beta_t U(x)}) - \beta_t' U(x) \phi(f_t(x) e^{\beta_t U(x)}) e^{-\beta_t U(x)} \Big] \mathrm{d}x \\
=& -\frac{1}{2} \int_{\mathbb{R}^d} |\nabla (f_t(x) e^{\beta_t U(x)})|^2 \phi''(f_t(x) e^{\beta_t U(x)}) e^{-\beta_t U(x)} \mathrm{d}x + \beta_t' \int_{\mathbb{R}^d} U(x) \psi(f_t(x) e^{\beta_t U(x)}) e^{-\beta_t U(x)} \mathrm{d}x.
\end{aligned}$$

For the last equality (first term), we used (5) and an integration by parts.

We now apply (6) with the convex function $\phi(u) = u \log(1+u)$, for which $\psi(u) = \frac{u^2}{1+u} \leq u$, to find, throwing away the nonpositive term, $h_t' \leq \beta_t' u_t$, where we have set

$$h_t = \int_{\mathbb{R}^d} f_t(x) \log(1 + f_t(x) e^{\beta_t U(x)}) \mathrm{d}x \quad \text{and} \quad u_t = \int_{\mathbb{R}^d} U(x) f_t(x) \mathrm{d}x = \mathbb{E}[U(X_t)].$$

But

$$h_t \geq \int_{\mathbb{R}^d} f_t(x) \log(f_t(x) e^{\beta_t U(x)}) \mathrm{d}x = \int_{\mathbb{R}^d} f_t(x) \log(f_t(x)) \mathrm{d}x + \beta_t u_t \geq (\beta_t - \alpha_0) u_t + \log(a_0).$$

We used that $\int_{\mathbb{R}^d} f(x) \log(f(x)/g(x)) \mathrm{d}x \geq 0$ for any pair of probability densities f and g on $\mathbb{R}^d$, whence $\int_{\mathbb{R}^d} f_t(x) \log(f_t(x)) \mathrm{d}x \geq \int_{\mathbb{R}^d} f_t(x) \log(a_0 \exp(-\alpha_0 U(x)) \mathrm{d}x = \log(a_0) - \alpha_0 u_t$.

We conclude, since $h_0 = \kappa(f_0)$, that

$$(\beta_t - \alpha_0) u_t \leq h_t - \log(a_0) \leq \kappa(f_0) - \log(a_0) + \int_0^t \beta_s' u_s \mathrm{d}s = \kappa(f_0) - \log(a_0) + \int_0^t \frac{\beta_s'}{\beta_s - \alpha_0} (\beta_s - \alpha_0) u_s \mathrm{d}s,$$

whence, by the Gronwall lemma,

$$(\beta_t - \alpha_0) u_t \leq [\kappa(f_0) - \log(a_0)] \exp\Big(\int_0^t \frac{\beta_s' \mathrm{d}s}{\beta_s - \alpha_0} \Big) = [\kappa(f_0) - \log(a_0)] \frac{\beta_t - \alpha_0}{\beta_0 - \alpha_0}.$$

Consequently, $\mathbb{E}[U(X_t)] = u_t \le [\kappa(f_0) - \log(a_0)]/[\beta_0 - \alpha_0]$ for all $t \ge 0$. □

We now try to deduce from this informal computation the rigorous results we need.

Lemma 6. *If ∇U is bounded together with all its derivatives and if the initial density f_0 belongs to $C_c(\mathbb{R}^d)$, the* a priori *estimate of Lemma 5 rigorously holds true for the solution* (1) *starting from $X_0 \sim f_0$.*

Proof. We first justify rigorously (6), for all $t \in (0,\infty)$, with $\phi(u) = u\log(1+u)$. Recall that f_t is the law of X_t. Since U has at most linear growth and ∇U is bounded, it is (widely) enough to check that $(f_t(x))_{t>0,x\in\mathbb{R}^d}$ is a strong solution to (5), i.e. $2\partial_t f_t(x) = \Delta f_t(x) + \beta_t \nabla U(x)\cdot\nabla f_t(x) + \beta_t f_t(x)\Delta U(x)$ on $(0,\infty)\times\mathbb{R}^d$ and satisfies, for all $0 < t_0 < t_1$, for some constants $C_{t_0,t_1} > 0$ and $\lambda_{t_0,t_1} > 0$,

$$\forall t \in [t_0,t_1],\ x \in \mathbb{R}^d, \quad f_t(x) + |\partial_t f_t(x)| + |\nabla f_t(x)| + |D^2 f_t(x)| \le C_{t_0,t_1}\exp(-\lambda_{t_0,t_1}|x|^2).$$

To prove those bounds, we use classical results found in Friedman [4], that apply to uniformly parabolic equations with bounded and Lipschitz coefficients (actually, Hölder is enough): by [4, Chapter 1, Theorem 12], we have $f_t(x) = \int_{\mathbb{R}^d}\Gamma(x,t;\xi,0)f_0(\xi)\mathrm{d}\xi$, with, for some $C_T > 0$ and $\lambda > 0$, for all $t \in [0,T]$, all $x \in \mathbb{R}^d$,

$$|\Gamma(x,t;\xi,0)| + t^{1/2}|\nabla_x\Gamma(x,t;\xi,0)| + t|D^2\Gamma(x,t;\xi,0)| \le C_T t^{-d/2}e^{-\lambda|x-\xi|^2/t}. \tag{7}$$

The above estimates for Γ and $\nabla\Gamma$ are nothing but [4, Chapter 1, Equations (6.12) and (6.13)], and the estimate on $D^2\Gamma$ is proved similarly, using [4, Chapter 1, Equation (4.11)]. The Gaussian upper-bounds of $f_t(x)$, $|\nabla f_t(x)|$ and $|D^2 f_t(x)|$ follow, because $f_0 \in C_c(\mathbb{R}^d)$. Finally, the bound on $\partial_t f_t(x)$ follows from the fact that $2|\partial_t f_t(x)| \le |\Delta f_t(x)| + \beta_t||\nabla U||_\infty|\nabla f_t(x)| + \beta_t||\Delta U||_\infty f_t(x)$.

Hence, all the arguments in the proof of Lemma 5 are correct for $t \in (0,\infty)$, and we conclude that for all $t_0 > 0$, $\sup_{t\ge t_0}\mathbb{E}[U(X_t)] \le (\beta_{t_0} - \alpha_0)^{-1}(\kappa(f_{t_0}) - \log(a_0))$. To complete the proof, the only issue is to show that $\lim_{t_0\to0+}\kappa(f_{t_0}) = \kappa(f_0)$. This can be deduced from the continuity of $f_t(x)$ on $[0,\infty)\times\mathbb{R}^d$, see [4, Chapter 1, Section 7], and the fact that there are $C_T > 0$ and $\lambda_T > 0$ such that $f_t(x) \le C_T e^{-\lambda_T|x|^2}$ for all $t \in [0,T]$ and $x \in \mathbb{R}^d$. This follows from (7), the fact that $f_t(x) = \int_{\mathbb{R}^d}\Gamma(x,t;\xi,0)f_0(\xi)\mathrm{d}\xi$ and that $f_0 \in C_c(\mathbb{R}^d)$. □

We can now prove the main result of this section.

Proof of Proposition 4. We assume (A) and that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x < \infty$ for some $\alpha_0 > 0$. We fix $c > 0$, $x_0 \in \mathbb{R}^d$ and $\beta_0 > 0$ and aim to check that for $(X_t)_{t\ge0}$ the solution to (1), $\liminf_{t\to\infty}|X_t| < \infty$ a.s. We divide the proof in four steps.

Step 1. We of course may assume additionally that $\beta_0 > \alpha_0$: fix $t_0 \ge 0$ large enough so that $\beta_{t_0} > \alpha_0$ and observe that $(X_{t_0+t})_{t\ge0}$ solves (1), with x_0 replaced by X_{t_0} and β_0 replaced by β_{t_0} (and with the Brownian motion $(B_{t_0+t} - B_{t_0})_{t\ge0}$). Since $\liminf_{t\to\infty}|X_t| = \liminf_{t\to\infty}|X_{t_0+t}|$, the conclusion follows.

Step 2. From now on, we assume that $\beta_0 > \alpha_0$. We introduce the stopping time $\tau \in [0,1]$ as in Lemma 3. We recall that $\sup_{[0,\tau]}|X_t - x_0| \le 1$ and that for $h \in L^1([0,1]\times B(x_0,1))$ the density of (τ, X_τ), there is $C > 0$ (depending on x_0 and β_0) such that $h(u,x) \le C\mathbf{1}_{\{u\in[0,1],x\in B(x_0,1)\}}$.

Step 3. For $n \ge |x_0|+1$, we introduce $U_n \in C^\infty(\mathbb{R}^d)$ such that $U_n(x) = U(x)$ for all $x \in B(0,n)$ and $U_n(x) = |x|$ as soon as $|x| \ge n+1$, with furthermore $U_n(x) \ge \min(U(x),|x|) - 1$ for all $x \in \mathbb{R}^d$. Then ∇U_n is bounded together all its derivatives. We denote by $(X_t^n)_{t\ge0}$ the solution to (1), with U_n instead of U. By a classical uniqueness argument (using that ∇U is locally Lipschitz continuous), X and X^n coincide until they reach $B(0,n)^c$. In particular, $X_t = X^n_t$ for all $t \in [0,\tau]$ and, setting

$$\zeta_n = \inf\{t \geq 0 : |X_{\tau+t}| \geq n\} = \inf\{t \geq 0 : |X^n_{\tau+t}| \geq n\},$$

it a.s. holds that $X^n_{\tau+t} = X_{\tau+t}$ for all $t \in [0,\zeta_n]$. Since $\lim_n \zeta_n = \infty$ a.s., we conclude that for all $t \geq 0$, $\lim_n U_n(X^n_{\tau+t}) = U(X_{\tau+t})$ a.s.

As we will check in Step 4,

$$\sup_{n\geq|x_0|+1} \sup_{t\geq 0} \mathbb{E}[U_n(X^n_{\tau+t})] < \infty. \tag{8}$$

By the Fatou lemma, we will conclude that $\sup_{t\geq 0} \mathbb{E}[U(X_{\tau+t})] < \infty$. By the Fatou Lemma again, this will imply that $\mathbb{E}[\liminf_{t\to\infty} U(X_t)] < \infty$. Since $\lim_{|x|\to\infty} U(x) = \infty$ by (A), this will show that $\liminf_{t\to\infty} |X_t| < \infty$ a.s. and thus complete the proof.

Step 4. Here we verify (8). Denote, for $x \in \mathbb{R}^d$ and $\beta > 0$, by $f^{n,x,\beta}_t$ the law at time t of the solution to (1) with $x_0 = x$, with β_0 replaced by β and with U_n instead of U. We then have, since h is the density of $(\tau, X_\tau) = (\tau, X^n_\tau)$,

$$\mathbb{E}[U_n(X^n_{\tau+t})] = \mathbb{E}[\mathbb{E}[U_n(X^n_{\tau+t})|\mathcal{F}_\tau]] = \int_{[0,1]\times B(x_0,1)} h(u,x)\Big[\int_{\mathbb{R}^d} U_n(y) f^{n,x,\beta_u}_t(\mathrm{d}y)\Big]\mathrm{d}u\mathrm{d}x.$$

Consider any probability density $f_0 \in C_c(\mathbb{R}^d)$ such that $f_0 > c\mathbf{1}_{B(x_0,1)}$, for some constant $c > 0$. We thus have $h(u,x) \leq C\mathbf{1}_{\{u\in[0,1],x\in B(x_0,1)\}} \leq (C/c) f_0(x)$, and write

$$\mathbb{E}[U_n(X^n_{\tau+t})] \leq \frac{C}{c} \sup_{u\in[0,1]} \int_{\mathbb{R}^d} f_0(x)\Big[\int_{\mathbb{R}^d} U_n(y) f^{n,x,\beta_u}_t(\mathrm{d}y)\Big]\mathrm{d}x = \frac{C}{c} \sup_{u\in[0,1]} \mathbb{E}[U_n(Y^{n,u}_t)],$$

where $(Y^{n,u}_t)_{t\geq 0}$ is the solution to (1) starting from $X_0 \sim f_0$, with β_0 replaced by β_u and U by U_n. To conclude the step, it only remains to verify that $\sup_{n\geq|x_0|+1} \sup_{u\in[0,1]} \sup_{t\geq 0} \mathbb{E}[U_n(Y^{n,u}_t)] < \infty$.

But Lemmas 5 and 6 tell us that, setting $\kappa_{n,u}(f_0) = \int_{\mathbb{R}^d} f_0(x)\log(1 + f_0(x)e^{\beta_u U_n(x)})\mathrm{d}x$ and $a_n = [\int_{\mathbb{R}^d} e^{-\alpha_0 U_n(x)}\mathrm{d}x]^{-1}$, it holds that

$$\mathbb{E}[U_n(Y^{n,u}_t)] \leq \frac{\kappa_{n,u}(f_0) - \log a_n}{\beta_u - \alpha_0}.$$

This last quantity is uniformly bounded, because

- $\beta_u \geq \beta_0 > \alpha_0$ for all $u \in [0,1]$ (by Step 1);
- $\sup_{n\geq|x_0|+1,u\in[0,1]} \kappa_{n,u}(f_0) < \infty$, since $f_0 \in C_c(\mathbb{R}^d)$, $\beta_u \leq \beta_1$ for all $u \in [0,1]$ and $U_n(x) = U(x)$ for all $x \in \text{Supp } f_0$ if n is large enough;
- $\sup_{n\geq|x_0|+1}(-\log a_n) < \infty$, since $\int_{\mathbb{R}^d} e^{-\alpha_0 U_n(x)}\mathrm{d}x \leq e^{\alpha_0}[\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x + \int_{\mathbb{R}^d} e^{-\alpha_0|x|}\mathrm{d}x] < \infty$, recall that $U_n(x) \geq \min\{U(x), |x|\} - 1$. □

4. Localization and absorption

Here we prove that on the event where $\sup_{t\geq 0} |X_t| < \infty$, the simulated annealing procedure is successful. We also check that each time the process $(X_t)_{t\geq 0}$ comes back in a given compact, it has a large probability to be absorbed forever in a (larger) compact.

Lemma 7. *Assume (A), fix $c > c_*$, $x_0 \in \mathbb{R}^d$ and $\beta_0 > 0$ and consider the solution $(X_t)_{t\geq 0}$ to (1). For any $\varepsilon > 0$,*

$$\lim_{t\to\infty} \mathbb{P}\Big(\sup_{s\geq 0} |X_s| < \infty \text{ and } U(X_t) > \varepsilon\Big) = 0.$$

Proposition 8. *Assume* (A) *and fix* $c > c_*$. *For any* $A \geq 1$, *there is* $b_A > 1$ *and* $K_A > A$ *such that if* $x_0 \in \{U \leq A\}$ *and* $\beta_0 \geq b_A$, *for* $(X_t)_{t\geq 0}$ *the solution to* (1), *we have*

$$\mathbb{P}\Big(\sup_{t\geq 0} U(X_t) \leq K_A\Big) \geq \frac{1}{2}.$$

The rest of the section is dedicated to the proof of these two results. Lemma 7 will easily follow from a result of Holley-Kusuoka-Stroock [7] concerning the compact case.

Concerning Proposition 8, let us recall from Holley-Kusuoka-Stroock [7], see also Miclo [12], that in the compact setting, $\limsup_{t\to\infty} U(X_t) = c$ a.s. and moreover for any $\varepsilon > 0$, if x_0 belongs to a connected component of $\{U \leq c+\varepsilon\}$ containing a global minimum of U, it holds that $\mathbb{P}(\sup_{t\geq 0} U(X_t) \leq c+\varepsilon) > 0$. This immediately extends to the non-compact setting, since the set $\{U \leq c+\varepsilon\}$ is compact. Unfortunately, such a result is not uniform in $\beta_0 > 0$, and we really need a uniform bound, see Step 2 of the proof of Proposition 2 in Section 5. We believe it is not possible to deduce Proposition 8 from [7, 12]. At this end, we have to work hard, following the ideas of [7], taking much less care about many constants and obtaining much less precise results (e.g. it might be possible to control K_A in Proposition 8) but carefuly tracking the dependence in β_0 and x_0.

In the whole section, we assume (A) and work with some fixed $c > c_*$. We introduce some notation.

Notation 9. *Let* $K \geq 1$.

(a) We consider $L_K > 0$ *such that* $\{U \leq K\} \subset [-(L_K-1),(L_K-1)]^d$. *We denote by* M_K *the torus* $[-L_k, L_K)^d$, *that is* $\mathbb{R}^d$ *quotiented by the equivalence relation* $x \sim y$ *if and only if for all* $i = 1,\dots,d$, $(x_i - y_i)/(2L_K) \in \mathbb{Z}$.

(b) We also consider $U_K \in C^\infty(M_K)$ *such that* $\min_{M_K} U_K = 0$, *such that* $U_K(x) = U(x)$ *for all* $x \in \{U \leq K\}$, *and such that*

$$c_*^K = \sup\{E_K(x,y) : x,y \in M_K\} \leq c_*,$$

where $E_K(x,y) = \inf\{\max_{t\in[0,1]} U_K(\gamma_t) - U_K(x) - U_K(y) \;:\; \gamma \in C([0,1],M_K), \gamma_0 = x, \gamma_1 = y\}$.

(c) For $x_0 \in \{U \leq K\} \subset M_K$ *and* $\beta_0 > 0$, *we introduce the inhomogeneous* M_K*-valued diffusion*

$$X_t^K = x_0 + B_t - \frac{1}{2}\int_0^t \beta_s \nabla U_K(X_s^K)\mathrm{d}s \text{ modulo } 2L_K, \tag{9}$$

where $(B_t)_{t\geq 0}$ *is a* d*-dimensional Brownian motion, where* $\beta_t = c^{-1}\log(e^{c\beta_0}+t)$ *as in* (1) *and*

$$\text{for } x = (x_1,\dots,x_d) \in \mathbb{R}^d, \quad x \text{ modulo } 2L_K = \Big(x_i - 2L_K\Big\lfloor \frac{x_i + L_K}{2L_K}\Big\rfloor\Big)_{i=1,\dots,d} \in [-L_K, L_K)^d.$$

For point (b), it suffices to choose a smooth version of $U_K = \min\{U,K\}$, see [2, Step 1 of the proof of Lemma 6]. Since $U_K = U$ on $\{U \leq K\}$ and since U is locally Lipschitz continuous, a simple uniqueness argument shows the following.

Remark 10. *For any* $K \geq 1$, *any* $x_0 \in \{U \leq K\}$, *any* $\beta_0 > 0$, *for* $(X_t)_{t\geq 0}$ *the solution to* (1) *and* $(X_t^K)_{t\geq 0}$ *the solution to* (9), *both driven by the same Brownian motion, it holds that*

$$\Big\{\sup_{t\geq 0} U_K(X_t^K) \leq K\Big\} = \Big\{\sup_{t\geq 0} U_K(X_t^K) \leq K, \sup_{t\geq 0}|X_t^K - X_t| = 0\Big\} = \Big\{\sup_{t\geq 0} U(X_t) \leq K\Big\}.$$

We can now give the

Proof of Lemma 7. By [7, Theorem 2.7] and since $c > c_* \geq c_*^K$, $U_K(X_t^K) \to 0$ in probability, as $t \to \infty$, for each $K \geq 1$. We fix $\eta > 0$. Since $\lim_{|x|\to\infty} U(x) = \infty$, there is $K_\eta > 0$ such that $\mathbb{P}(\sup_{s\geq 0} |X_s| < \infty, \sup_{s\geq 0} U(X_s) > K_\eta) \leq \eta$. We then write, using Remark 10,

$$\begin{aligned}\mathbb{P}\Big(\sup_{s\geq 0}|X_s| < \infty \text{ and } U(X_t) > \varepsilon\Big) \leq& \eta + \mathbb{P}\Big(\sup_{s\geq 0} U(X_s) \leq K_\eta \text{ and } U(X_t) > \varepsilon\Big)\\ =&\eta + \mathbb{P}\Big(\sup_{s\geq 0} U_{K_\eta}(X_s^{K_\eta}) \leq K_\eta \text{ and } U_{K_\eta}(X_t^{K_\eta}) > \varepsilon\Big)\\ \leq&\eta + \mathbb{P}\Big(U_{K_\eta}(X_t^{K_\eta}) > \varepsilon\Big).\end{aligned}$$

We conclude that $\limsup_{t\to\infty} \mathbb{P}(\sup_{s\geq 0} |X_s| < \infty \text{ and } U(X_t) > \varepsilon) \leq \eta$, whence the result since $\eta > 0$ is arbitrarily small. ☐

We next introduce the invariant probability measure of the time-homogeneous version of (9).

Remark 11. *There is a constant $\kappa_0 > 0$ such that, for all $K \geq 1$, all $\beta > 0$, it holds that*

$$\mathcal{Z}_\beta^K := \int_{M_K} \exp(-\beta U_K(x))\mathrm{d}x \geq \kappa_0(\beta+1)^{-d}.$$

We also have $\mathcal{Z}_\beta^K \leq (2L_K)^d$. We introduce the probability density

$$\mu_\beta^K(x) = (\mathcal{Z}_\beta^K)^{-1}\exp(-\beta U_K(x)), \quad x \in M_K.$$

Proof. Since $\min_{\mathbb{R}^d} U = 0$, there is $x_* \in \mathbb{R}^d$ such that $U(x_*) = 0$. Fix $r_* > 0$ such that $B(x_*, r_*) \subset \{U \leq 1\} \subset M_K$. Denote by $C = \sup_{B(x_*,r_*)} |\nabla U|$. For all $K \geq 1$, all $x \in B(x_*, r_*)$, we have that $x \in \{U \leq 1\} \subset M_K$ and $U_K(x) = U(x) \leq C|x - x_*|$. Hence for all $\beta > 0$,

$$\mathcal{Z}_\beta^K \geq \int_{B(x_*,r_*)} \exp(-\beta C|x-x_*|)\mathrm{d}x \geq e^{-1}\mathrm{Vol}(B(x_*, r_* \wedge (1/(C\beta))),$$

from which the lower-bound follows. The upper-bound is trivial. ☐

As a final preliminary, we recall the crucial spectral gap estimate of Holley-Kusuoka-Stroock [7, Theorem 1.14 and Remark 1.16], in the special case of the torus. We use that $c_*^K \leq c_*$, see Notation 9-(b) (in the notation of [7], $m = c_*^K$).

Lemma 12 (Holley-Kusuoka-Stroock)**.** *Fix $K \geq 1$. There is a constant $\gamma_K > 0$ such that for all $\phi \in C^1(M_K)$, for all $\beta > 0$,*

$$\int_{M_K} |\nabla\phi(x)|^2 \mu_\beta^K(x)\mathrm{d}x \geq \lambda_K(\beta)\int_{M_K}\Big(\phi(x) - \int_{M_K}\phi(y)\mu_\beta^K(y)\mathrm{d}y\Big)^2 \mu_\beta^K(x)\mathrm{d}x,$$

with

$$\lambda_K(\beta) = \gamma_K(\beta+1)^{2-5d}\exp(-\beta c_*).$$

The constant γ_K drastically depends on K but, as we will see, this is not an issue.

Lemma 13. *Fix $K \geq 1$. There is a constant $b_K^{(1)} > 0$ such that if $\beta_0 \geq b_K^{(1)}$, then for any density $f_0^K \in C(M_K)$, for f_t^K the density of X_t^K, the solution to (9) starting from $X_0^K \sim f_0^K$,*

$$\forall\, t \geq 0, \quad \int_{M_K} \frac{(f_t^K(x))^2}{\mu_{\beta_t}^K(x)}\mathrm{d}x \leq \max\Big(2, \int_{M_K}\frac{(f_0^K(x))^2}{\mu_{\beta_0}^K(x)}\mathrm{d}x\Big).$$

Proof. The function $(f_t^K(x))_{t\geq 0, x\in M_K}$ is a weak solution to the uniformly parabolic equation $\partial_t f_t^K(x) = \frac{1}{2}\mathrm{div}(\nabla f_t^K(x) + \beta_t f_t^K(x)\nabla U_K(x))$. It can be seen as a periodic solution of the same equation in $\mathbb{R}^d$, with U_K and f_0^K replaced by their periodic continuation. We thus can apply some classical results, see Friedman [4, Chapter 1, Theorems 10 and 12] and conclude that $(f_t^K(x))_{t\geq 0, x\in M_K}$ belongs to $C([0,\infty)\times M_K)\cap C^{1,2}((0,\infty)\times M_K)$. The periodic continuation of f_0^K has an infinite mass, but this is allowed by [4]. Since furthermore M_K is bounded, all the computations below are easily justified.

We introduce

$$\varphi(t) = \int_{M_K} \frac{(f_t^K(x))^2}{\mu_{\beta_t}^K(x)}\mathrm{d}x = \mathcal{Z}_{\beta_t}^K \int_{M_K} (f_t^K(x))^2 e^{\beta_t U_K(x)}\mathrm{d}x.$$

Since $(\mathcal{Z}_{\beta_t}^K)' = -\beta_t' \int_{M_K} U_K(x) e^{-\beta_t U_K(x)}\mathrm{d}x \leq 0$, we have, for all $t > 0$,

$$\varphi'(t) \leq \mathcal{Z}_{\beta_t}^K \int_{M_K} 2[\partial_t f_t^K(x)] f_t^K(x) e^{\beta_t U_K(x)}\mathrm{d}x + \beta_t' \mathcal{Z}_{\beta_t}^K \int_{M_K} U_K(x)(f_t^K(x))^2 e^{\beta_t U_K(x)}\mathrm{d}x.$$

Recalling that $\partial_t f_t^K(x) = \frac{1}{2}\mathrm{div}(\nabla f_t^K(x) + \beta_t f_t^K(x)\nabla U_K(x))$, proceeding to an integration by parts in the first term and to a rough upper-bound in the second one, we find

$$\begin{aligned}\varphi'(t) \leq & -\mathcal{Z}_{\beta_t}^K \int_{M_K} |\nabla f_t^K(x) + \beta_t f_t^K(x)\nabla U_K(x)|^2 e^{\beta_t U_K(x)}\mathrm{d}x + \beta_t' ||U_K||_\infty \varphi(t) \\ = & -\int_{M_K} \Big|\nabla\Big(\frac{f_t^K(x)}{\mu_{\beta_t}^K(x)}\Big)\Big|^2 \mu_{\beta_t}^K(x)\mathrm{d}x + \beta_t' ||U_K||_\infty \varphi(t).\end{aligned}$$

By Lemma 12 with $\phi(x) = f_t^K(x)/\mu_{\beta_t}^K(x)$, for which $\int_{M_K} \phi(y)\mu_{\beta_t}^K(y)\mathrm{d}y = 1$, we conclude that

$$\varphi'(t) \leq -\lambda_K(\beta_t)\int_{M_K} \Big[\frac{f_t^K(x)}{\mu_{\beta_t}^K(x)} - 1\Big]^2 \mu_{\beta_t}^K(x)\mathrm{d}x + \beta_t' ||U_K||_\infty \varphi(t) = -\lambda_K(\beta_t)[\varphi(t) - 1] + \beta_t' ||U_K||_\infty \varphi(t).$$

But we know from Lemma 12 that for all $\beta > 0$,

$$\lambda_K(\beta) \geq \gamma_K(\beta+1)^{2-5d} e^{-\beta c_*} \geq \gamma_K' e^{-\beta(c+c_*)/2}$$

for some other constant $\gamma_K' > 0$, since $c > c_*$. Setting $\alpha = (c - c_*)/(2c) \in (0,1)$, so that $(c + c*)/2 = c(1-\alpha)$, recalling that $\beta_t = \log(e^{c\beta_0} + t)/c$, we conclude that

$$\varphi'(t) \leq -\frac{\gamma_K'}{(e^{c\beta_0}+t)^{1-\alpha}}[\varphi(t) - 1] + \frac{||U_K||_\infty}{c(e^{c\beta_0}+t)}\varphi(t).$$

Let $b_K^{(1)} = \frac{1}{\alpha c}\log(2||U_K||_\infty/(\gamma_K' c))$, so that if $\beta_0 \geq b_K^{(1)}$, for all $t \geq 0$,

$$\frac{||U_K||_\infty}{c(e^{c\beta_0}+t)} \leq \frac{\gamma_K'}{2(e^{c\beta_0}+t)^{1-\alpha}},$$

whence

$$\varphi'(t) \leq -\frac{\gamma_K'}{2(e^{c\beta_0}+t)^{1-\alpha}}[\varphi(t) - 2].$$

We classically conclude that indeed, if $\beta_0 \geq b_K^{(1)}$, then for all $t \geq 0$, $\varphi(t) \leq \max(2, \varphi(0))$. □

From the previous lemma and the Cauchy-Schwarz inequality, we deduce the following.

Lemma 14. *For $A \geq 1$, let $D_A = 2C_A^{(1)} + C_A^{(2)} + 1 + 4c$ and $K_A = D_A + 1$, where $C_A^{(1)}$ was introduced in Lemma 3 and where $C_A^{(2)} = \sup_{x \in \{U \leq A\}} \sup_{y \in B(x,2)} U(y)$. There is a constant $C_A^{(3)} > 0$ such that, if $\beta_0 \geq b_{K_A}^{(1)}$ (see Lemma 13) and $x_0 \in \{U \leq A\}$, it holds that $\sup_{[0,\tau]} U_{K_A}(X_t^{K_A}) \leq D_A$ a.s. and*

$$\forall\, t \geq 0, \quad \mathbb{P}(U_{K_A}(X_{\tau+t}^{K_A}) \geq D_A) \leq \frac{C_A^{(3)}}{(e^{c\beta_0} + t)^2},$$

where $(X_t^{K_A})_{t \geq 0}$ is the solution to (9) starting from x_0 and where τ is the stopping time introduced in Lemma 3 (for the solution $(X_t)_{t\geq 0}$ to (1) driven by the same Brownian motion as $(X_t^{K_A})_{t \geq 0}$).

Proof. We fix $A \geq 1$, $\beta_0 \geq b_{K_A}^{(1)}$ and $x_0 \in \{U \leq A\}$. First, since $B(x_0, 1) \subset \{U \leq D_A\}$ (because $D_A \geq C_A^{(2)}$), since $\sup_{[0,\tau]} |X_t - x_0| \leq 1$ and since $D_A \leq K_A$, Remark 10 tells us that $X_t = X_t^{K_A}$ for all $t \in [0, \tau]$. In particular, $\sup_{[0,\tau]} U_{K_A}(X_t^{K_A}) \leq D_A$ and the law of $(\tau, X_\tau^{K_A}) = (\tau, X_\tau)$ has a density $h(u, x)$ bounded by $e^{C_A^{(1)}(\beta_0+1)} \mathbf{1}_{\{u \in [0,1], x \in B(x_0,1)\}}$, see Lemma 3.

Denote, for $x \in \mathbb{R}^d$ and $\beta > 0$, by $f_t^{K_A,x,\beta}$ the law of the solution of (9) with $K = K_A$, with $x_0 = x$ and with β_0 replaced by β. We then have

$$\begin{aligned}\mathbb{P}(U_{K_A}(X_{\tau+t}^{K_A}) \geq D_A) =& \mathbb{E}[\mathbb{P}(U_{K_A}(X_{\tau+t}^{K_A}) \geq D_A | \mathcal{F}_\tau)] \\ =& \int_{[0,1] \times B(x_0,1)} h(u,x) \Big[\int_{\{U_{K_A} \geq D_A\}} f_t^{K_A,x,\beta_u}(\mathrm{d}y) \Big] \mathrm{d}u \mathrm{d}x.\end{aligned}$$

Consider a probability density $f_0 \in C_c(\mathbb{R}^d)$ such that $(2v_d)^{-1} \mathbf{1}_{B(x_0,1)} \leq f_0 \leq \mathbf{1}_{B(x_0,2)}$, v_d being the volume of the unit ball. We write

$$\begin{aligned}\mathbb{P}(U_{K_A}(X_{\tau+t}^{K_A}) \geq D_A) \leq& 2v_d e^{C_A^{(1)}(\beta_0+1)} \sup_{u \in [0,1]} \int_{\mathbb{R}^d} \Big[\int_{\{U_{K_A} \geq D_A\}} f_t^{K_A,x,\beta_u}(\mathrm{d}y) \Big] f_0(x) \mathrm{d}x \\ =& 2v_d e^{C_A^{(1)}(\beta_0+1)} \sup_{u \in [0,1]} \mathbb{P}(U_{K_A}(Y_t^{A,u}) \geq D_A),\end{aligned} \tag{10}$$

where $(Y_t^{A,u})_{t \geq 0}$ is the solution to (9) with $K = K_A$, starting from $Y_0 \sim f_0$, with β_0 replaced by β_u. We now denote by $f_t^{A,u}$ the density of $Y_t^{A,u}$ and use the Cauchy-Schwarz inequality to write

$$\begin{aligned}\mathbb{P}(U_{K_A}(Y_t^{A,u}) \geq D_A) =& \int_{\{U_{K_A} \geq D_A\}} f_t^{A,u}(x) \mathrm{d}x \\ \leq& \Big(\int_{\{U_{K_A} \geq D_A\}} \mu_{\beta_{t+u}}^{K_A}(x) \mathrm{d}x \Big)^{1/2} \Big(\int_{M_{K_A}} \frac{[f_t^{A,u}(x)]^2 \mathrm{d}x}{\mu_{\beta_{t+u}}^{K_A}(x)} \Big)^{1/2}.\end{aligned} \tag{11}$$

By Lemma 13, we know that, since $\beta_u \geq \beta_0 \geq b_{K_A}^{(1)}$,

$$\int_{M_{K_A}} \frac{[f_t^{A,u}(x)]^2 \mathrm{d}x}{\mu_{\beta_{t+u}}^{K_A}(x)} \leq 2 \vee \int_{M_{K_A}} \frac{[f_0(x)]^2 \mathrm{d}x}{\mu_{\beta_u}^{K_A}(x)} \leq 2 \vee \int_{B(x_0,2)} \frac{\mathrm{d}x}{\mu_{\beta_u}^{K_A}(x)} = 2 \vee \int_{B(x_0,2)} \mathcal{Z}_{\beta_u}^{K_A} e^{\beta_u U(x)} \mathrm{d}x.$$

Recalling the definition of $C_A^{(2)}$ and that $\mathcal{Z}_{\beta_u}^{K_A} \leq (2L_{K_A})^d$, see Remark 11, we find

$$\int_{M_{K_A}} \frac{[f_t^{A,u}(x)]^2 \mathrm{d}x}{\mu_{\beta_{t+u}}^{K_A}(x)} \leq 2 \vee [2^d v_d (2L_{K_A})^d e^{C_A^{(2)} \beta_u}] = 2^d v_d (2L_{K_A})^d e^{C_A^{(2)} \beta_u}. \tag{12}$$

Next, since the volume of M_{K_A} is smaller than $(2L_{K_A})^d$, we have

$$\int_{\{U_{K_A}\geq D_A\}} \mu^{K_A}_{\beta_{t+u}}(x)\mathrm{d}x \leq \frac{(2L_{K_A})^d e^{-\beta_{t+u}D_A}}{\mathcal{Z}^{K_A}_{\beta_{t+u}}}.$$

By Remark 11 again,

$$\int_{\{U_{K_A}\geq D_A\}} \mu^{K_A}_{\beta_{t+u}}(x)\mathrm{d}x \leq \frac{(2L_{K_A})^d(\beta_{t+u}+1)^d e^{-\beta_{t+u}D_A}}{\kappa_0} \leq C_A e^{-\beta_{t+u}(D_A-1)}, \tag{13}$$

for some constant $C_A > 0$ of which we now allow the value to change from line to line. Gathering (10)-(11)-(12)-(13), we find

$$\mathbb{P}(U_{K_A}(X^{K_A}_{\tau+t}) \geq D_A) \leq C_A e^{C^{(1)}_A(\beta_0+1)} \sup_{u\in[0,1]} e^{-\beta_{t+u}(D_A-1)/2+C^{(2)}_A\beta_u/2}.$$

Since $s\mapsto\beta_s$ is non-decreasing and $D_A-1 > C^{(2)}_A$,

$$\mathbb{P}(U_{K_A}(X^{K_A}_{\tau+t}) \geq D_A) \leq C_A e^{C^{(1)}_A\beta_t} \sup_{u\in[0,1]} e^{-\beta_{t+u}(D_A-1-C^{(2)}_A)/2} \leq C_A e^{-\beta_t(D_A-1-C^{(2)}_A-2C^{(1)}_A)/2}.$$

Recalling finally that $D_A = 2C^{(1)}_A + C^{(2)}_A + 1 + 4c$ and that $\beta_t = c^{-1}\log(e^{c\beta_0}+t)$, we conclude that

$$\mathbb{P}(U_{K_A}(X^{K_A}_{\tau+t}) \geq D_A) \leq C_A e^{-2c\beta_t} = \frac{C_A}{(e^{c\beta_0}+t)^2}$$

as desired. □

We finally give the

Proof of Proposition 8. We fix $A\geq 1$ and introduce D_A, $K_A = D_A+1$, $b^{(1)}_{K_A}$ and $C^{(3)}_A$ as in Lemma 14. We will show that one can find $b_A > b^{(1)}_{K_A}$ such that if $\beta_0 > b_A$ and $x_0\in\{U\leq A\}$, the solution $(X^{K_A}_t)_{t\geq 0}$ to (9) satisfies

$$\mathbb{P}\Big(\sup_{t\geq 0} U_{K_A}(X^{K_A}_t) \leq K_A\Big) \geq \frac{1}{2}.$$

By Remark 10, this will show the result. By Lemma 14, we have $\sup_{[0,\tau]} U_{K_A}(X^{K_A}_t) \leq D_A \leq K_A$ a.s., so that we only have to check that

$$\mathbb{P}\Big(\sup_{t\geq 0} U_{K_A}(X^{K_A}_{\tau+t}) \leq K_A\Big) \geq \frac{1}{2}.$$

We consider $\phi_A\in C^\infty(\mathbb{R}_+)$, with values in $[0,1]$, such that $\phi_A = 0$ outside $[D_A,K_A]$ and such that $\phi_A((D_A+K_A)/2) = 1$, and we introduce $\psi_A = \phi_A\circ U_{K_A} : M_{K_A}\to[0,1]$. Setting

$$\mathcal{L}^A_{\beta_t}\psi_A(x) = \frac{1}{2}(\Delta\psi_A(x) - \beta_t\nabla\psi_A(x)\cdot\nabla U_{K_A}(x)),$$

we have $|\mathcal{L}^A_{\beta_t}\psi_A(x)| \leq C^{(4)}_A(1+\beta_t)\mathbf{1}_{\{U_{K_A}(x)\geq D_A\}}$, where $C^{(4)}_A$ is a constant involving the supremum on M_{K_A} of U_{K_A} and its two first derivatives.

We now fix $b_A > b^{(1)}_{K_A}$ such that for all $\beta_0\geq b_A$,

$$\int_0^\infty \frac{C^{(3)}_A C^{(4)}_A[1+\log(e^{c\beta_0}+t+1)]}{c(e^{c\beta_0}+t)^2}\mathrm{d}t = \int_{e^{c\beta_0}}^\infty \frac{C^{(3)}_A C^{(4)}_A[1+\log(s+1)]}{cs^2}\mathrm{d}s \leq \frac{1}{40}.$$

By Itô's formula and since $\psi_A(X^{K_A}_\tau)=0$ (because $U_{K_A}(X^{K_A}_\tau)\le D_A$),

$$\psi_A(X^{K_A}_{\tau+t})=M_t+R_t,$$

where $(M_t)_{t\ge 0}$ is a martingale issued from 0 and where

$$R_t=\int_0^t \mathcal{L}^A_{\beta_{\tau+s}}\psi_A(X^{K_A}_{\tau+s})\mathrm{d}s.$$

By Lemma 14, since $|\mathcal{L}^A_{\beta_{\tau+t}}\psi_A(x)|\le C^{(4)}_A(1+\beta_{t+1})\mathbf{1}_{\{U_{K_A}(x)\ge D_A\}}$ and since $\beta_0\ge b_A\ge b^{(1)}_{K_A}$,

$$\mathbb{E}\Big[\sup_{t\ge 0}|R_t|\Big]\le C^{(4)}_A\int_0^\infty(1+\beta_{t+1})\mathbb{P}(U_{K_A}(X^{K_A}_{\tau+t})\ge D_A)\mathrm{d}t\le\int_0^\infty\frac{C^{(3)}_AC^{(4)}_A(1+\beta_{t+1})}{(e^{c\beta_0}+t)^2}\mathrm{d}t\le\frac{1}{40}.$$

Consequently, for $E=\{\sup_{t\ge0}|R_t|<1/10\}$, we have $\mathbb{P}(E^c)\le 1/4$.

On E, we have $M_t=M_{t\wedge\sigma}$, where $\sigma=\inf\{t\ge0:M_t\notin[-1/10,11/10]\}$, because $M_t+R_t=\psi_A(X^{K_A}_{\tau+t})$ takes values in $[0,1]$. On $\{\sup_{t\ge0}U_{K_A}(X^{K_A}_{\tau+t})\ge K_A\}$, the process $\psi_A(X^{K_A}_{\tau+t})$ must up-cross $[0,1]$ at least once, so that on $E\cap\{\sup_{t\ge0}U_{K_A}(X^{K_A}_{\tau+t})\ge K_A\}$, the martingale $M_t=M_{t\wedge\sigma}$ must up-cross $[1/10,9/10]$ at least once. Hence

$$\mathbb{P}\Big(\sup_{t\ge0}U_{K_A}(X^{K_A}_{\tau+t})\ge K_A\Big)\le\mathbb{P}(E^c)+\mathbb{P}(E,(M_{t\wedge\sigma})_{t\ge0}\text{ up-crosses }[1/10,9/10])\le 1/4+p,$$

where $p=\mathbb{P}((M_{t\wedge\sigma})_{t\ge0}\text{ up-crosses }[1/10,9/10])$.

By Doob's up-crossing inequality, see e.g. Revuz-Yor [13, Proposition 2.1 page 61] we know that, for any continuous martingale $(Z_t)_{t\ge0}$, any $a<b$, denoting by $U_{T,a,b}$ the number of up-crossings of $[a,b]$ by $(Z_t)_{t\ge0}$ during $[0,T]$, it holds that $(b-a)\mathbb{E}[U_{T,a,b}]\le\mathbb{E}[(Z_T-a)_-]$.

Thus for N_T the number of up-crossings of $[1/10,9/10]$ by the martingale $(M_{t\wedge\sigma})_{t\ge0}$ during $[0,T]$, it holds that

$$p=\lim_{T\to\infty}\mathbb{P}(N_T\ge1)\le\lim_{T\to\infty}\mathbb{E}[N_T]\le\lim_{T\to\infty}\frac{\mathbb{E}[(M_{T\wedge\sigma}-1/10)_-]}{8/10}\le\frac{2/10}{8/10}=\frac{1}{4}.$$

We used that $M_{T\wedge\sigma}\ge-1/10$ by definition of σ. We conclude that, for all $\beta>b_A$, we have $\mathbb{P}(\sup_{t\ge0}U_{K_A}(X^{K_A}_{\tau+t})\ge K_A)\le 1/2$ as desired. ☐

5. Success of the simulated annealing

We now show that no escape in large time implies the success of the simulated annealing.

Proof of Proposition 2. We assume (A), fix $c>c_*$, $x_0\in\mathbb{R}^d$, $\beta_0>0$ and consider the solution $(X_t)_{t\ge0}$ to (1). Since $\lim_{|x|\to\infty}U(x)=\infty$, our goal is to show that for any fixed $\varepsilon>0$,

$$\lim_{t\to\infty}\mathbb{P}\Big(\liminf_{s\to\infty}U(X_s)<\infty\text{ and }U(X_t)>\varepsilon\Big)=0.$$

Step 1. It suffices to show that for each $A\ge1$, setting

$$\Omega_A=\{\liminf_{s\to\infty}U(X_s)<A\},$$

it holds that $\Omega_A \subset \{\sup_{s\geq 0}|X_s|<\infty\}$. Indeed, if this hold true, we fix $\eta>0$, consider $A_\eta>0$ large enough so that $\mathbb{P}(A_\eta \leq \liminf_{s\to\infty} U(X_s)<\infty)<\eta$ and write

$$\mathbb{P}\Big(\liminf_{s\to\infty} U(X_s)<\infty \text{ and } U(X_t)>\varepsilon\Big) \leq \eta + \mathbb{P}(\Omega_{A_\eta} \text{ and } U(X_t)>\varepsilon) \leq \eta + \mathbb{P}\Big(\sup_{s\geq 0}|X_s|<\infty \text{ and } U(X_t)>\varepsilon\Big).$$

Thus $\limsup_{t\to\infty}\mathbb{P}(\liminf_{s\to\infty} U(X_s)<\infty \text{ and } U(X_t)>\varepsilon)\leq \eta$ by Lemma 7. Since $\eta>0$ is arbitrarily small, the conclusion follows.

Step 2. We fix $A\geq 1$ and show that for $\Omega_A=\{\liminf_{s\to\infty} U(X_s)<A\}$, we have $\Omega_A\subset\{\sup_{s\geq 0}|X_s|<\infty\}$.

We introduce $b_A>1$ and $K_A>A$ as in Proposition 8 and consider $t_A\geq 0$ large enough so that $\beta_{t_A}\geq b_A$. We set $S_0=t_A$ and, for all $k\geq 1$,

$$T_k=\inf\{t>S_{k-1}: U(X_t)\leq A\} \quad \text{and} \quad S_k=\inf\{t>T_k: U(X_t)\geq K_A\},$$

with the convention that $\inf\emptyset=\infty$.

We start from

$$\mathbb{P}(S_{k+1}<\infty|S_k<\infty) = \mathbb{P}(T_{k+1}<\infty, S_{k+1}<\infty|S_k<\infty) = \mathbb{E}\Big[\mathbf{1}_{\{T_{k+1}<\infty\}}\mathbb{P}(S_{k+1}<\infty|\mathcal{F}_{T_{k+1}})\Big|S_k<\infty\Big].$$

But on $\{T_{k+1}<\infty\}$ and conditionally on $\mathcal{F}_{T_{k+1}}$, $(X_{T_{k+1}+t})_{t\geq 0}$ is a solution to (1), starting from $X_{T_{k+1}}\in\{U\leq A\}$, with β_0 replaced by $\beta_{T_{k+1}}\geq\beta_{t_A}\geq b_A$. Hence, using Proposition 8, a.s.,

$$\mathbf{1}_{\{T_{k+1}<\infty\}}\mathbb{P}(S_{k+1}<\infty|\mathcal{F}_{T_{k+1}}) = \mathbf{1}_{\{T_{k+1}<\infty\}}\mathbb{P}\Big(\sup_{t\geq 0} U(X_{T_{k+1}+t})\geq K_A\Big)\leq 1/2.$$

All this shows that for all $k\geq 1$, $\mathbb{P}(S_{k+1}<\infty|S_k<\infty)\leq 1/2$.

Consequently, there a.s. exists $k\geq 1$ such that $S_k=\infty$, and we introduce

$$k_0=\inf\{k\geq 1: S_k=\infty\}.$$

We then have $S_{k_0-1}<\infty=S_{k_0}$. By definition of Ω_A, it holds that $T_{k_0}<\infty$ on Ω_A. Since $U(X_t)<K_A$ for all $t\in[T_{k_0},S_{k_0})=[T_{k_0},\infty)$ (on Ω_A), this implies that

$$\Omega_A\subset\Big\{\limsup_{s\to\infty} U(X_s)\leq K_A\Big\}\subset\Big\{\sup_{s\geq 0}|X_s|<\infty\Big\}$$

as desired. □

We conclude the section with the

Proof of Theorem 1. We assume (A) and that there is $\alpha_0>0$ such that $\int_{\mathbb{R}^d} e^{-\alpha_0 U(x)}\mathrm{d}x<\infty$. We fix $c>0$, $x_0\in\mathbb{R}^d$, $\beta_0>0$ and consider the unique solution $(X_t)_{t\geq 0}$ to (1). By Proposition 4, $\liminf_{t\to\infty}|X_t|<\infty$ a.s. If moreover $c>c_*$, $\lim_{t\to\infty} U(X_t)=0$ in probability by Proposition 2. □

6. Appendix: non-explosion

It remains to study the non-explosion of our process. Surprisingly, this is rather tedious, except if assuming some Lyapunov condition, for example that $-x\cdot\nabla U(x)\leq C(1+|x|^2)$, which forbids too nasty oscillations. We will prove the following result, which is much stronger (but more natural) than what we really need, since $U\geq 0$ under (A).

Theorem 15. *Assume that $U : \mathbb{R}^d \to \mathbb{R}$ and $\beta : \mathbb{R}_+ \to (0,\infty)$ are of class C^∞. Fix $x_0 \in \mathbb{R}^d$ and consider the pathwise unique maximal solution $(X_t)_{t\in[0,\zeta)}$ to*

$$X_t = x_0 + B_t - \frac{1}{2}\int_0^t \beta_s \nabla U(X_s)\mathrm{d}s, \tag{14}$$

where $\zeta = \lim_n \zeta_n$, with $\zeta_n = \inf\{t \geq 0 : |X_t| \geq n\}$. Assume that

$$\text{there is } L > 0 \text{ such that for all } x \in \mathbb{R}^d,\ U(x) \geq -L(1+|x|^2). \tag{15}$$

Then it holds that $\zeta = \infty$ a.s.

Since ∇U is locally Lipschitz continuous, the existence of a pathwise unique possibly exploding solution is classical. This result is rather natural: as is well-known, the solution to (14), with $U(x) = -(1+|x|^2)^\alpha$ explodes if and only if $\alpha > 1$. The difficulty relies in the fact that we do not want to assume any local property on ∇U. Let us mention that the proof below, assuming that $U \geq 0$, would be slightly simpler but less transparent.

Our proof is inspired by methods found in Ichihara [9], who uses Dirichlet forms, and Grigor'yan [5] and [6, Section 9], who studies manifold-valued diffusions. Both deal with the time-homogeneous case ($\beta_t = \beta_0$ for all $t \geq 0$). In [6], non-explosion is proved under some very weak conditions (allowing e.g. for some additional logarithmic factors in (15)), while [9] is more stringent (roughly, he treats only the case where $U(x) \geq -L(1+|x|)$).

We start with the following remark.

Remark 16. *(i) To prove Theorem 15, one may assume additionally that*

$$\text{there is } t_0 > 0 \text{ such that } \beta_t = \beta_{t_0} \text{ for all } t \geq t_0. \tag{16}$$

(ii) For any $x_0 \in \mathbb{R}^d$, for $(X_t)_{t\in[0,\zeta)}$ the solution to (14) and for $t > 0$, the measure f_t defined by $f_t(A) = \mathbb{P}(\zeta > t, X_t \in A)$ is absolutely continuous with respect to the Lebesgue measure on $\mathbb{R}^d$.

(iii) It suffices to prove Theorem 15 for a.e. $x_0 \in \mathbb{R}^d$.

Proof. (i) Assume that Theorem 15 holds under the additional condition (16) and consider $\beta : \mathbb{R}_+ \to (0,\infty)$ of class C^∞. We fix $T > 0$, introduce $\bar\beta : \mathbb{R}_+ \to (0,\infty)$ of class C^∞ satisfying (16), such that $\beta_t = \bar\beta_t$ on $[0,T]$ and we introduce the corresponding solution $(\bar X_t)_{t\in[0,\bar\zeta)}$. We have $(X_t)_{t\in[0,T\wedge\zeta)} = (\bar X_t)_{t\in[0,T\wedge\bar\zeta)}$, whence in particular $\{\zeta \leq T\} = \{\bar\zeta \leq T\}$. Since $\bar\zeta = \infty$ a.s., we conclude that $\mathbb{P}(\zeta \leq T) = 0$. Since T is arbitrarily large, this implies that $\zeta = \infty$ a.s.

(ii) Fix a Lebesgue-null set $A \in \mathbb{R}^d$. Since ∇U is bounded on compact sets, we deduce from the Girsanov theorem that $\mathbb{P}(\zeta_n > t, X_t \in A) = 0$ for all $n \geq 1$. By monotone convergence, we conclude that $\mathbb{P}(\zeta > t, X_t \in A) = 0$ as desired.

(iii) Assume that for any $\beta : \mathbb{R}_+ \to (0,\infty)$ of class C^∞, $\mathbb{P}_{0,x}(\zeta < \infty) = 0$ for a.e. $x \in \mathbb{R}^d$. Then for a given $\beta : \mathbb{R}_+ \to (0,\infty)$ of class C^∞, for all $t \geq 0$, $\mathbb{P}_{t,x}(\zeta < \infty) = 0$ for a.e. $x \in \mathbb{R}^d$. Since $\zeta > 0$ a.s. by continuity, we may write, for all $x_0 \in \mathbb{R}^d$,

$$\mathbb{P}_{0,x_0}(\zeta < \infty) = \lim_{t\to 0} \mathbb{P}_{0,x_0}(t < \zeta < \infty) = \lim_{t\to 0} \mathbb{E}_{0,x_0}[\mathbf{1}_{\{\zeta > t\}}\mathbb{P}_{t,X_t}(\zeta < \infty)] = 0.$$

We used the Markov property and that $\mathbf{1}_{\{\zeta>t\}}\mathbb{P}_{t,X_t}(\zeta < \infty) = 0$ a.s. when $t > 0$ by point (ii) and since $\mathbb{P}_{t,x}(\zeta < \infty) = 0$ for a.e. $x \in \mathbb{R}^d$. ☐

Above and in the whole section, we denote by $\mathbb{E}_{t_0,x_0}$ the expectation concerning the process starting from $x_0 \in \mathbb{R}^d$ at time $t_0 \geq 0$: under $\mathbb{E}_{t_0,x_0}$, the process $(X_t)_{t\geq 0}$ solves (in law) the S.D.E. $X_t = x_0 + B_t - \frac{1}{2}\int_0^t \beta_{t_0+s}\nabla U(X_s)\mathrm{d}s$.

In the whole section, we denote by v_d the volume of the unit ball and, for $r > 0$, we set

$$B_r = \{x \in \mathbb{R}^d : |x| < r\}, \quad \bar{B}_r = \{x \in \mathbb{R}^d : |x| \le r\} \quad \text{and} \quad \partial B_r = \{x \in \mathbb{R}^d : |x| = r\}.$$

We will study of the following Kolmogorov backward equation, which consists of a particular case of the Feynman-Kac formula.

Lemma 17. *Adopt the assumptions of Theorem 15 and suppose* (16). *Fix $n \ge 1$ and $\alpha > 0$. There is a function $u_{n,\alpha} \in C^{1,2}(\mathbb{R}_+ \times \bar{B}_n)$ such that $u_{n,\alpha} = 1$ on $\mathbb{R}_+ \times \partial B_n$ and*

$$\partial_t u_{n,\alpha}(t,x) + \mathcal{L}_{\beta_t} u_{n,\alpha}(t,x) = \alpha u_{n,\alpha}(t,x) \quad \text{for } (t,x) \in [0,\infty) \times B_n. \tag{17}$$

For $\varphi : \mathbb{R}^d \to \mathbb{R}$ of class C^2, $\beta > 0$ and $x \in \mathbb{R}^d$, we have set

$$\mathcal{L}_\beta \varphi(x) = \frac{1}{2}[\Delta\varphi(x) - \beta \nabla U(x) \cdot \nabla \varphi(x)].$$

For any $t \ge 0$, any $x \in \bar{B}_n$, it holds that $u_{n,\alpha}(t,x) = \mathbb{E}_{t,x}[\exp(-\alpha\zeta_n)]$.

Proof. This relies one more time on classical results found in Friedman [4]. We fix some $t_0 \ge 0$ such that $\beta_t = \beta_{t_0}$ for all $t \ge t_0$. All the coefficients of (17) are smooth and bounded, since restricted to $\bar{B}_n$, whose boundary is smooth. Hence all the results cited below do indeed apply.

By [4, Chapter 3, Theorem 19], there exists a solution $v_{n,\alpha} \in C^2(\bar{B}_n)$ to the elliptic boundary problem $\mathcal{L}_{\beta_{t_0}} v_{n,\alpha} = \alpha v_{n,\alpha}$ on B_n and $v_{n,\alpha} = 1$ on ∂B_n.

By [4, Chapter 3, Theorem 7] (after time-reversing), there exists a solution $w_{n,\alpha}$ belonging to $C^{1,2}([0,t_0] \times \bar{B}_n)$ to the parabolic problem $\partial_t w_{n,\alpha} + \mathcal{L}_{\beta_t} w_{n,\alpha} = \alpha w_{n,\alpha}$ on $(0,t_0) \times B_n$, with boundary condition $w_{n,\alpha} = 1$ on $[0,t_0] \times \partial B_n$ and terminal condition $w_{n,\alpha}(t_0,x) = v_{n,\alpha}(x)$ on B_n.

The function $u_{n,\alpha}$ defined by $u_{n,\alpha}(t,x) = v_{n,\alpha}(x)$ if $t \ge t_0$ and $u_{n,\alpha}(t,x) = w_{n,\alpha}(t,x)$ if $t \in [0,t_0]$ satisfies the conditions of the statement.

Finally, using the Itô formula and (17), one checks that for all $t \ge 0$, all $x \in B_n$, all $T \ge 0$,

$$\mathbb{E}_{t,x}[u_{n,\alpha}(T \wedge \zeta_n, X_{T\wedge\zeta_n}) e^{-\alpha(T\wedge\zeta_n)}] = u_{n,\alpha}(t,x).$$

We let $T \to \infty$ and find that $\mathbb{E}_{t,x}[e^{-\alpha\zeta_n}] = u_{n,\alpha}(t,x)$ by dominated convergence and since $u_{n,\alpha}(\zeta_n, X_{\zeta_n}) = 1$ a.s. ☐

Remark 18. *By the Green formula, for all $\beta > 0$, for all $r > 0$, for all $\varphi : \bar{B}_r \to \mathbb{R}$ of class C^1 and $\psi : \bar{B}_r \to \mathbb{R}$ of class C^2,*

$$2\int_{B_r} \varphi(x)\mathcal{L}_\beta\psi(x)e^{-\beta U(x)}\mathrm{d}x = -\int_{B_r} \nabla\varphi(x)\cdot\nabla\psi(x)e^{-\beta U(x)}\mathrm{d}x + \int_{\partial B_r} \varphi(x)[\nabla\psi(x)\cdot\nu(x)]e^{-\beta U(x)}\mathrm{d}S,$$

where $\nu(x) = x/|x|$ is the unit vector normal to ∂B_r and where $\mathrm{d}S$ is its surface element.

Although this is already known, see Grigor'yan [6, Section 9], we recall for the sake of completeness how to treat the homogeneous case. We use an approach closer to the one of Ichihara [9], who however assumes more than (15) and whose proof is more intricate and relies on the study of $v(x) = \mathbb{E}_x[e^{-\sigma_1}]$, where $\sigma_1 = \inf\{t \ge 0 : |X_t| \le 1\}$.

Proposition 19. *Assume that $U : \mathbb{R}^d \to \mathbb{R}$ is C^∞ and satisfies* (15). *If $\beta_t = \beta_0 > 0$ for all $t \ge 0$, then $\mathbb{P}_x(\zeta < \infty) = 0$ for a.e. $x \in \mathbb{R}^d$.*

Proof. For $\alpha > 0$ and $n \geq 1$, we set $u_\alpha(x) = \mathbb{E}_x[e^{-\alpha\zeta}]$ and $u_{n,\alpha}(x) = \mathbb{E}_x[e^{-\alpha\zeta_n}]$. We divide the proof into 2 steps. We recall that L is defined in (15).

Step 1. Here we prove that for all $r > 0$, there is a constant $C_r > 0$ such that

$$\forall \alpha > 0, \quad \int_{B_r} u_\alpha^2(x) e^{-\beta_0 U(x)} \mathrm{d}x \leq C_r e^{-\alpha/(2\beta_0 L)}. \tag{18}$$

By Proposition 17, $u_{n,\alpha} \in C^2(\bar{B}_n)$, $u_{n,\alpha} = 1$ on ∂B_n and $\mathcal{L}_{\beta_0} u_{n,\alpha} = \alpha u_{n,\alpha}$ on B_n. For any $r \in (0, n]$, we have

$$\begin{aligned}\Phi_{n,\alpha}(r) :=& \int_{B_r} (2\alpha u_{n,\alpha}^2(x) + |\nabla u_{n,\alpha}(x)|^2) e^{-\beta_0 U(x)} \mathrm{d}x \\ =& \int_{\partial B_r} u_{n,\alpha}(x)[\nabla u_{n,\alpha}(x) \cdot \nu(x)] e^{-\beta_0 U(x)} \mathrm{d}S.\end{aligned}$$

Indeed, it suffices to write $2\alpha u_{n,\alpha}^2 = 2u_{n,\alpha}\mathcal{L}_{\beta_0} u_{n,\alpha}$ and to use Remark 18 with $\varphi = \psi = u_{n,\alpha}$. Hence for all $r \in (0, n]$, since $2\alpha a^2 + b^2 \geq 2\sqrt{2\alpha}ab$,

$$\begin{aligned}\Phi'_{n,\alpha}(r) =& \int_{\partial B_r} (2\alpha u_{n,\alpha}^2(x) + |\nabla u_{n,\alpha}(x)|^2) e^{-\beta_0 U(x)} \mathrm{d}S \\ \geq& 2\sqrt{2\alpha} \int_{\partial B_r} u_{n,\alpha}(x)|\nabla u_{n,\alpha}(x)| e^{-\beta_0 U(x)} \mathrm{d}S \geq 2\sqrt{2\alpha}\Phi_{n,\alpha}(r).\end{aligned}$$

Thus $\Phi_{n,\alpha}(r) \leq \Phi_{n,\alpha}(n) e^{2\sqrt{2\alpha}(r-n)}$ for all $r \in (0, n]$.

But, writing $2\alpha u_{n,\alpha} = 2\mathcal{L}_{\beta_0} u_{n,\alpha}$ and using Remark 18 with $\varphi = 1$ and $\psi = u_{n,\alpha}$,

$$2\int_{B_n} \alpha u_{n,\alpha}(x) e^{-\beta_0 U(x)} \mathrm{d}x = \int_{\partial B_n} [\nabla u_{n,\alpha}(x) \cdot \nu(x)] e^{-\beta_0 U(x)} \mathrm{d}S = \Phi_{n,\alpha}(n),$$

because $u_{n,\alpha} = 1$ on ∂B_n. Hence $\Phi_{n,\alpha}(n) \leq 2\alpha \int_{B_n} e^{-\beta_0 U(x)} \mathrm{d}x \leq 2\alpha v_d n^d e^{\beta_0 L(1+n^2)}$ by (15). All this shows that for all $\alpha > 0$, all $n \geq 1$, all $r \in (0, n]$,

$$\int_{B_r} u_{n,\alpha}^2(x) e^{-\beta_0 U(x)} \mathrm{d}x \leq \frac{1}{2\alpha}\Phi_{n,\alpha}(r) \leq v_d n^d e^{\beta_0 L(1+n^2)} e^{2\sqrt{2\alpha}(r-n)}.$$

But $u_\alpha(x) \leq u_{n,\alpha}(x)$ for all $n \geq 1$, all $x \in \mathbb{R}^d$. Hence for $r > 0$ fixed, with the choice $n = r + \sqrt{\alpha}/(\beta_0 L)$, we conclude that, for some constant $C_r > 0$ depending on r (and on L and d),

$$\int_{B_r} u_\alpha^2(x) e^{-\beta_0 U(x)} \mathrm{d}x \leq v_d (r + \sqrt{\alpha}/(\beta_0 L))^d e^{\beta_0 L(1+2r^2)+2\alpha/(\beta_0 L)} e^{-2\sqrt{2}\alpha/(\beta_0 L)} \leq C_r e^{-\alpha/(2\beta_0 L)}.$$

Step 2. We now conclude. Assume by contradiction that $\int_{\mathbb{R}^d} \mathbb{P}_x(\zeta < \infty) \mathrm{d}x > 0$ and fix $\eta > 0$.

It holds that $\int_{\mathbb{R}^d} \mathbb{P}_x(\zeta \leq \eta) \mathrm{d}x > 0$. Else we would have, by the Markov property,

$$\int_{\mathbb{R}^d} \mathbb{P}_x(\zeta \leq 2\eta) \mathrm{d}x = \int_{\mathbb{R}^d} \mathbb{P}_x(\eta < \zeta \leq 2\eta) \mathrm{d}x = \int_{\mathbb{R}^d} \mathbb{E}_x[\mathbf{1}_{\{\zeta > \eta\}} \mathbb{P}_{X_\eta}(\zeta \leq \eta)] \mathrm{d}x = 0$$

thanks to Remark 16-(ii). Iterating the argument, we would find that $\int_{\mathbb{R}^d} \mathbb{P}_x(\zeta \leq K\eta) \mathrm{d}x = 0$ for all $K \geq 1$, whence $\int_{\mathbb{R}^d} \mathbb{P}_x(\zeta < \infty) \mathrm{d}x = 0$.

Consequently, we can find $r_0 > 0$ such that $q := \int_{B_{r_0}} [\mathbb{P}_x(\zeta \le \eta)]^2 e^{-\beta_0 U(x)} \mathrm{d}x > 0$. We then have, since $u_\alpha(x) = \mathbb{E}_x[e^{-\alpha\zeta}] \ge e^{-\alpha\eta}\mathbb{P}_x(\zeta \le \eta)$,

$$\forall \alpha > 0, \quad \int_{B_{r_0}} u_\alpha^2(x) e^{-\beta_0 U(x)} \mathrm{d}x \ge q e^{-2\alpha\eta}.$$

With the choice $\eta = 1/(8\beta_0 L)$, this contradicts (18). □

Using in particular some clever ideas found in Grigor'yan [6, Section 9], who studies, in the homogeneous case, the P.D.E. satisfied by $w(t,x) = \mathbb{P}_x[\zeta < t]$, we can now give the

Proof of Theorem 15. We consider $U : \mathbb{R}^d \to \mathbb{R}$ and $\beta : \mathbb{R}_+ \to (0,\infty)$ of class C^∞. We recall that $\zeta = \lim_n \zeta_n$, with $\zeta_n = \inf\{t \ge 0 : |X_t| \ge n\}$. We set $u_n(t,x) = \mathbb{E}_{t,x}[e^{-\zeta_n}]$ and $u(t,x) = \mathbb{E}_{t,x}[e^{-\zeta}]$, omitting the subscript α since we now always work with $\alpha = 1$. By Remark 16, we may moreover suppose that there is $t_0 > 0$ such that $\beta_t = \beta_{t_0}$ for all $t \ge t_0$, and it suffices to prove that $u(0,x) = 0$ for a.e. $x \in \mathbb{R}^d$. Since $u(t_0,x) = 0$ for a.e. $x \in \mathbb{R}^d$ by Proposition 19, it is sufficient to prove that

$$\exists \delta_0 > 0, \forall t_1 \in [0,t_0], \Big\{ \int_{\mathbb{R}^d} u(t_1,x)\mathrm{d}x = 0 \Big\} \Rightarrow \Big\{ \forall t \in [(t_1-\delta_0)\vee 0, t_1], \int_{\mathbb{R}^d} u(t,x)\mathrm{d}x = 0 \Big\}. \tag{19}$$

Step 1. Here we check that for all $a \in [0,1]$, all $b \ge 0$, all $\varepsilon > 0$, all $\eta > 0$,

$$ab \le \frac{a}{\eta\varepsilon} + \frac{e^{\eta b - 1/\varepsilon}}{\eta}.$$

We fix $a \in [0,1]$, $\varepsilon > 0$, and $\eta > 0$ and study $f(b) = \frac{a}{\varepsilon} + e^{\eta b - 1/\varepsilon} - \eta ab$. We have $f(0) > 0$, $f(\infty) = \infty$ and $f'(b) = \eta[e^{\eta b - 1/\varepsilon} - a]$. If $a \le e^{-1/\varepsilon}$, then f is non-decreasing, so that f is nonnegative on $\mathbb{R}_+$. If now $a > e^{-1/\varepsilon}$, then f attains its minimum at $b_0 = \frac{1}{\eta}[\log a + \frac{1}{\varepsilon}]$ and $f(b_0) = a - a\log a > 0$.

Step 2. Here we prove that are some constants $\delta > 0$ and $\kappa_0 > 0$ such that for all $t_1 \in [0,t_0]$, all $R > 1$, there is a C^1 function $\alpha_{t_1,R} : [(t_1-\delta)\vee 0, t_1] \times \mathbb{R}^d \to [0,1]$ enjoying the properties that

$$\alpha_{t_1,R} = 1 \text{ on } [(t_1-\delta)\vee 0, t_1] \times B_R, \qquad \alpha_{t_1,R} = 0 \text{ on } [(t_1-\delta)\vee 0, t_1] \times B_{4R}^c$$

and, for all $t \in [(t_1-\delta)\vee 0, t_1]$,

$$m_{t_1,R}(t) := \int_{\mathbb{R}^d} \Big(|\nabla \alpha_{t_1,R}(t,x)|^2 - \partial_t[\alpha_{t_1,R}^2(t,x)] \Big)_+ e^{-\beta_t U(x)} \mathrm{d}x \le \kappa_0 e^{-R^2}.$$

We start with a C^∞-function $\eta_R : \mathbb{R}^d \to [0,1]$ such that $\eta_R = 1$ on B_{2R}, $\eta_R = 0$ on B_{4R}^c and $|\nabla \eta_R| \le 1/R$.

We also introduce the C^1 function on $[(t_1-\delta)\vee 0, t_1] \times \mathbb{R}^d$ defined by

$$\xi_{t_1,R}(t,x) = \frac{(|x|-R)_+^2}{2(2\delta + t - t_1)},$$

which equals 0 on $[(t_1-\delta)\vee 0, t_1] \times B_R$ and solves $\partial_t \xi_{t_1,R} + \frac{1}{2}|\nabla \xi_{t_1,R}|^2 = 0$ on $[(t_1-\delta)\vee 0, t_1] \times B_R^c$.

If $\delta > 0$ is small enough, the function $\alpha_{t_1,R}(t,x) = \eta_R(x)\exp(-\xi_{t_1,R}(t,x)/2)$ enjoys the desired properties: it is C^1, $[0,1]$-valued, we have $\alpha_{t_1,R}(t,x) = 1$ if $|x| \le R$ and $\alpha_R(t,x) = 0$ if $|x| \ge 4R$, and we have

$$\begin{aligned} |\nabla \alpha_{t_1,R}|^2 - \partial_t[\alpha_{t_1,R}^2] =& \Big| \nabla \eta_{t_1,R} - \frac{1}{2}\eta_{t_1,R}\nabla\xi_{t_1,R} \Big|^2 e^{-\xi_{t_1,R}} + \eta_{t_1,R}^2 e^{-\xi_{t_1,R}} \partial_t \xi_{t_1,R} \\ \le& \Big(2|\nabla \eta_{t_1,R}|^2 + \frac{1}{2}\eta_{t_1,R}^2 |\nabla \xi_{t_1,R}|^2 + \eta_{t_1,R}^2 \partial_t \xi_{t_1,R} \Big) e^{-\xi_{t_1,R}} = 2|\nabla \eta_{t_1,R}|^2 e^{-\xi_{t_1,R}}. \end{aligned}$$

Since $|\nabla \eta_{t_1,R}| \le R^{-1}\mathbf{1}_{B_{4R}\setminus B_{2R}}$ and since $\xi_{t_1,R} \ge \frac{R^2}{4\delta}$ on $[(t_1-\delta)\vee 0, t_1]\times B_{2R}^c$, we deduce from (15), that

$$m_{t_1,R}(t) \le 2R^{-2}e^{-R^2/(4\delta)}e^{\beta_t L(1+16R^2)}\ \mathrm{Vol}(B_{4R}\setminus B_{2R}).$$

Since β is bounded on $[0,t_0]$, it indeed suffices to choose $\delta>0$ small enough to complete the step.

Step 3. We consider $\delta>0$ as in Step 2, fix $t_1\in[0,t_0]$ and set, for $R>1$, $n\ge 5R$ and $t\in[(t_1-\delta)\vee 0, t_1]$,

$$\varphi_{n,t_1,R}(t) = \int_{\mathbb{R}^d} u_n^2(t,x)\alpha_{t_1,R}^2(t,x)e^{-\beta_t U(x)}\mathrm{d}x.$$

The goal of this step is to verify that there is a constant $\kappa_1>0$ such that

$$(20)\quad \forall t_1\in[0,t_0],\ \forall R>1,\ \forall n\ge 5R,\ \forall t\in[(t_1-\delta)\vee 0,t_1],\ \ \varphi'_{n,t_1,R}(t)\ge -\kappa_1\Big[R^2\varphi_{n,t_1,R}(t)+e^{-R^2}\Big].$$

By (17) (with $\alpha=1$), we know that $\partial_t u_n(t,x)=u_n(t,x)-\mathcal{L}_{\beta_t}u_n(t,x)$ on $[0,\infty)\times B_n$. Since Supp $\alpha_{t_1,R}(t,\cdot)\subset B_{4R}$ and since $n\ge 5R$, we may write

$$\varphi'_{n,t_1,R}(t) = I_{n,t_1,R}(t)+J_{n,t_1,R}(t)-K_{n,t_1,R}(t),$$

where

$$\begin{aligned} I_{n,t_1,R}(t) =& \int_{\mathbb{R}^d} 2[u_n(t,x)-\mathcal{L}_{\beta_t}u_n(t,x)]u_n(t,x)\alpha_{t_1,R}^2(t,x)e^{-\beta_t U(x)}\mathrm{d}x,\\ J_{n,t_1,R}(t) =& \int_{\mathbb{R}^d} u_n^2(t,x)\partial_t[\alpha_{t_1,R}^2(t,x)]e^{-\beta_t U(x)}\mathrm{d}x,\\ K_{n,t_1,R}(t) =& \beta'_t\int_{\mathbb{R}^d} U(x)u_n^2(t,x)\alpha_{t_1,R}^2(t,x)e^{-\beta_t U(x)}\mathrm{d}x. \end{aligned}$$

Using Remark 18 with any $r>4R$, since $\alpha_{t_1,R}(t,\cdot)$ is supported in B_{4R}, we have

$$\begin{aligned} I_{n,t_1,R}(t) \ge& -2\int_{\mathbb{R}^d}\mathcal{L}_{\beta_t}u_n(t,x)[u_n(t,x)\alpha_{t_1,R}^2(t,x)]e^{-\beta_t U(x)}\mathrm{d}x\\ =&\int_{\mathbb{R}^d}\nabla u_n(t,x)\cdot\nabla[u_n(t,x)\alpha_{t_1,R}^2(t,x)]e^{-\beta_t U(x)}\mathrm{d}x\\ =&\int_{\mathbb{R}^d}\Big[|\nabla u_n(t,x)|^2\alpha_{t_1,R}^2(t,x)+2u_n(t,x)\alpha_{t_1,R}(t,x)\nabla u_n(t,x)\cdot\nabla\alpha_{t_1,R}(t,x)\Big]e^{-\beta_t U(x)}\mathrm{d}x\\ \ge& -\int_{\mathbb{R}^d}u_n^2(t,x)|\nabla\alpha_{t_1,R}(t,x)|^2e^{-\beta_t U(x)}\mathrm{d}x. \end{aligned}$$

We finally used that $a^2-2ab\ge -b^2$ with $a=|\nabla u_n|\alpha_{t_1,R}$ and and $b=u_n|\nabla\alpha_{t_1,R}|$. Thus

$$\begin{aligned} I_{n,t_1,R}(t)+J_{n,t_1,R}(t) \ge& \int_{\mathbb{R}^d}u_n^2(t,x)\Big(\partial_t[\alpha_{t_1,R}^2(t,x)]-|\nabla\alpha_{t_1,R}(t,x)|^2\Big)e^{-\beta_t U(x)}\mathrm{d}x\\ \ge& -\int_{\mathbb{R}^d}\Big(|\nabla\alpha_{t_1,R}(t,x)|^2-\partial_t[\alpha_{t_1,R}^2(t,x)]\Big)_+e^{-\beta_t U(x)}\mathrm{d}x\ge -\kappa_0e^{-R^2} \end{aligned}$$

by Step 2. We used that $u_n^2(t,x)\in[0,1]$.

We next write $K_{n,t_1,R}(t)=K_{n,t_1,R}^{(1)}(t)+K_{n,t_1,R}^{(2)}(t)$, where

$$K_{n,t_1,R}^{(1)}(t)=\beta'_t\int_{\mathbb{R}^d}\mathbf{1}_{\{U(x)\le 0\}}U(x)u_n^2(t,x)\alpha_{t_1,R}^2(t,x)e^{-\beta_t U(x)}\mathrm{d}x\le CR^2\varphi_{n,t_1,R}(t),$$

because $|\beta'|$ is bounded on $[0,t_0]$ and because $|\mathbf{1}_{\{U\le 0\}}U|\le L(1+(4R)^2)$ on Supp $\alpha_{t_1,R}(t,\cdot)\subset B_{4R}$ by (15), and

$$K^{(2)}_{n,t_1,R}(t)=\beta'_t\int_{\mathbb{R}^d}\mathbf{1}_{\{U(x)\ge 0\}}U(x)u_n^2(t,x)\alpha^2_{t_1,R}(t,x)e^{-\beta_tU(x)}\mathrm{d}x.$$

By Step 1 with $a=u_n^2(t,x)\alpha^2_{t_1,R}(t,x)\in[0,1]$, $b=U(x)\ge 0$, $\eta=\beta_t>0$ and $\varepsilon=(2R)^{-2}$,

$$\begin{aligned}K^{(2)}_{n,t_1,R}\le&\frac{|\beta'_t|}{\beta_t}\int_{B_{4R}}\Big[2R^2u_n^2(t,x)\alpha^2_{t_1,R}(t,x)+e^{\beta_tU(x)-2R^2}\Big]e^{-\beta_tU(x)}\mathrm{d}x\\=&\frac{|\beta'_t|}{\beta_t}\Big[2R^2\varphi_{n,t_1,R}(t)+\mathrm{Vol}(B_{4R})e^{-2R^2}\Big]\\\le&C\Big[R^2\varphi_{n,t_1,R}(t)+e^{-R^2}\Big],\end{aligned}$$

since $|\beta'_t|/\beta_t$ is bounded on $[0,t_0]$. This ends the step.

Step 4. We now conclude that (19) holds true with $\delta_0=\min\{\delta,1/(2\kappa_1)\}$, where $\delta>0$ and $\kappa_1>0$ were introduced in Steps 2 and 3. We thus fix $t_1\in[0,t_0]$ and assume that $\int_{\mathbb{R}^d}u(t_1,x)\mathrm{d}x=0$.

Integrating (20), we find that for all $t\in[(t_1-\delta_0)\vee 0,t_1]$, all $R>1$ and all $n\ge 5R$,

$$\varphi_{n,t_1,R}(t)\le\varphi_{n,t_1,R}(t_1)e^{\kappa_1R^2(t_1-t)}+R^{-2}e^{-R^2}[e^{\kappa_1R^2(t_1-t)}-1]\le e^{R^2/2}\varphi_{n,t_1,R}(t_1)+e^{-R^2/2},$$

the last inequality following from the fact that $t_1-t\le\delta_0\le 1/(2\kappa_1)$.

Since $\lim_n u_n(t,x)=u(t,x)$ by dominated convergence and since $\alpha_{t_1,R}(t,\cdot)$ is compactly supported, we have $\lim_n\varphi_{n,t_1,R}(t)=\varphi_{t_1,R}(t)$, where $\varphi_R(t)=\int_{\mathbb{R}^d}u^2(t,x)\alpha^2_{t_1,R}(t,x)e^{-\beta_tU(x)}\mathrm{d}x$. We thus find, for all $t\in[(t_1-\delta_0)\vee 0,t_1]$, all $R>1$

$$\varphi_{t_1,R}(t)\le e^{R^2/2}\varphi_{t_1,R}(t_1)+e^{-R^2/2}.$$

But since $u(t_1,x)=0$ for a.e. $x\in\mathbb{R}^d$, it holds that $\varphi_{t_1,R}(t_1)=0$ for all $R>1$. Hence for all fixed $t\in[(t_1-\delta_0)\vee 0,t_1]$, all fixed $R_0>0$, all $R>R_0>1$, since $\alpha_{t_1,R}(t,\cdot)\ge\mathbf{1}_{B_{R_0}}$,

$$\int_{B_{R_0}}u^2(t,x)e^{-\beta_tU(x)}\mathrm{d}x\le\varphi_{t_1,R}(t)\le e^{-R^2/2},$$

whence $\int_{B_{R_0}}u^2(t,x)e^{-\beta_tU(x)}\mathrm{d}x=0$ and thus $u(t,x)=0$ for a.e. $x\in\mathbb{R}^d$ as desired. □

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