

# Talagrand's convolution conjecture up to $\log \log$ via perturbed reverse heat

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## Abstract

We prove that under the heat semigroup  $(P_\tau)$  on the Boolean hypercube, any nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  exhibits a uniform tail bound that is better than that by Markov's inequality. Specifically, for any  $\eta > e^3$  and  $\tau > 0$ ,

$$\mathbb{P}_{X \sim \mu} \left( P_\tau f(X) > \eta \int f d\mu \right) \leq c_\tau \frac{\log \log \eta}{\eta \sqrt{\log \eta}},$$

where  $\mu$  is the uniform measure on the Boolean hypercube  $\{-1, 1\}^n$  and  $c_\tau$  is a constant that only depends on  $\tau$ . This resolves Talagrand's convolution conjecture up to a dimension-free  $\log \log \eta$  factor. Its proof relies on properties of the reverse heat process on the Boolean hypercube and a coupling construction based on carefully engineered perturbations of this reverse heat process.

## 1 Introduction

In 1989, Talagrand (in Problem 1 and 2 [Tal89]) put forward a conjecture on the regularization effect generated by convolution applied to  $L^1$  functions on the Boolean hypercube. Consider the Boolean hypercube  $\{-1, 1\}^n$ . Given  $t \geq 0$ , let  $\xi_t$  be a random vector on  $\{-1, 1\}^n$ , whose coordinates  $\xi_t^{[i]}$  are independent and identically distributed with

$$\mathbb{P}(\xi_t^{[i]} = 1) = \frac{1 + e^{-t}}{2}, \quad \mathbb{P}(\xi_t^{[i]} = -1) = \frac{1 - e^{-t}}{2}.$$

Consider the *heat semigroup*  $(P_t)_{t \geq 0}$  defined for any function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}$  by, for any  $x \in \{-1, 1\}^n$ ,

$$P_t f(x) := \mathbb{E}[f(x \odot \xi_t)], \tag{1}$$

where  $\odot$  denotes element-wise product. Let  $\mu_t^n$  denote the law of  $\xi_t$ , then  $P_t$  can also be written as a convolution  $P_t f(x) = \int f(x \odot y) d\mu_t^n(y) = f * \mu_t^n$ , where the convolution operator  $*$  is defined via the multiplicative group structure on  $\{-1, 1\}^n$ . For this reason, the heat semigroup  $P_t$  was referred to as “convolution by a biased coin” in [Tal89].

Introduce the shorthand  $\mu := \mu_\infty^n$ , which is the uniform measure on  $\{-1, 1\}^n$ . For  $p \geq 1$ ,  $f : \{-1, 1\}^n \rightarrow \mathbb{R}$ , define its  $L^p(\mu)$ -norm to be  $\|f\|_p := (\int |f|^p d\mu)^{\frac{1}{p}}$ . Talagrand's convolution conjecture, also restated on his website with the title “Regularization from  $L^1$  by convolution” [Tal16], aims to precisely quantify the regularization effect of the heat semigroup when applied to  $L^1(\mu)$  functions, as follows.

**Conjecture 1** ([Tal89]). *For every  $\tau > 0$ , there exists a constant  $c_\tau > 0$  only depends on  $\tau$ , such that for every nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  with  $\|f\|_1 \neq 0$ , and any  $\eta > 1$ , we have*

$$\mathbb{P}_{X \sim \mu}(P_\tau f(X) > \eta \|f\|_1) \leq \frac{c_\tau}{\eta \sqrt{\log \eta}}.$$

In this conjecture, the regularization effect refers to the gain of a  $1/\sqrt{\log \eta}$  factor compared to Markov's inequality while retaining the constant dimension-free. In this paper, we prove the following theorem, which resolves the conjecture up to a  $\log \log \eta$  factor, with a dimension-free constant.

**Theorem 1.** *For every  $\tau > 0$ , there exists a universal constant  $c > 0$ , such that for every nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  with  $\|f\|_1 \neq 0$ , and any  $\eta > e^3$ , we have*

$$\mathbb{P}_{X \sim \mu}(P_\tau f(X) > \eta \|f\|_1) \leq c \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log \eta}{\eta \sqrt{\log \eta}}.$$

While  $1/\sqrt{\log \eta}$  is conjectured to be the extra factor, Talagrand also mentioned that “I do not know if it is true that  $\lim_{\eta \rightarrow \infty} \psi(\eta) = 0$ ” [Tal16], where  $\psi(\eta) := \sup_{n \in \mathbb{N}} \sup_{f \geq 0} \{\eta \mathbb{P}(P_\tau f \geq \eta \|f\|_1)\}$  (see also Problem 1 in [Tal89]). Our Theorem 1 is the first result with a dimension-free upper bound which confirms that  $\lim_{\eta \rightarrow \infty} \psi(\eta) = 0$ .

**Remark 1.** *Without loss of generality, by rescaling, we may assume  $\|f\|_1 = 1$ . Additionally, it suffices to prove the case for strictly positive functions first, and then obtain the general case by passing on limits.*

Before we proceed to the main proofs, we make a few comments about its relation to classical results and summarize the progress on this conjecture.

## 1.1 A few comments on the conjecture

First, to bound the tail probability of  $P_\tau f(X) > \eta \|f\|_1$ , the first idea that comes to mind is Markov's inequality. Since  $\mathbb{E}_{X \sim \mu}[P_\tau f(X)] = \mathbb{E}_{X \sim \mu}[f(X)] = \|f\|_1$ , Markov's inequality gives

$$\mathbb{P}_{X \sim \mu}(P_\tau f(X) > \eta \|f\|_1) \leq \frac{1}{\eta}. \quad (2)$$

This bound holds for any  $\tau \geq 0$ . For  $\tau > 0$ , Talagrand's conjecture is a strengthening of Markov's inequality when a heat semigroup is applied.

Second, from Eq. (2), one immediately obtains a bound with an extra  $1/\sqrt{\log \eta}$  factor if a dimension-dependent constant is allowed.

$$\mathbb{P}_{X \sim \mu}(P_\tau f(X) > \eta \|f\|_1) \leq \frac{1}{\eta} = \frac{\sqrt{\log \eta}}{\eta \sqrt{\log \eta}} \stackrel{(i)}{\leq} \frac{\sqrt{n \log 2}}{\eta \sqrt{\log \eta}}.$$

(i) follows from the trivial bound  $f \leq 2^n \|f\|_1$  (see Lemma 4), as well as the fact that if  $\eta > 2^n$ , then the probability on the left-hand side is 0. Hence, allowing dimension-dependent constants in Conjecture 1 is not very interesting, unless the constants are much smaller than  $\sqrt{n}$ .

Third, as shown in Proposition 5 of [Tal16], if one aims for a uniform dimension-free tail bound which holds for any  $f \geq 0$  and any  $\eta > 2$ , then the best bound one can hope for is  $1/(\eta \sqrt{\log \eta})$  up to

a constant that depends on  $\tau$ . For this, [Tal16] constructed an explicit lower bound by considering the product function  $f(x) = \prod_{i=1}^n (1 + x_i)$  and a carefully chosen threshold  $\eta$ .

Fourth, one may ask why the normalization has to be with  $\|f\|_1$  rather than with  $\|f\|_p$  for  $p > 1$ . As pointed out in [Tal89], as long as  $p > 1$ ,  $P_\tau$  is known to be a “regularizing” operator. Specifically, hypercontractivity for the uniform measure on  $\{-1, 1\}^n$  implies that, for  $q = 1 + e^{-2\tau}(p - 1)$ ,  $\|P_\tau f\|_q \leq \|f\|_p$ . Then Markov’s inequality gives

$$\mathbb{P}(P_\tau f(X) > \eta \|f\|_p) \leq \frac{1}{\eta^q},$$

which is better than  $1/(\eta \sqrt{\log \eta})$  for large  $\eta$  as long as  $p > 1$ . While hypercontractivity is powerful for  $p > 1$ , it does not tell anything about the action of  $P_\tau$  on  $L^1$  functions. This leads to the original main motivation of the conjecture: to clarify the regularizing properties of  $P_\tau$  on  $L^1$  functions.

Finally, since the author comes from a background of studying isoperimetric inequalities, it is worth mentioning that Conjecture 1 is closely related to isoperimetric inequalities with extra logarithmic factors and the geometry of small sets (see Section 1 [EL18]).

## 1.2 Remarks on the Gaussian counterpart

In an attempt to attack Conjecture 1, a natural Gaussian counterpart of the conjecture, related to the Ornstein-Uhlenbeck (OU) semigroup, has been formulated [BBB<sup>+</sup>13] and studied.

Let  $\gamma_n$  denote the standard Gaussian measure in  $\mathbb{R}^n$  with density  $x \mapsto \frac{1}{(2\pi)^{n/2}} \exp(-\|x\|_2^2/2)$ , with  $\|\cdot\|_2$  being the Euclidean norm. For  $p \geq 1$ , let  $L^p(\gamma_n) := \{f : \mathbb{R}^n \rightarrow \mathbb{R} \mid \int |f|^p d\gamma_n < \infty\}$ . Given  $f \in L^1(\gamma_n)$ , the OU semigroup is defined by Mehler’s representation as

$$P_t^{\text{OU}} f(x) := \int f(e^{-t}x + \sqrt{1 - e^{-2t}}y) d\gamma_n(y), \quad x \in \mathbb{R}^n, t \geq 0.$$

The Gaussian counterpart of the conjecture asks whether it is true that for every nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  with  $\|f\|_1 \neq 0$ , and any  $\eta > 1$ , we have

$$\mathbb{P}_{X \sim \gamma_n}(P_\tau^{\text{OU}} f(X) > \eta \|f\|_1) \leq \frac{c_\tau}{\eta \sqrt{\log \eta}}, \quad (3)$$

for a constant  $c_\tau$  that only depends on  $\tau > 0$ . In words, the Gaussian counterpart replaces the heat semigroup on the Boolean hypercube with OU semigroup, and the uniform measure on the Boolean hypercube with the standard Gaussian. The Gaussian counterpart is fully resolved. Ball, Barthe, Bednorz, Oleszkiewicz and Wolff [BBB<sup>+</sup>13] first formulated this problem and provided a bound with a constant  $c_{\tau,n}$  that depends on the dimension  $n$  and an extra  $\log \log \eta$  factor in the numerator. Eldan and Lee [EL18], using Föllmer’s process and a coupling construction via stochastic calculus, proved a dimension-free bound with an extra  $\sqrt{\log \log \eta}$  factor in the numerator. Following the main ideas in [EL18], Lehec [Leh16] refined their stochastic analysis to remove the extra  $\sqrt{\log \log \eta}$  factor, fully resolving the Gaussian counterpart.

In both [EL18] and [Leh16], they crucially use the second-order smoothness (or semi-log-convexity) brought by the OU semigroup, as follows: for any  $f : \mathbb{R}^n \rightarrow \mathbb{R}_+$  and  $t > 0$ , we have

$$\nabla^2 \log P_t^{\text{OU}} f \succeq -\frac{1}{2t} \mathbb{I}_n.$$

In fact, this semi-log-convexity is the only role of the OU semigroup in resolving the Gaussian counterpart of the conjecture. It is a well-known fact that the Gaussian counterpart of the conjecture follows from Talagrand’s Conjecture 1 by the central limit theorem. On the other hand, whether the Gaussian proof is helpful for proving Conjecture 1 is unknown.

There are several recent works which attempt to extend the success in the Gaussian setting to other measures and/or other semigroups. [GMRS19] gave an alternative proof of the Gaussian counterpart in dimension 1. [GLM<sup>+</sup>23] studied another continuous analogue by replacing OU semigroup with perturbations of OU semigroup in dimension 1, as well as other variants for the  $M/M/\infty$  queuing process on the integers and Laguerre semigroup in dimension 1.

**Notation** Let  $[n]$  denote the set  $\{1, 2, \dots, n\}$ .  $(e_1, e_2, \dots, e_n)$  denotes the canonical basis of  $\mathbb{R}^n$ . For  $a, b \in \mathbb{R}$ ,  $a \wedge b := \min\{a, b\}$ . Let  $\odot$  denote the element-wise product. For  $x \in \mathbb{R}^n$ ,  $\varsigma_i(x) := (x_1, \dots, x_{i-1}, -x_i, x_{i+1}, \dots)$  is the vector obtained by flipping the  $i$ -th coordinate. Let  $\Delta_i h$  denote the “flip  $i$ -th coordinate and take difference” function  $x \mapsto h(\varsigma_i(x)) - h(x)$ . Denote  $\mathbb{R}_+ := [0, \infty)$ . For  $x \in \mathbb{R}$ ,

$$\text{sign}(x) := \begin{cases} +1 & \text{if } x > 0 \\ 0 & \text{if } x = 0 \\ -1 & \text{otherwise.} \end{cases}$$

For  $x \in \mathbb{R}^n$ ,  $\text{sign}(x)$  is the vector obtained by applying sign coordinate-wise. RHS means right-hand side and LHS means left-hand side.  $c$  and  $c'$  denote universal constants, which may differ depending on the context.

## 2 Preliminaries

We introduce a few basic facts about Boolean function analysis, general continuous-time Markov processes and the heat semigroup on the Boolean hypercube.

### 2.1 Boolean function analysis basics

Concepts are introduced without proofs. For a detailed exposition on Boolean function analysis, we refer interested readers to the book [O'D14].

**Inner product for functions on  $\{-1, 1\}^n$ .** For a pair of functions  $g, h : \{-1, 1\}^n \rightarrow \mathbb{R}$ , we define their inner product as

$$\langle g, h \rangle := \int g(x)h(x)d\mu(x) = \mathbb{E}_\mu[gh].$$

**Multilinear expansion of a function on  $\{-1, 1\}^n$**  For a subset  $S \subseteq [n]$ , define the monomial corresponding to  $S$  as  $x^S := \prod_{i \in S} x_i$ , with  $x^\emptyset = 1$  by convention. With the above inner product,  $\{x^S \mid S \subseteq [n]\}$  form an orthonormal basis for the vector space of functions  $\{-1, 1\}^n \rightarrow \mathbb{R}$  (see e.g.

Theorem 1.5 in [O'D14]). Additionally, every function  $g : \{-1, 1\}^n \rightarrow \mathbb{R}$  can be uniquely expressed as a multilinear polynomial,

$$g(x) = \sum_{S \subseteq [n]} \hat{g}(S)x^S, \quad (4)$$

where  $\hat{g}(S) := \langle g, x^S \rangle$  is called the Fourier coefficient of  $g$  on  $S$  (see e.g. Theorem 1.1 in [O'D14]). With the multilinear polynomial representation,  $g$  can be treated as a function on  $\mathbb{R}^n$ . This allows us to define the derivative of  $g$  in the usual sense, for  $i \in [n]$

$$\partial_i g(x) := \lim_{h \rightarrow 0} \frac{g(x + he_i) - g(x)}{h} = \frac{g(\dots, x_{i-1}, +1, x_{i+1}, \dots) - g(\dots, x_{i-1}, -1, x_{i+1}, \dots)}{2}.$$

Additionally, the first Fourier coefficient satisfies, if  $g \geq 0$ , then  $\hat{g}(\emptyset) = \|g\|_1 = \int g d\mu = g(0)$ .

**Explicit form of the heat semigroup** Using the multilinear expansion, the heat semigroup (1) can be written as

$$P_t g(x) = \int g(x \odot y) d\mu_t^n(y) = \sum_{y \in \{-1, 1\}^n} \sum_{S \subseteq [n]} \hat{g}(S)x^S y^S \prod_{i \in [n]} \left( \frac{1 + y_i e^{-t}}{2} \right) \stackrel{(i)}{=} g(e^{-t}x). \quad (5)$$

(i) follows by summing over  $y$  first. Vaguely speaking, applying the heat semigroup “moves” the input space from  $\{-1, 1\}^n$  to the inner hypercube  $\{-e^{-t}, e^{-t}\}^n$ , which may benefit from additional regularity of a multilinear polynomial in the inner hypercube.

## 2.2 Continuous-time Markov processes

In this subsection, we introduce a few concepts related to Markov processes and Markov semigroups. Interested readers are referred to [And12] for continuous-time Markov chains and [Paz12] for a semigroup viewpoint for additional details.

Given a Markov process  $(X_t)_{t \geq 0}$  with  $X_t$  taking values in a finite space  $\Omega$ . All Markov processes considered are càdlàg (right continuous with left limits).

**Homogeneous case** When  $(X_t)_{t \geq 0}$  is time-homogeneous (i.e., the law of  $X_t \mid X_s = x$  stays the same as  $X_{t-s} \mid X_0 = x, \forall t \geq s \geq 0$ ), we define the associated *Markov semigroup*  $Q_t$  as

$$Q_0 = \mathbb{I}$$

$$Q_t h(x) = \mathbb{E}[h(X_t) \mid X_0 = x],$$

for every bounded function  $h : \Omega \rightarrow \mathbb{R}$ , and every  $x \in \Omega$ . It also acts on measures through the duality  $\int h d(\nu P_t) = \int P_t h d\nu$ . Its *generator* is defined as (if the limit is well-defined)

$$Lh(x) := \lim_{t \rightarrow 0^+} \frac{Q_t h(x) - h(x)}{t}.$$

A measure  $\nu$  on  $\{-1, 1\}^n$  is said to be *invariant* for  $(Q_t)$  if  $\int Q_t h d\nu = \int h d\nu, \forall t \geq 0$ . The Markov property guarantees that it satisfies the semigroup property, namely,  $Q_{t+s} = Q_t Q_s, \forall 0 \leq s \leq t$ .

**In-homogeneous case** When  $X_t$  is time-inhomogeneous, we work with a two-parameter semi-group (also called evolution system)  $(Q_{s,t})_{0 \leq s \leq t}$  acting on bounded functions  $\Omega \rightarrow \mathbb{R}$ , such that

$$Q_{s,s} = \mathbb{I}$$

$$Q_{s,t}h(x) = \mathbb{E}[h(X_t) | X_s = x].$$

The Markov property guarantees that it satisfies the two-parameter semigroup property  $Q_{s,t} = Q_{s,r}Q_{r,t}, 0 \leq s \leq r \leq t$ . Additionally, on a finite space  $\Omega$ ,  $Q_{s,t}$  can be seen as a matrix of size  $|\Omega| \times |\Omega|$ . Its time-dependent generator  $L_t$  is defined via the Kolmogorov forward and backward equations (if the partial derivative with respect to  $t$  is well-defined):

$$\partial_t Q_{s,t} = Q_{s,t}L_t, \quad \partial_s Q_{s,t} = -L_s Q_{s,t}.$$

### 2.3 Heat semigroup and its associated Markov process

In the heat semigroup definition in Eq. (1),  $\xi_t$  only specifies one-time marginals of the process. We introduce a Markov process which fulfills the one-time marginals via a jump stochastic differential equation (SDE), making the name ‘‘heat semigroup’’ consistent with our semigroup definition in Section 2.2.

Let  $E := \mathbb{R}^2$ , equipped with Lebesgue measure. Let  $N$  be a Poisson random measure (PRM) on  $\mathbb{R}^+ \times E$ , which equips the probability space with a natural filtration  $\{\mathcal{F}_t\}_{t \in \mathbb{R}_+}$ .  $\tilde{N}$  is its associated compensated Poisson random measure and  $\nu$  is its intensity such that  $\nu(dt, dz) = dt dz_1 dz_2$ . Let  $f$  be a function  $\{-1, 1\}^n \rightarrow (0, \infty)$  with  $\|f\|_1 = 1$ . Define  $\nu_f := f \cdot \mu$ , which is probability measure with density  $f$  with respect to the uniform measure on  $\{-1, 1\}^n$ . Let  $T > 0$ .

**Forward jump process** We define the forward jump process through the following jump SDE,

$$U_0 \sim \nu_f = f \cdot \mu,$$

$$dU_t := \sum_{i=1}^n (-2U_{t-}e_i) \int_E \mathbf{1}_{z_1 \in (i, i+1]} \mathbf{1}_{0 < z_2 < \frac{1}{2}} N(dt, dz). \quad (6)$$

Since the intervals  $\{(i, i+1]\}_{i=1, \dots, n}$  are disjoint, the driving noise in one coordinate is independent of that in another. Notation-wise, it is sometimes simpler to treat the driving noises as  $n$  independent Poisson random measures  $N^{[i]}$  on  $\mathbb{R}^+ \times \mathbb{R}$  instead of  $\mathbb{R}^+ \times E$ , and  $i$ -th coordinate evolves independently as follows

$$U_0 \sim f \cdot \mu$$

$$dU_t^{[i]} = -2U_{t-}^{[i]} \int_{\mathbb{R}} \mathbf{1}_{0 < z < \frac{1}{2}} N^{[i]}(dt, dz). \quad (7)$$

We use these two notation interchangeably for convenience.

For any  $T > 0$ , the existence and uniqueness of the solution of the SDE on  $[0, T]$  follows from the bounded total jump rate for pure jump process (see e.g., Chapter 4.7 [EK09]). Additionally, since each coordinate of  $U_t$  evolves independently, the distribution of  $U_t$  is characterized by that in each coordinate. For the first coordinate, it follows a Poisson process with rate  $1/2$ . Its conditional mean has an explicit form, after solving an ordinary differential equation (ODE),

$$\mathbb{E}\left[U_t^{[1]} | U_0^{[1]} = x\right] = xe^{-t}.$$

Then the transition probability follows since  $U_t^{[1]}$  only takes value in  $\{-1, 1\}$ :  $\mathbb{P}(U_t^{[1]} = 1 \mid U_0^{[1]} = x) = \frac{1+xe^{-t}}{2}$ . In other words,  $U_t \mid U_0 = x$  matches the distribution of  $x \odot \xi_t$ . Hence, the associated semigroup to  $(U_t)_{t \geq 0}$  is exactly the heat semigroup  $(P_t)_{t \geq 0}$  defined in Eq. (1).

Next, we describe its generator and its marginal law. Its generator takes the form, for any test function  $h : \{-1, 1\}^n \rightarrow \mathbb{R}$ ,

$$L^U h(x) = \frac{1}{2} \sum_{i=1}^n (h(\zeta_i(x)) - h(x)). \quad (8)$$

In its matrix form,  $L^U(x, y) = \frac{1}{2} \sum_{i=1}^n \mathbf{1}_{y=\zeta_i(x)}$ ,  $x, y \in \{-1, 1\}^n$ . Additionally, the uniform measure  $\mu$  is the invariant measure for  $(P_t)_{t \geq 0}$ . For time  $t > 0$ , the marginal law of  $U_t$  has measure  $p_t := \nu_f P_t$ , which has an explicit form  $p_t(x) = f(e^{-t}x)\mu(x)$ . Conceptually, as  $t$  tends to  $\infty$ , one may think the process  $(U_t)_{t \geq 0}$  as creating a stochastic bridge from the probability measure  $\nu_f$  to the uniform measure  $\mu$ .

## 2.4 Time reversal of a Markov process

Given a Markov process  $(X_t)$  on a finite space  $\Omega$  and its associated semigroup  $(Q_{s,t})_{0 \leq s \leq t}$  with generator  $L_t$ . Let  $\pi_t = \pi_0 Q_{0,t}$  be a family of probability measures of the law of  $X_t$ . The *time-reversed semigroup* (with respect to  $(\pi_t)$ ) is defined as

$$\tilde{Q}_{s,t}(x, y) := \frac{\pi_s(x)}{\pi_t(y)} Q_{s,t}(x, y), \forall s \leq t, \forall x, y \in \Omega.$$

Its reversed generator satisfies the *flux equation*

$$\begin{aligned} \tilde{L}_t(y, x) &= \frac{\pi_t(x)}{\pi_t(y)} L_t(x, y), \text{ if } x \neq y, \\ \tilde{L}_t(y, y) &= - \sum_{x \neq y} \tilde{L}_t(y, x). \end{aligned}$$

The time reversal has a pathwise interpretation. Define  $\tilde{X}_t := X_{T-t}$  for  $t \in [0, T]$ . Then  $\tilde{X}_t$  is a Markov process with initial law  $\pi_T$ , with  $\tilde{Q}_{T-t, T-s}$  as its associated semigroup and  $\tilde{L}_{T-t}$  as its generator. See e.g., Chapter 7 [And12] for more details about time-reversed Markov processes.

## 2.5 Time reversal of the heat process

Using the time reversal formula, we derive the time reversal of the heat process in Eq. (6).

**Reverse jump process** Define  $(V_t)_{t \in [0, T]}$  as  $V_t := U_{T-t}$ , which satisfies the following SDE

$$\begin{aligned} V_0 &= U_T, \\ dV_t &= \sum_{i=1}^n (-2V_{t-}e_i) \int_{\mathbb{R}} \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(e^{-(T-t)}V_{t-})} N^{[i]}(dt, dz), \end{aligned} \quad (9)$$

where the *score function* for  $i$ -th coordinate  $S_i : [-1, 1]^n \rightarrow \mathbb{R}$ , considering multilinear expansion of  $f$ , is defined as

$$S_i(x) := \frac{x_i \partial_i f(x)}{f(x)}, \quad \forall i \in [n]. \quad (10)$$

The reverse jump rate is derived as the unique solution to the flux equation. Recall that for the heat semigroup, the marginal law is  $p_t(x) = f(e^{-t}x)\mu(x)$  and  $L^U(x, y) = \frac{1}{2} \sum_{i=1}^n \mathbf{1}_{y=\varsigma_i(x)}$ . The flux equation provides an explicit form of the generator, for any function  $h : \{-1, 1\}^n \rightarrow \mathbb{R}$ ,

$$L_t^V h(x) = \frac{1}{2} \sum_{i=1}^n \frac{f(\varsigma_i(e^{-(T-t)}x))}{f(e^{-(T-t)}x)} (h(\varsigma_i(x)) - h(x)).$$

Since  $f > 0$  and the space  $\{-1, 1\}^n$  is finite, the jump rate is finite on  $[0, T]$ . The existence and uniqueness of the solution of the SDE follows from the bounded total jump rate for pure jump process (see e.g., Chapter 4.7 [EK09]).

Unlike the forward process, the reverse jump process is time-inhomogeneous due to its time-dependent jump rates. In view of the jump rate, it is natural to introduce the *scaled reverse jump process*

$$\mathcal{V}_t := e^{-(T-t)} V_t, \quad (11)$$

which lives in the inner cube  $[-1, 1]^n$  and becomes a time-homogeneous Markov process.

**Remark 2.** *In light of the recent trendy development on score-based diffusion models for sampling high dimensional natural images [SSDK<sup>+</sup>21] via time-reversal of Ornstein-Uhlenbeck process, we remark that  $(V_t)_{t \geq 0}$  is the Boolean hypercube analogue of the Gaussian diffusion models. Here, the Gaussian noise is replaced by Poisson jumps.*

Note that as a vector,  $S(\mathcal{V}_t) = V_t \odot \nabla \log P_{T-t} f(V_t)$ . Its resemblance to Föllmer's drift (or the score) in the Gaussian setting [EL18] is the reason we name it the score, too. It is known that Föllmer's drift is a martingale in the Gaussian setting (see e.g. Section 2 [EL18]). The score  $S(\mathcal{V}_t)$ , in our definition, is also a martingale, which we show in Appendix (Lemma 13).

### 3 Main proof

Fix  $\tau > 0$ ,  $T > \tau$  to be chosen and  $T_o = T - \tau$ . For  $t \in [0, T]$ , let  $\rho_t = e^{-(T-t)}$ . Based on Remark 1, we restrict ourselves to strictly positive function  $f : \{-1, 1\}^n \rightarrow (0, \infty)$  with  $\|f\|_1 = 1$ . To prove Theorem 1, our high-level proof strategy is to construct a coupling, which is inspired by the main strategy in the Gaussian counterpart [EL18]. However, the coupling construction and technical details differ significantly due to the discrete nature of the Boolean hypercube  $\{-1, 1\}^n$ . The first step is to show that it suffices to prove the following anti-concentration due to the heat semigroup.

**Lemma 1** (Anti-concentration). *Let  $\nu_{P_\tau f}$  be the probability measure on  $\{-1, 1\}^n$  with density  $P_\tau f$  with respect to the uniform measure  $\mu$ . There exists a universal constant  $c > 0$ , such that for any  $\eta > e^3$ ,*

$$\mathbb{P}_{Y \sim \nu_{P_\tau f}} (P_\tau f(Y) \in (\eta, e\eta]) \leq c \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log \eta}{\sqrt{\log \eta}}.$$

Theorem 1 directly follows from Lemma 1, using the same proof in the Gaussian space (see Section 2 [EL18]). A short proof is provided for completeness.

*Proof of Theorem 1.* We have

$$\begin{aligned}
\mathbb{P}_{X \sim \mu}(P_\tau f(X) > \eta) &= \sum_{k=0}^{\infty} \mathbb{P}_{X \sim \mu}(P_\tau f(X) \in (e^k \eta, e^{k+1} \eta]) \\
&\leq \sum_{k=0}^{\infty} \frac{1}{e^k \eta} \mathbb{E}_{X \sim \mu} \left[ P_\tau f(X) \mathbf{1}_{P_\tau f(X) \in (e^k \eta, e^{k+1} \eta]} \right] \\
&= \sum_{k=0}^{\infty} \frac{1}{e^k \eta} \mathbb{P}_{Y \sim \nu_{P_\tau f}} \left( P_\tau f(Y) \in (e^k \eta, e^{k+1} \eta] \right) \\
&\stackrel{(i)}{\leq} \sum_{k=0}^{\infty} \frac{1}{e^k \eta} c \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log(e^k \eta)}{\sqrt{\log(e^k \eta)}} \\
&\stackrel{(ii)}{\leq} 2c \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log(\eta)}{\eta \sqrt{\log(\eta)}} \sum_{k=0}^{\infty} \frac{1}{e^k} \\
&= \frac{2ce}{e-1} \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log(\eta)}{\eta \sqrt{\log(\eta)}}.
\end{aligned}$$

(i) follows from Lemma 1. Let  $q : x \mapsto \log \log(x) / \sqrt{\log(x)}$ . (ii) follows from the fact that  $q(\eta) \geq \frac{1}{2} \max_{x > \eta} q$  for  $\eta > e^3$ .  $\square$

The second step is to construct a coupling via the reverse jump process to prove Lemma 1. While this idea is natural after reading the Gaussian proof [EL18], one cannot apply the same type of perturbation because any drift perturbation moves the process outside the Boolean hypercube  $\{-1, 1\}^n$ . New ideas are needed. We would like to construct a coupling of two Markov processes  $(V_t, W_t)$  such that, marginally at time  $T_o$ ,  $V_{T_o}$  has law  $\nu_{P_\tau f}$  (already achieved according to the construction of the reverse process (9)),  $W_{T_o}$  has law  $\nu^W$ , and they satisfy the following two properties, vaguely speaking:

1. the two measures  $\nu_{P_\tau f}$  and  $\nu^W$  are close in total variation (TV);
2. with high probability,  $P_\tau f(V_{T_o})$  is strictly larger than  $P_\tau f(W_{T_o})$ , given that  $P_\tau f(W_{T_o}) \geq \eta$ .

More precisely, these properties are formalized in the following two lemmas.

**Lemma 2** (Total variation control). *Let  $\eta > e^3$ . For any  $0 < \bar{\delta} < \frac{1}{2}$ , there exists a coupling construction  $(V_{T_o}, W_{T_o})$ , described in Section 3.1, satisfying*

$$d_{TV}(\nu_{P_\tau f}, \nu^W) \leq \frac{ce^{-\tau}}{1 - e^{-\tau}} \bar{\delta} \sqrt{\log \eta}.$$

Here  $\nu^W$  denotes the law of  $W_{T_o}$  and  $c > 0$  is a universal constant.

Its proof is in Section 3.2.

**Lemma 3** (Approximate monotone coupling at tail). *Let  $\eta > e^3$ . For any  $\frac{\frac{1}{2} \log \log \eta + 0.91}{\log \eta} \leq \bar{\delta} < \frac{1}{2}$ , there exists a coupling construction  $(V_{T_o}, W_{T_o})$ , described in Section 3.1, such that*

$$\mathbb{P}(\log P_\tau f(V_{T_o}) > \log \eta + 1) \geq \mathbb{P}(\log P_\tau f(W_{T_o}) > \log \eta) - \frac{3}{\sqrt{\log \eta}}.$$

Its proof is in Section 3.3. Lemma 1 easily follows from the above two lemmas.

*Proof of Lemma 1.* Take  $\bar{\delta} = \frac{\frac{1}{2} \log \log \eta + 0.91}{\log \eta}$ . The TV distance control in Lemma 2 gives

$$|\mathbb{P}(P_\tau f(W_{T_o}) > \eta) - \mathbb{P}(P_\tau f(V_{T_o}) > \eta)| \leq \frac{ce^{-\tau}}{1 - e^{-\tau}} \bar{\delta} \sqrt{\log \eta}.$$

Using this equation to eliminate  $W_{T_o}$  term in Lemma 3, we obtain

$$\begin{aligned} \mathbb{P}(P_\tau f(V_{T_o}) \in (\eta, e\eta]) &\leq \frac{3}{\sqrt{\log \eta}} + \frac{ce^{-\tau}}{1 - e^{-\tau}} \bar{\delta} \sqrt{\log \eta} \\ &\leq c' \max \left\{ 1, \frac{e^{-\tau}}{1 - e^{-\tau}} \right\} \frac{\log \log \eta}{\sqrt{\log \eta}}. \end{aligned}$$

□

The rest of this section is organized as follows. In Section 3.1, we introduce our coupling construction. In Section 3.2 and Section 3.3, we prove Lemma 2 and Lemma 3 respectively.

### 3.1 Main coupling construction

The Föllmer process [Fö105], as the (time-reparametrized) time-reversed Ornstein-Uhlenbeck (OU) process, played an important role for constructing a coupling in the Gaussian counterpart of Talagrand's conjecture [EL18]. Following this idea, we perturb the reverse jump process (9) to construct a coupling. The perturbation is no longer on the drift, but on the jump rate. Recall that the reverse jump process  $(V_t)_{t \in [0, T]}$  satisfies the following SDE

$$\begin{aligned} V_0 &= U_T \\ dV_t &= \sum_{i=1}^n (-2V_{t-} e_i) \int_{\mathbb{R}} \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(e^{-(T-t)} V_{t-})} N^{[i]}(dt, dz), \end{aligned}$$

where the score function is  $S_i(x) = \frac{x \partial_i f(x)}{f(x)}$ .

**Perturbed reverse jump process** Let  $0 < \bar{\delta} < \frac{1}{2}$ . We define for  $t \in [0, T]$ ,

$$\begin{aligned} W_0 &:= V_0 \\ dW_t &:= \sum_{i=1}^n (-2W_{t-} e_i) \int_{\mathbb{R}} \mathbf{1}_{0 < z \leq \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}}) S_i(e^{-(T-t)} V_{t-})} N^{[i]}(dt, dz), \end{aligned} \tag{12}$$

where the stopping time is defined as

$$\mathfrak{T} := \inf \left\{ t \in [0, \infty) \mid \max \left\{ \log P_{T-t} f(V_t) - \frac{1}{2} \log \log \eta - 1, \log P_{T-t} f(W_t) \right\} > \log \eta \right\} \wedge T_o, \tag{13}$$

and  $\delta_i$  is a shorthand for  $\delta_i(e^{-(T-t)}V_{t-})$ , where

$$\delta_i(x) := \bar{\delta} \left[ \mathbf{1}_{S_i(x)>0} + \frac{1 - 2S_i(x)}{1 - 2\bar{\delta}S_i(x)} \mathbf{1}_{S_i(x)\leq 0} \right], \quad i \in [n], \quad x \in [-1, 1]^n. \quad (14)$$

In words,  $\mathfrak{T}$  is the first time either the process  $\log P_{T-t}f(W_t)$  hits value  $\log \eta$  or  $\log P_{T-t}f(V_t)$  hits value  $\log \eta + \frac{1}{2} \log \log \eta + 1$ , with the convention that  $\mathfrak{T}$  takes value  $T_o$  if they never reach  $\log \eta$ . The jump perturbation rate is of order  $\bar{\delta}$ , but has two forms depending on whether the score  $S_i$  is positive or not.

**Remark 3.** In Eldan and Lee's proof for the Gaussian counterpart [EL18], a  $\delta$  perturbation is added to the score function, which results in a  $\delta$  perturbation of the drift of Föllmer's process. Here, we cannot add perturbations to the drift as it moves out of  $\{-1, 1\}^n$ . But the idea that we should perturb the score function, once the score on the Boolean hypercube is properly defined, remains valid and essential.

While a constant  $\delta$  perturbation of the score suffices in Eldan and Lee's proof for the Gaussian counterpart [EL18], our coupling construction takes full advantage of the perturbation along the stochastic process: the perturbation  $\delta_i$  is no longer a constant. It is state-dependent and coordinate-dependent.

The processes  $(V_t, W_t)_{t \in [0, T]}$  are coupled in that

- they share the same initialization  $W_0 = V_0$ ;
- they share the same Poisson random measure  $N^{[i]}, \forall i \in [n]$ ;
- $W$  alone is not Markov, its jump rate depends on  $V$ .

To make sure the SDE solution is well-defined, we verify that the jump rate is nonnegative and never explodes. The following lemma checks the range of  $S_i$ .

**Lemma 4** (Edge ratio bound). *For any nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  with  $f \neq 0$ , consider its multilinear expansion. Then for any  $x \in (-1, 1)^n$ ,  $f$  is upper and lower bounded pointwise*

$$0 < \|f\|_1 \prod_{j=1}^n (1 - |x_j|) \leq f(x) \leq \|f\|_1 \prod_{j=1}^n (1 + |x_j|).$$

Additionally, for any  $i \in [n]$ ,  $i$ -th edge ratio is also bounded

$$\frac{1 - |x_i|}{1 + |x_i|} \leq \frac{f(\varsigma_i(x))}{f(x)} \leq \frac{1 + |x_i|}{1 - |x_i|}, \quad \forall x \in (-1, 1)^n.$$

Its proof is deferred to Section 4.1. The next lemma verifies the existence and uniqueness of the SDE solutions.

**Lemma 5.** *For  $0 < \bar{\delta} < \frac{1}{2}$ , the coupled SDE for  $(V, W)$  in Eq. (9) and (12) has a unique solution. Additionally,  $0 \leq \delta_i \leq 2\bar{\delta}, \forall i \in [n]$ .*

*Proof of Lemma 5.* First, since we consider strictly positive function  $f$ , the jump rate in Eq. (9) is always finite on a finite state space. Second, Lemma 4 gives

$$\frac{-|x_i|}{1-|x_i|} \leq S_i(x) \leq \frac{|x_i|}{1+|x_i|}, \quad \forall x \in (-1, 1)^n. \quad (15)$$

In particular, we obtain that for  $t \in [0, T_o]$ ,  $\frac{1-e^{-\tau}}{1+e^{-\tau}} \leq \frac{1}{2} - S_i(e^{-(T-t)}V_{t-}) \leq \frac{1+e^{-\tau}}{1-e^{-\tau}}$ . Back to Eq. (12), we verify that the jump rate on the  $i$ -th coordinate of  $W_t$  is nonnegative and finite, as long as  $0 < \bar{\delta} < \frac{1}{2}$ . For  $t \in [0, T]$ ,  $x = e^{-(T-t)}V_{t-}$ ,

$$\frac{1}{2} - S_i(x) + \delta_i \mathbf{1}_{t < \mathfrak{T}} S_i(x) = \begin{cases} \frac{1}{2} - S_i(x) + \bar{\delta} \mathbf{1}_{t < \mathfrak{T}} S_i(x) \geq \frac{1}{2} - S_i(x) \geq 0 & \text{if } S_i(x) > 0, \\ \left( \frac{1}{2} - S_i(x) \right) \left[ \mathbf{1}_{t \geq \mathfrak{T}} + \mathbf{1}_{t < \mathfrak{T}} \frac{1}{1 - 2\bar{\delta}S_i(x)} \right] \geq 0 & \text{otherwise.} \end{cases}$$

The bounded total jump rate ensures the existence and uniqueness of the solution of the SDE (12) (Chapter 4.7 [EK09]). Additionally, as long as  $0 < \bar{\delta} < \frac{1}{2}$ , we have

$$0 \leq \frac{1 - 2S_i(x)}{1 - 2\bar{\delta}S_i(x)} \leq 2,$$

which leads to  $0 < \delta_i \leq 2\bar{\delta}$ .  $\square$

**Joint generator representation** The use of the stopping time  $\mathfrak{T}$  makes the joint process  $(V_t, W_t)_{t \in [0, T]}$  no longer Markov. To make it Markov again, we could enlarge the state space with a flag variable  $I_t := \mathbf{1}_{t < \mathfrak{T}}$ , taking value on  $\{0, 1\}$ . Then the process  $(V_t, W_t, I_t)_{t \in [0, T]}$  is Markov. However, to simplify notation, we decide to not do so. Applying Itô's formula, for any function  $h : \{-1, 1\}^{2n} \rightarrow \mathbb{R}$ , we have

$$dh(V_t, W_t) = \mathcal{G}_t h(V_{t-}, W_{t-}) dt + dM_t^h,$$

where  $M_t^h$  is a local martingale.  $\mathcal{G}_t$  is a path-dependent and time-dependent operator adapted to  $\mathcal{F}_t$ , which we also call joint generator of  $(V_t, W_t)$ , with the form

$$\mathcal{G}_t := \bar{L}_t^0 + \mathbf{1}_{t < \mathfrak{T}} (\bar{L}_t - \bar{L}_t^0). \quad (16)$$

Here, with  $\rho_t = e^{-(T-t)}$ ,

$$\begin{aligned} \bar{L}_t^0 h(x, y) &= \sum_{i=1}^n [h(\varsigma_i(x), \varsigma_i(y)) - h(x, y)] \left( \frac{1}{2} - S_i(\rho_t x) \right), \\ A_t &= \bar{L}_t - \bar{L}_t^0, \\ A_t h(x, y) &= \sum_{i=1}^n \left\{ \mathbf{1}_{S_i(\rho_t x) \geq 0} [h(\varsigma_i(x), y) - h(\varsigma_i(x), \varsigma_i(y))] \delta_i(\rho_t x) S_i(\rho_t x) \right. \\ &\quad \left. + \mathbf{1}_{S_i(\rho_t x) < 0} [h(x, \varsigma_i(y)) - h(x, y)] [-\delta_i(\rho_t x)] S_i(\rho_t x) \right\}. \end{aligned}$$

We make a few remarks about  $\mathcal{G}_t$ .

- In words,  $\mathcal{G}_t$  does,
  - before  $\mathfrak{T}$  (always  $\leq T_o$ ), follow  $\bar{L}_t$ , the joint Markov semigroup with perturbation;
  - after  $\mathfrak{T}$ , follow  $\bar{L}_t^0$ , the joint Markov semigroup without perturbation.
- The path-dependency of  $\mathcal{G}_t$  only comes from the stopping time in  $\mathbf{1}_{t < \mathfrak{T}}$ .
- Without perturbation, as captured in  $\bar{L}_t^0$ , the two processes jump together. Consequently,  $\text{sign}(x \odot y)$  is preserved along  $\bar{L}_t^0$ .
- The perturbation part  $A_t$  always involves a jump on  $y$ .

### 3.2 Proof of Lemma 2 on the total variation control

In this subsection, we upper-bound the TV distance

$$d_{\text{TV}}(\text{Law}(V_{T_o}), \text{Law}(W_{T_o})) = \sup_{\phi: \{-1, 1\}^n \rightarrow \{0, 1\}} |\mathbb{E}[\phi(V_{T_o})] - \mathbb{E}[\phi(W_{T_o})]|.$$

The main idea is to apply Duhamel's formula from 0 to  $T_o$  by treating the joint generator (16) as unperturbed generator  $\bar{L}_t^0$  plus a small perturbation. A key observation on how the heat semigroup  $P_\tau$  helps in bounding TV distance is the following identity, which we prove later in Lemma 8. For any test function  $\phi : \{-1, 1\}^n \rightarrow \{0, 1\}$ ,

$$\mathbb{E}[\phi(V_{T_o}) - \phi(W_{T_o})] = \mathbb{E}[P_\tau \phi(V_T) - P_\tau \phi(W_T)].$$

Intuitively, instead of working with arbitrary bounded test functions in the TV distance definition, we only have to deal with “smoothed” test functions due to  $P_\tau$ .

However, upon testing our proof strategy with a single-stage Duhamel's formula, we realize that it cannot fully take advantage of the “smoothness” gained from  $P_\tau$ . We introduce a multi-stage Duhamel proof. We introduce  $m$  early-stopped perturbed processes, which interpolate between  $(V_t, V_t)$  and  $(V_t, W_t)$  as follows. Fix a partition of time intervals

$$0 = t_0 < t_1 < \dots < t_m = T_o,$$

with  $t_k - t_{k-1} = v$ , to be chosen.

**Early-stopped processes construction** For any  $k \in \{0, 1, \dots, m\}$ , define the early-stopped process  $(V_t, W_t^{(k)})_{t \in [0, T]}$ , using the same PRM as  $(V_t, W_t)_{t \in [0, T]}$ :

- on  $[0, t_k]$ , the same dynamics as  $(V_t, W_t)$  is used;
- on  $[t_k, T]$ , the perturbation is switched off;
- $(V_t)$  is never changed, which is why we kept the same notation.

In other words, its (path-dependent) generator satisfies

$$\mathcal{G}_t^{(k)} = \bar{L}_t^0 + \mathbf{1}_{t < \mathfrak{T} \wedge t_k} (\bar{L}_t - \bar{L}_t^0). \quad (17)$$

Just as how  $(V_t, W_t)$  is defined, these early-stopped processes are well-defined. Note that

$$\text{Law}(V_{T_o}) = \text{Law}(W_{T_o}^{(0)}), \quad \text{Law}(W_{T_o}) = \text{Law}(W_{T_o}^{(m)}).$$

By triangle inequality, we have

$$d_{\text{TV}} \left( \text{Law}(W_{T_o}^{(0)}), \text{Law}(W_{T_o}^{(m)}) \right) \leq \sum_{k=1}^m d_{\text{TV}} \left( \text{Law}(W_{T_o}^{(k-1)}), \text{Law}(W_{T_o}^{(k)}) \right). \quad (18)$$

What remains is to apply Duhamel to each term on the RHS. Before completing the proof of Lemma 2, we need three lemmas, with proofs deferred to Section 4.2.

**Lemma 6** (Basic level-1 inequality). *Let  $h : \{-1, 1\}^n \rightarrow \{0, 1\}$ . Consider its multilinear expansion. For any  $x \in (-1, 1)^n$ , we have*

$$\sum_{i=1}^n (1 - x_i^2) (\partial_i h(x))^2 \leq h(x) - h(x)^2.$$

This is a well-known consequence of Parseval's inequality for biased Fourier analysis, see, e.g., Section 3 of [EMR23] or Appendix 1 of [EG20].

**Lemma 7** (Expected total squared score bound). *Let  $n \geq 3, T \geq 100 \log(n)$ . For the reverse jump process (11), with  $\mathcal{V}_t = e^{-(T-t)} V_t$ , we have*

$$\mathbb{E} \left[ \int_0^{\mathfrak{T}} \sum_{i=1}^n S_i(\mathcal{V}_{t-})^2 dt \right] \leq \frac{4}{\alpha} \left( \log \eta + \frac{1}{2} \log \log \eta + 0.99 \right),$$

where  $\alpha = \frac{1-e^{-\tau}}{1+e^{-\tau}}$ .

Intuitively, as a consequence of Itô's formula applied to  $\log f(\mathcal{V}_t)$ , this lemma expresses that the total squared score  $\int_0^t \sum_{i=1}^n S_i(\mathcal{V}_{s-})^2 ds$  is closely related to  $\log f(\mathcal{V}_t) - \log f(\mathcal{V}_0)$ , up to a multiplicative factor.

**Lemma 8** (Reverse-time martingale identity). *For any  $k \in [m]$  and any  $\phi : \{-1, 1\}^n \rightarrow \{0, 1\}$ , we have*

$$\mathbb{E} \left[ \phi(W_{t_k}^{(k-1)}) - \phi(W_{t_k}^{(k)}) \right] = \mathbb{E} \left[ P_{T-t_k} \phi(W_T^{(k-1)}) - P_{T-t_k} \phi(W_T^{(k)}) \right].$$

This lemma is the main manifestation of the gained smoothness from the heat semigroup  $P_\tau$ . We are now ready to complete the proof of Lemma 2.

*Proof of Lemma 2.* Introduce the shorthand  $Z_t^{(k)} := (V_t, W_t^{(k)})$ . Let  $R_{s,t}^0$  and  $R_{s,t}$  be the Markov semigroups associated to the generators  $\bar{L}_t^0$  and  $\bar{L}_t$  respectively.

First, we derive Duhamel's formula. Given a test function  $h : \{-1, 1\}^{2n} \rightarrow \mathbb{R}$ , let  $u_t(z)$  be the post-switch process starting at time  $t \geq 0$ ,

$$u_t(z) := R_{t,T}^0 h(z).$$

Note that by definition,  $u_t$  satisfies the Kolmogorov backward equation

$$\frac{\partial u_t}{\partial t} + \bar{L}_t^0 u_t = 0.$$

Consider  $u_t(V_t, W_t^{(k)})$ , and apply Itô's formula for  $t \in [0, \mathfrak{T} \wedge t_k]$  to obtain

$$du_t(V_t, W_t^{(k)}) = \left( \frac{\partial u_t}{\partial t} + \bar{L}_t u \right) (V_{t-}, W_{t-}^{(k)}) ds + dM_t.$$

$M_t$  is a martingale. Integrating from 0 to  $\mathfrak{T} \wedge t_k$ , taking expectation and applying the optional stopping theorem, we obtain

$$\mathbb{E}[h(Z_{T_o}^{(k)})] - \mathbb{E}[h(Z_{T_o})] = \mathbb{E}[u_{\mathfrak{T} \wedge t_k}(Z_{\mathfrak{T} \wedge t_k}^{(k)})] - \mathbb{E}[u_0(Z_0)] = \mathbb{E} \left[ \int_0^{\mathfrak{T} \wedge t_k} (\bar{L}_s - \bar{L}_s^0) u_s(Z_{s-}^{(k)}) ds \right].$$

Doing the same for  $k-1$ , and noticing that  $Z_s^{(k)}$  is identical to  $Z_s^{(k-1)}$  until  $\mathfrak{T} \wedge t_{k-1}$ , we obtain Duhamel's formula

$$\mathbb{E}[h(Z_{T_o}^{(k)})] - \mathbb{E}[h(Z_{T_o}^{(k-1)})] = \mathbb{E} \left[ \int_{\mathfrak{T} \wedge t_{k-1}}^{\mathfrak{T} \wedge t_k} (\bar{L}_s - \bar{L}_s^0) u_s(Z_{s-}^{(k)}) ds \right]. \quad (19)$$

Second, we examine the terms in the above integral and bound it. Recall that  $A_t = \bar{L}_t - \bar{L}_t^0$ ,

$$\begin{aligned} A_t h(x, y) &= \sum_{i=1}^n \left\{ \mathbf{1}_{S_i(\rho_t x) \geq 0} [h(\varsigma_i(x), y) - h(\varsigma_i(x), \varsigma_i(y))] \delta_i(\rho_t x) S_i(\rho_t x) \right. \\ &\quad \left. + \mathbf{1}_{S_i(\rho_t x) < 0} [h(x, \varsigma_i(y)) - h(x, y)] [-\delta_i(\rho_t x)] S_i(\rho_t x) \right\}. \end{aligned}$$

Thanks to Lemma 8, we are only interested in test functions of the form  $h(x, y) = \varphi(y)$ , where  $\varphi = P_{T-t_k} \phi$  (we omit the  $k$ -dependency to simplify notation). Then

$$\begin{aligned} u_s(x, y) &= \mathbb{E}[h(V_{T_o}, W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (x, y)] \\ &= \mathbb{E}[\varphi(W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (x, y)] \\ \Delta_i^y u_s(x, y) &= \mathbb{E}[\varphi(W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (x, \varsigma_i(y))] - \mathbb{E}[\varphi(W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (x, y)] \\ &\stackrel{(i)}{=} \mathbb{E}[\Delta_i \varphi(W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (x, y)] \\ \Delta_i^y u_s(\varsigma_i(x), y) &= \mathbb{E}[\Delta_i \varphi(W_{T_o}^{(0)}) \mid (V_s, W_s^{(0)}) = (\varsigma_i(x), y)]. \end{aligned}$$

(i) follows from the fact that  $W^{(0)}$  has jump rates that only depend on  $V$ , so a flip at initialization results in a flip in the end. Consequently, with  $\mathcal{V}_t = \rho_t V_t$ ,

$$\begin{aligned} A_s u_s(Z_{s-}^{(k)}) &= \sum_{i=1}^n \left\{ \mathbf{1}_{S_i(\mathcal{V}_{s-}) \geq 0} [\Delta_i^y u_s(\varsigma_i(V_{s-}), W_{s-}^{(k)})] + \mathbf{1}_{S_i(\mathcal{V}_{s-}) < 0} [\Delta_i^y u_s(V_{s-}, W_{s-}^{(k)})] \right\} \delta_i(\mathcal{V}_{s-}) S_i(\mathcal{V}_{s-}). \quad (20) \end{aligned}$$

Applying Cauchy-Schwarz inequality and  $0 \leq \delta_i \leq 2\bar{\delta}$  from Lemma 5, we bound the second sum in Eq. (20)

$$\begin{aligned} & \left| \sum_{i=1}^n \mathbf{1}_{S_i(\mathcal{V}_{s-}) < 0} \left[ \Delta_i^y u_s(V_{s-}, W_{s-}^{(k)}) \right] \delta_i(\mathcal{V}_{s-}) S_i(\mathcal{V}_{s-}) \right| \\ & \leq 2\bar{\delta} \mathbb{E} \left[ \left( \sum_{i=1}^n \left( \Delta_i \varphi(W_{T_o}^{(0)}) \right)^2 \right)^{\frac{1}{2}} \mid (V_s, W_s^{(0)}) = (V_{s-}, W_{s-}^{(k)}) \right] \left( \sum_{i=1}^n S_i^2(\mathcal{V}_{s-}) \right)^{\frac{1}{2}} \\ & \stackrel{(i)}{\leq} 2\bar{\delta} \left( \frac{4e^{-2(T-t_k)}}{1 - e^{-2(T-t_k)}} \right)^{\frac{1}{2}} \left( \sum_{i=1}^n S_i^2(\mathcal{V}_{s-}) \right)^{\frac{1}{2}}. \end{aligned}$$

(i) applies the level-1 inequality pointwise from Lemma 6 using that fact that  $\varphi = P_{T-t_k}\phi = \phi(e^{-(T-t_k)})$ , which exploits the fact that the argument is in the inner cube. The first sum in Eq. (20) is bounded in the same way. Combining both bounds into Eq. (19), we obtain

$$\begin{aligned} \left| \mathbb{E}[h(Z_{T_o}^{(k)})] - \mathbb{E}[h(Z_{T_o}^{(k-1)})] \right| & \leq 4\bar{\delta} \left( \frac{4e^{-2(T-t_k)}}{1 - e^{-2(T-t_k)}} \right)^{\frac{1}{2}} \mathbb{E} \left[ \int_{t_{k-1}}^{t_k} \mathbf{1}_{s < \mathfrak{T}} \left( \sum_{i=1}^n S_i^2(\mathcal{V}_{s-}) \right)^{\frac{1}{2}} ds \right] \\ & \stackrel{(i)}{\leq} 4\bar{\delta} \left( \frac{4e^{-2(T-t_k)}}{1 - e^{-2(T-t_k)}} \right)^{\frac{1}{2}} (t_k - t_{k-1})^{\frac{1}{2}} \left( \mathbb{E} \left[ \int_0^{\mathfrak{T}} \sum_{i=1}^n S_i(\mathcal{V}_{s-})^2 ds \right] \right)^{\frac{1}{2}} \\ & \leq \frac{8\bar{\delta}e^{-\tau}}{(1 - e^{-2\tau})^{\frac{1}{2}}} e^{-T_o + kv} \sqrt{v} \left( \mathbb{E} \left[ \int_0^{\mathfrak{T}} \sum_{i=1}^n S_i(\mathcal{V}_{s-})^2 ds \right] \right)^{\frac{1}{2}}. \end{aligned}$$

(i) applies Cauchy-Schwarz inequality. The expected total squared score is bounded via Lemma 7,

$$\mathbb{E} \left[ \int_0^{\mathfrak{T}} \sum_{i=1}^n S_i(\mathcal{V}_{s-})^2 ds \right] \leq \frac{4}{\alpha} \left( \log \eta + \frac{1}{2} \log \log \eta + 0.99 \right).$$

Summing over  $k$  from 1 to  $m$ , using  $mv = T_o$ , we have

$$\sum_{k=1}^m e^{-T_o + kv} \sqrt{v} = \frac{\sqrt{v}}{1 - e^{-v}} (1 - e^{-T_o}) \stackrel{(i)}{\leq} \frac{\sqrt{2}}{1 - e^{-1}}.$$

(i) follows because we choose  $m = \lfloor T_o \rfloor$  and  $T_o > 1$ , then  $1 \leq v \leq 2$ .

Finally, applying Lemma 8 and triangle inequality in Eq. (18), we have

$$\begin{aligned} d_{\text{TV}} \left( \text{Law}(W_{T_o}^{(0)}), \text{Law}(W_{T_o}^{(m)}) \right) & \leq c \frac{e^{-\tau}}{\alpha^{\frac{1}{2}} (1 - e^{-2\tau})^{\frac{1}{2}}} \bar{\delta} \sqrt{\log \eta} \\ & \leq c \frac{e^{-\tau}}{1 - e^{-\tau}} \bar{\delta} \sqrt{\log \eta}. \end{aligned}$$

In fact, we also have an explicit bound on the constant,  $c \leq 32$ . □

**Remark 4.** The single-stage Duhamel proof is loose with a  $\sqrt{T}$  factor from the application of Cauchy-Schwarz inequality. With our choice of  $T$ , it would be of order  $\sqrt{\log n}$ , making the final bound no longer dimension-free. The purpose of our multi-stage Duhamel proof is to save this extra  $\sqrt{\log n}$  factor.

**Remark 5.** A natural alternative idea to bound the TV distance is through a Kullback-Leibler (KL) divergence bound and Pinsker's inequality. The KL divergence can be bounded via Girsanov's theorem applied to jump processes (see e.g. [Léo12]). However, to bound KL divergence this way requires a bound on  $\sum_{i=1}^n (S_i(\rho_t V_t) - S_i(\rho_t W_t))^2$ , and the author was unable to obtain a good bound of this type. Intuitively, while in the Gaussian counterpart the perturbed process and the original process are closed in  $L^2$  distance, the discrete nature of the Boolean hypercube  $\{-1, 1\}^n$  makes them far apart in  $L^2$  distance. This is, according to the author, the main difficulty in working with the perturbed reverse process on the Boolean hypercube.

Another idea to bound the TV distance is to follow the proof in [EL18] and [Leh16]. They crucially use the semi-log-convexity gained from the heat semigroup (see Eq. (5.6) in [Leh16]), and the second-order Taylor expansion derived from it. As we show in Lemma 12 in Appendix, the heat semigroup on the Boolean hypercube also provides a similar semi-log-convexity and allows us to write a similar second-order Taylor expansion as follows

$$\log P_\tau f(W_{T_o}) \geq \log P_\tau f(V_{T_o}) + \langle \nabla \log P_\tau f(V_{T_o}), W_{T_o} - V_{T_o} \rangle - \frac{c_\tau}{2} \|W_{T_o} - V_{T_o}\|_2^2,$$

for a constant  $c_\tau$  that only depends on  $\tau$ . However, again, the difficulty to proceed from here is that the author was unable to obtain a good dimension-free  $L^2$  bound on  $\|W_{T_o} - V_{T_o}\|_2$ , which is intuitively quite large as the distance between two points on the Boolean hypercube. Our whole proof was designed to avoid such  $L^2$  bounds.

### 3.3 Proof of Lemma 3 on the approximate monotone coupling at tail

In this section, we show that our coupling construction  $(V, W)$  makes  $\log P_\tau f(V_{T_o})$  strictly larger than  $\log P_\tau f(W_{T_o})$  conditioned on  $\log P_\tau f(W_{T_o})$  being large, via stochastic calculus. It is more convenient to work with scaled processes, with  $\rho_t = e^{-(T-t)}$ ,

$$\begin{aligned} \mathcal{V}_t &= \rho_t V_t, \\ \mathcal{W}_t &:= \rho_t W_t. \end{aligned}$$

Then  $P_{T-t}f(V_t) = f(\mathcal{V}_t)$  and  $P_{T-t}f(W_t) = f(\mathcal{W}_t)$ . Applying Itô's formula to  $\log f(\mathcal{V}_t)$  and  $\log f(\mathcal{W}_t)$ , we obtain

$$\begin{aligned} d \log f(\mathcal{V}_t) &= \sum_{i=1}^n \left[ S_i(\mathcal{V}_{t-}) dt + \int \log(1 - 2S_i(\mathcal{V}_{t-})) \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(\mathcal{V}_{t-})} N^{[i]}(dt, dz) \right], \\ d \log f(\mathcal{W}_t) &= \sum_{i=1}^n \left[ S_i(\mathcal{W}_{t-}) dt + \int \log(1 - 2S_i(\mathcal{W}_{t-})) \mathbf{1}_{0 < z \leq \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}}) S_i(\mathcal{V}_{t-})} N^{[i]}(dt, dz) \right], \end{aligned}$$

where recall that  $\delta_i \equiv \delta_i(\mathcal{V}_{t-})$ , with  $0 < \bar{\delta} < \frac{1}{2}$ ,

$$\delta_i(x) = \bar{\delta} \left[ \mathbf{1}_{S_i(x) > 0} + \frac{1 - 2S_i(x)}{1 - 2\bar{\delta}S_i(x)} \mathbf{1}_{S_i(x) \leq 0} \right], \quad i \in [n], \quad x \in [-1, 1]^n.$$

Introduce the shorthand  $(v_i, w_i) := (S_i(\mathcal{V}_{t-}), S_i(\mathcal{W}_{t-}))$ , where we omit the dependency on  $t$  as long as it is clear from the context. Then the two SDEs above become

$$\begin{aligned} d \log f(\mathcal{V}_t) &= \sum_{i=1}^n \left[ v_i dt + \int \log(1 - 2v_i) \mathbf{1}_{0 < z \leq \frac{1}{2} - v_i} N^{[i]}(dt, dz) \right], \\ d \log f(\mathcal{W}_t) &= \sum_{i=1}^n \left[ w_i dt + \int \log(1 - 2w_i) \mathbf{1}_{0 < z \leq \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}})v_i} N^{[i]}(dt, dz) \right]. \end{aligned} \quad (21)$$

To complete the proof of Lemma 3, we need three lemmas which bound quantities in Eq. (21) with high probability. Their proofs are deferred to Section 4.3.

**Lemma 9.** *With probability at least  $1 - \frac{1}{\sqrt{\log \eta}}$ , we have*

$$\log f(\mathcal{V}_{T_o}) > \log f(\mathcal{V}_{\mathfrak{T}}) - \frac{1}{2} \log \log \eta.$$

Since  $\mathfrak{T}$  is always upper bounded by  $T_o$ , from Eq. (21),  $\log f(\mathcal{V}_{T_o}) - \log f(\mathcal{V}_{\mathfrak{T}})$  has nonnegative drift terms. Lemma 9 states that the noise term does not alter the nonnegativity too much.

**Lemma 10.** *With probability at least  $1 - \frac{1}{\sqrt{\log \eta}}$ , we have*

$$\log f(\mathcal{W}_{\mathfrak{T}}) - \log f(\mathcal{W}_0) < \left[ 2 \sum_{i=1}^n \int_0^{\mathfrak{T}} (1 - \delta_i) w_i v_i dt \right] + \frac{1}{2} \log \log \eta.$$

In words, Lemma 10 upper bounds  $\log f(\mathcal{W}_{\mathfrak{T}})$  with the corresponding score terms with high probability.

**Lemma 11.** *With probability at least  $1 - \frac{1}{\sqrt{\log \eta}}$ , we have*

$$\log f(\mathcal{W}_{T_o}) - \log f(\mathcal{V}_{T_o}) < \left[ -2 \sum_{i=1}^n \int_0^{\mathfrak{T}} \delta_i \left( \mathbf{1}_{v_i > 0} + \mathbf{1}_{v_i \leq 0} \frac{1}{1 - 2v_i} \right) w_i v_i dt \right] + \frac{1}{2} \log \log \eta.$$

Roughly speaking, Lemma 11 shows that with high probability,  $\log f(\mathcal{V}_{T_o})$  is slightly larger than  $\log f(\mathcal{W}_{T_o})$  by a term proportional to  $\bar{\delta}$ . We are now ready to prove Lemma 3.

*Proof of Lemma 3.* Define the events

$$\begin{aligned} \mathcal{E}_1 &:= \left\{ \log f(\mathcal{V}_{T_o}) > \log f(\mathcal{V}_{\mathfrak{T}}) - \frac{1}{2} \log \log \eta \right\} \\ \mathcal{E}_2 &:= \left\{ \log f(\mathcal{W}_{\mathfrak{T}}) - \log f(\mathcal{W}_0) < \left[ 2 \sum_{i=1}^n \int_0^{\mathfrak{T}} (1 - \delta_i) w_i v_i dt \right] + \frac{1}{2} \log \log \eta \right\}, \\ \mathcal{E}_3 &:= \left\{ \log f(\mathcal{W}_{T_o}) - \log f(\mathcal{V}_{T_o}) < \left[ -2 \sum_{i=1}^n \int_0^{\mathfrak{T}} \delta_i \left( \mathbf{1}_{v_i > 0} + \mathbf{1}_{v_i \leq 0} \frac{1}{1 - 2v_i} \right) w_i v_i dt \right] + \frac{1}{2} \log \log \eta \right\}. \end{aligned}$$

Applying Lemma 9, 10 and 11, we have

$$\mathbb{P}(\mathcal{E}_1 \cap \mathcal{E}_2 \cap \mathcal{E}_3) \geq 1 - \frac{3}{\sqrt{\log \eta}}. \quad (22)$$

The rest of proof is conditioned on all three events. Our choice of  $\delta_i$  allows us to connect the two quantities on the RHS. Recall that

$$\delta_i = \bar{\delta} \left[ \mathbf{1}_{v_i > 0} + \frac{1 - 2v_i}{1 - 2\bar{\delta}v_i} \mathbf{1}_{v_i \leq 0} \right], \quad i \in [n], \quad x \in [-1, 1]^n.$$

Observe that

$$1 - \delta_i = (1 - \bar{\delta}) \mathbf{1}_{v_i > 0} + \left(1 - \bar{\delta} \frac{1 - 2v_i}{1 - 2\bar{\delta}v_i}\right) \mathbf{1}_{v_i \leq 0} = (1 - \bar{\delta}) \left[ \mathbf{1}_{v_i > 0} + \frac{1}{1 - 2\bar{\delta}v_i} \mathbf{1}_{v_i \leq 0} \right]$$

$$\delta_i \left( \mathbf{1}_{v_i > 0} + \mathbf{1}_{v_i \leq 0} \frac{1}{1 - 2v_i} \right) = \bar{\delta} \left[ \mathbf{1}_{v_i > 0} + \frac{1}{1 - 2\bar{\delta}v_i} \mathbf{1}_{v_i \leq 0} \right] \stackrel{(i)}{=} \frac{\bar{\delta}}{1 - \bar{\delta}} (1 - \delta_i).$$

(i) uses the expression of  $1 - \delta_i$  in the first line. Consequently,

$$\delta_i w_i v_i \left( \mathbf{1}_{v_i > 0} + \mathbf{1}_{v_i \leq 0} \frac{1}{1 - 2v_i} \right) = \frac{\bar{\delta}}{1 - \bar{\delta}} [(1 - \delta_i) w_i v_i].$$

This connects  $\mathcal{E}_2$  and  $\mathcal{E}_3$ , and allows us to obtain, under  $\mathcal{E}_2 \cap \mathcal{E}_3$ ,

$$\log f(\mathcal{W}_{T_o}) - \log f(\mathcal{V}_{T_o}) < -\frac{\bar{\delta}}{1 - \bar{\delta}} \left[ \log f(\mathcal{W}_{\mathfrak{T}}) - \log f(\mathcal{W}_0) - \frac{1}{2} \log \log \eta \right] + \frac{1}{2} \log \log \eta.$$

Rearranging, we obtain

$$\log f(\mathcal{V}_{T_o}) > \log f(\mathcal{W}_{T_o}) + \frac{\bar{\delta}}{1 - \bar{\delta}} [\log f(\mathcal{W}_{\mathfrak{T}}) - \log f(\mathcal{W}_0)] - \frac{1}{2(1 - \bar{\delta})} \log \log \eta. \quad (23)$$

The event  $\{\log f(\mathcal{W}_{T_o}) > \log \eta\}$  implies that, based on our definition of stopping time (13),

$$\text{either } \log f(\mathcal{V}_{\mathfrak{T}}) \geq \log \eta + \frac{1}{2} \log \log \eta + 1 \text{ or } \log f(\mathcal{W}_{\mathfrak{T}}) \geq \log \eta.$$

If the first case holds at  $\mathfrak{T}$ , then by Lemma 9, under  $\mathcal{E}_1$

$$\log f(\mathcal{V}_{T_o}) \geq \log f(\mathcal{V}_{\mathfrak{T}}) - \frac{1}{2} \log \log \eta \geq \log \eta + 1.$$

If the second case holds at  $\mathfrak{T}$ , then from Eq. (23), using Lemma 4,  $\log f(\mathcal{W}_0) \leq \log(1 + e^{-T})^n \leq 1/n^{99} \leq 0.01$  if  $T \geq 100 \log n$  and  $n \geq 3$ . For  $\eta > e^3$ ,  $\frac{\frac{1}{2} \log \log \eta + 0.91}{\log \eta} \leq 0.49$ . For  $\bar{\delta} \geq \frac{\frac{1}{2} \log \log \eta + 0.91}{\log \eta}$ , under  $\mathcal{E}_2 \cap \mathcal{E}_3$ ,

$$\log f(\mathcal{V}_{T_o}) > \log \eta + \frac{1}{1 - \bar{\delta}} \left[ \bar{\delta}(\log \eta - 0.01) - \frac{1}{2} \log \log \eta \right] \geq \log \eta + 1.$$

Combining both cases, we obtain the following implication

$$\mathcal{E}_1 \cap \mathcal{E}_2 \cap \mathcal{E}_3 \cap \{\log f(\mathcal{W}_{T_o}) > \log \eta\} \implies \{\log f(\mathcal{V}_{T_o}) > \log \eta + 1\}.$$

Together with Eq. (22), we conclude that

$$\mathbb{P}(\log f(\mathcal{V}_{T_o}) > \log \eta + 1) \geq \mathbb{P}(\log f(\mathcal{V}_{T_o}) > \log \eta) - \frac{3}{\sqrt{\log \eta}}.$$

□

**Remark 6.** The main difference between Poisson noise in the reverse heat process in the Boolean setting and Brownian motion in the reverse OU process in the Gaussian setting is that the former's law is not symmetric. This is why (1) we have to design state-dependent perturbation, (2) we lower bound the unperturbed process by the perturbed process while it is in the reverse direction in the Gaussian counterpart [EL18]. Lower bounding the noise in Lemma 11 is more challenging than upper bounding it.

In view of the exponential martingale bound in Lemma 11, it is reasonable to conjecture that one might be able to obtain a better bound to save the extra  $\log \log \eta$  factor via a similar strategy. One possibility is to obtain a better  $L^2$  bound on  $\sum_i (w_i - v_i)^2$  and use a larger  $\gamma$  in Eq. (28) in the proof of Lemma 11. However, as we discussed in Remark 5, the author was unable to prove a good dimension-free  $L^2$  bound. Our current construction is designed to avoid the appearance of terms like  $\sum_i (w_i - v_i)^2$ .

## 4 Proofs of other lemmas

In this section, we complete the missing proofs.

### 4.1 Proof related to smoothness

Here we prove Lemma 4, which quantifies one form of smoothness brought by the heat semigroup.

*Proof of Lemma 4.* Note that for  $z \in \{-1, 1\}^n$ , we may write

$$f(z) = \sum_{y \in \{-1, 1\}^n} f(y) \prod_{j=1}^n \left( \frac{1 + y_j z_j}{2} \right).$$

This gives another multilinear polynomial expansion, which takes value  $f(y)$  for any  $y \in \{-1, 1\}^n$ . By the uniqueness of the multilinear polynomial expansion, we conclude that this polynomial agrees with the one in Eq. (4). It shows that for any  $z \in [-1, 1]^n$ ,  $f(z) \geq 0$ , because  $f(y) \geq 0$  for  $y \in \{-1, 1\}^n$  and  $1 + y_i z_i \geq 0$ . Additionally, for any  $z \in (-1, 1)^n$ , because  $1 - |z_i| \leq 1 + y_i z_i \leq 1 + |z_i|$ ,

$$\|f\|_1 \prod_{j=1}^n (1 - |z_i|) \leq f(z) \leq \|f\|_1 \prod_{j=1}^n (1 + |z_i|).$$

Now for  $z \in [-1, 1]^n$ , write

$$f(z) = (1 + z_i) \underbrace{\sum_{y \in \{-1, 1\}^n, y_i=1} f(y) \prod_{j \in [n], j \neq i} \left( \frac{1 + y_j z_j}{2} \right)}_{=: R_1} + (1 - z_i) \underbrace{\sum_{y \in \{-1, 1\}^n, y_i=-1} f(y) \prod_{j \in [n], j \neq i} \left( \frac{1 + y_j z_j}{2} \right)}_{=: R_2}.$$

Note that  $R_1 \geq 0$  and  $R_2 \geq 0$ , for the same reason why  $f(z) \geq 0$ . We have

$$\begin{aligned} f(z) &= (1 + z_i)R_1 + (1 - z_i)R_2 \\ f(\varsigma_i(z)) &= (1 - z_i)R_1 + (1 + z_i)R_2 \end{aligned}$$

Then if  $z_i > 0$ ,

$$\frac{f(\varsigma_i(z))}{f(z)} = \frac{1 - z_i}{1 + z_i} + \frac{\left[(1 + z_i) - \frac{(1 - z_i)^2}{1 + z_i}\right] R_1}{(1 - z_i)R_1 + (1 + z_i)R_2} \geq \frac{1 - |z_i|}{1 + |z_i|}.$$

If  $z_i < 0$ ,

$$\frac{f(\varsigma_i(z))}{f(z)} = \frac{1 + z_i}{1 - z_i} + \frac{\left[(1 - z_i) - \frac{(1 + z_i)^2}{1 - z_i}\right] R_2}{(1 - z_i)R_1 + (1 + z_i)R_2} \geq \frac{1 - |z_i|}{1 + |z_i|}.$$

Overall,  $\frac{f(\varsigma_i(z))}{f(z)} \geq \frac{1 - |z_i|}{1 + |z_i|}$ . Finally, by considering  $\varsigma_i(x)$  in the place of  $x$ , we also obtain an upper bound.  $\square$

## 4.2 Proofs related to Lemma 2

Here we prove Lemma 6, 7 and 8.

*Proof of Lemma 6.* We first introduce the basics of  $p$ -biased analysis on the Boolean hypercube. For a reference, see [EG20] or Section 8 of [O'D14]. Let  $p = (p_1, \dots, p_n) \in [0, 1]^n$ , and let  $\mu_p$  be the following product measure on  $\{-1, 1\}^n$ , with

$$\mu_p(y) := \prod_{i=1}^n \frac{1 + y_i(2p_i - 1)}{2},$$

where the  $i$ -th marginal takes value 1 with probability  $p_i$  and value  $-1$  with probability  $1 - p_i$ . For  $i \in [n]$ , define  $\phi_i : \{-1, 1\}^n \rightarrow \mathbb{R}$  as

$$\phi_i(y) := \frac{1}{2} \left( \frac{1 - 2p_i}{\sqrt{p_i(1 - p_i)}} + y_i \frac{1}{\sqrt{p_i(1 - p_i)}} \right). \quad (24)$$

For  $S \subseteq [n]$ , define  $\phi_S := \prod_{i \in S} \phi_i$ , and  $\phi_\emptyset := 1$  by convention.

**Proposition 1** (Proposition 31 in [EG20]).  $(\phi_S)_{S \subseteq [n]}$  form an orthonormal basis for the space of functions on  $\{-1, 1\}^n$ , equipped with the inner product  $\langle f, g \rangle_{\mu_p} := \mathbb{E}_{\mu_p}[fg]$ . Any function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}$  can be written as

$$f(y) = \sum_{S \in [n]} \hat{f}_p(S) \phi_S(y), \quad \forall y \in \{-1, 1\}^n,$$

where  $\hat{f}_p(S) := \mathbb{E}_{\mu_p}[f\phi_S]$  is called the  $p$ -biased Fourier coefficients of  $f$ . Additionally, let  $\mathfrak{S} = \{i_1, \dots, i_k\} \subseteq [n]$  be a set of indices and  $z \in (-1, 1)^n$ , if  $p = \frac{1+z}{2}$ , then

$$\partial_{i_1} \dots \partial_{i_k} f(z) = \left( \prod_{i \in \mathfrak{S}} \frac{1}{\sqrt{1 - z_i^2}} \right) \hat{f}_p(\mathfrak{S}). \quad (25)$$

Remark that Eq. 25 differs from that in Proposition 31 in [EG20] by a factor 4 on each term in the product. We believe that it was a typo, so we provide a proof in Appendix A.1 for completeness.

Take  $p = \frac{1+x}{2}$ . Applying Parseval's inequality, we have

$$\langle h, h \rangle_{\mu_p} \geq \hat{f}_p(\emptyset)^2 + \sum_{i=1}^n \hat{f}_p(\{i\})^2. \quad (26)$$

Note that  $\langle h, h \rangle_{\mu_p} = \mathbb{E}_{\mu_p} h^2 \stackrel{(i)}{=} \mathbb{E}_{\mu_p} h = \hat{f}_p(\emptyset)$ , where (i) follows from the fact that  $h$  takes value in  $\{0, 1\}$ . Additionally, according to Proposition 1,

$$\hat{f}_p(\emptyset) = f(x), \quad \hat{f}_p(\{i\}) = \sqrt{1 - x_i^2} \partial_i f(x).$$

Conclude by plugging these values to the Parseval's inequality (26).  $\square$

*Proof of Lemma 7.* It is more convenient to work with the scaled reverse jump process  $\mathcal{V}_t = e^{-(T-t)} V_t$ . Applying Itô's formula to  $\log f(\mathcal{V}_t)$ , we obtain

$$\begin{aligned} d \log f(\mathcal{V}_t) &= \sum_{i=1}^n \left[ S_i(\mathcal{V}_{t-}) dt + \int \log(1 - 2S_i(\mathcal{V}_{t-})) \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(\mathcal{V}_{t-})} N^{[i]}(dt, dz) \right] \\ &= \sum_{i=1}^n \left[ S_i(\mathcal{V}_{t-}) + \left( \frac{1}{2} - S_i(\mathcal{V}_{t-}) \right) \log(1 - 2S_i(\mathcal{V}_{t-})) \right] dt \\ &\quad + \int \log(1 - 2S_i(\mathcal{V}_{t-})) \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(\mathcal{V}_{t-})} \tilde{N}^{[i]}(dt, dz). \end{aligned}$$

We claim that

$$x \log(x) - x + 1 \geq \frac{\alpha}{2}(x-1)^2 \text{ for } 0 \leq x \leq \frac{1}{\alpha}. \quad (27)$$

For  $t \leq T_o = T - \tau$ , Lemma 4 implies that  $0 \leq 1 - 2S_i(\mathcal{V}_t) \leq \frac{1}{\alpha}$  where  $\alpha = \frac{1-e^{-\tau}}{1+e^{-\tau}}$ . Applying the claim and integrating Itô's formula to obtain

$$\begin{aligned} \log f(\mathcal{V}_{\bar{\tau}}) &\geq \log f(\mathcal{V}_0) + \frac{\alpha}{4} \int_0^{\bar{\tau}} \sum_{i=1}^n S_i(\mathcal{V}_{t-})^2 dt \\ &\quad + \int_0^{\bar{\tau}} \sum_{i=1}^n \left[ \int \log(1 - 2S_i(\mathcal{V}_{t-})) \mathbf{1}_{0 < z \leq \frac{1}{2} - S_i(\mathcal{V}_{t-})} \tilde{N}^{[i]}(dt, dz) \right]. \end{aligned}$$

The martingale term has expectation 0 by the optional stopping theorem. By the trivial lower bound of  $f$  in Lemma 4,  $\log f(\mathcal{V}_0) = \log f(e^{-T} V_0) \geq n \log(1 - e^{-T}) \geq \frac{-ne^{-T}}{1-e^{-T}} \geq -0.01$ , when  $n \geq 3$  and  $T \geq 100 \log(n)$ . And  $\log f(\mathcal{V}_{\bar{\tau}}) \leq \log \eta + \frac{1}{2} \log \log \eta + 1$  by the stopping time definition (13). We conclude that

$$\mathbb{E} \left[ \int_0^{\bar{\tau}} \sum_{i=1}^n S_i(\mathcal{V}_{t-})^2 dt \right] \leq \frac{4}{\alpha} \left[ \log \eta + \frac{1}{2} \log \log \eta + 0.99 \right].$$

**Verify the claim (27)** Consider the function  $q(x) := x \log(x) - x + 1 - \frac{\alpha}{2}(x-1)^2$

$$\begin{aligned} q'(x) &= \log x - \alpha(x-1) \\ q''(x) &= \frac{1}{x} - \alpha \end{aligned}$$

For  $0 \leq x \leq \frac{1}{\alpha}$ ,  $q''(x) \geq 0$ ,  $q$  is convex.  $q(1) = 0$ ,  $q(0) \geq 1 - \frac{\alpha}{2} > 0$ ,  $q'(1) = 0$  and  $q'(x) \geq 0$  for  $x \geq 1$  as it is increasing. Then  $q$  is non-decreasing from  $x = 1$ . Hence,  $q(x) \geq 0$  for  $0 \leq x \leq \frac{1}{\alpha}$ .  $\square$

*Proof of Lemma 8.* First, observe that when  $k = 0$ ,  $W^{(0)} = V$ , it is easy to show the identity

$$\mathbb{E}[\phi(V_0)] \stackrel{(i)}{=} \int \phi P_T f d\mu \stackrel{(ii)}{=} \int f P_T \phi d\mu = \mathbb{E}[P_T \phi(V_T)].$$

This identity only uses (i) the law of  $V_0$  has density  $P_T f$  as the time reversal of heat process, and (ii)  $P_T$  is symmetric with respect to the invariant measure  $\mu$  and the law of  $V_T$  has density  $f$ . Next, we deal with general  $k \in [m]$ . Define the reversed pair, for  $t \in [0, T-t_k]$ ,

$$(U_t, \vec{W}_t) := (V_{T-t}, W_{T-t}^{(k)}).$$

$U_t = V_{T-t}$  is already known by definition, so the above definition defines  $\vec{W}_t$ . We claim that  $(U_t, \vec{W}_t)_{t \in [0, T-t_k]}$  is a (time-homogeneous) Markov process with generator  $\vec{L}$ , for any test function  $h : \{-1, 1\}^n \rightarrow \mathbb{R}$ ,

$$\vec{L} h(x, y) = \frac{1}{2} \sum_{i=1}^n [h(\varsigma_i(x), \varsigma_i(y)) - h(x, y)].$$

In words, each coordinate flips synchronously in both processes at rate 1/2 independent of other coordinates. This is because (i)  $U_t$  is the time-reversal of  $V_t$ , and it is the heat process with jump rate 1/2 on each coordinate; (ii) on  $[t_k, T]$ ,  $(V, W^{(k)})$  jump synchronously with rates only depending on  $V$ , which forces the reversed pair to jump synchronously. As a consequence, we have

$$\mathbb{E}[\phi(\vec{W}_{T-t_k}) \mid (U_0, \vec{W}_0)] = \mathbb{E}[\phi(\vec{W}_0 \odot U_0 \odot U_{T-t_k}) \mid (U_0, \vec{W}_0)] = P_{T-t_k} \phi(\vec{W}_0).$$

Taking expectation, applying tower property and rewriting, we obtain

$$\mathbb{E}[\phi(W_{t_k}^{(k)})] = \mathbb{E}[P_{T-t_k} \phi(W_T^{(k)})].$$

$\square$

### 4.3 Proofs related to Lemma 3

*Proof of Lemma 9.* Recall from Eq. (21) that  $\log f(\mathcal{V}_t)$  satisfies the following SDE

$$d \log f(\mathcal{V}_t) = \sum_{i=1}^n \left[ v_i dt + \int \log(1-2v_i) \mathbf{1}_{0 < z \leq \frac{1}{2}-v_i} N^{[i]}(dt, dz) \right],$$

where  $v_i = S_i(\mathcal{V}_{t-})$ . Let  $\psi_i := \log(1 - 2v_i) \mathbf{1}_{0 < z \leq \frac{1}{2} - v_i}$ . Let  $\gamma > 0$ . Introduce the exponentiated process

$$\Psi_t := \exp \left[ \gamma \int_0^t \int \sum_i \psi_i N^{[i]}(ds, dz) - \int_0^t \int \sum_i [\exp(\gamma\psi_i) - 1] dz ds \right].$$

Applying Itô's formula, we obtain

$$\begin{aligned} d\Psi_t &= \Psi_{t-} \left( - \int \sum_{i=1}^n [\exp(\gamma\psi_i) - 1] dz dt \right) + \sum_{i=1}^n \int [\Psi_{t-} \exp(\gamma\psi_i) - \Psi_{t-}] N^{[i]}(dt, dz) \\ &= \sum_{i=1}^n \int [\Psi_{t-} \exp(\gamma\psi_i) - \Psi_{t-}] \tilde{N}^{[i]}(dt, dz). \end{aligned}$$

$(\Psi_t)_{t \geq 0}$  is a local martingale. Take  $\gamma = -1$ , observe that  $\Psi_t = \frac{1}{f(\mathcal{V}_t)}$ . The optional stopping theorem gives  $\mathbb{E}[\Psi_{T_o} | \mathcal{F}_{\mathfrak{T}}] = \Psi_{\mathfrak{T}}$ . Apply Markov's inequality conditioned on  $\mathcal{F}_{\mathfrak{T}}$ , for any  $\theta > 0$ , we have

$$\mathbb{P}(\Psi_{T_o} \geq \theta \Psi_{\mathfrak{T}} | \mathcal{F}_{\mathfrak{T}}) \leq \frac{\mathbb{E}[\Psi_{T_o} | \mathcal{F}_{\mathfrak{T}}]}{\theta \Psi_{\mathfrak{T}}} \leq \frac{1}{\theta}.$$

Taking expectation gives

$$\mathbb{P}(-\log f(\mathcal{V}_{T_o}) \geq -\log f(\mathcal{V}_{\mathfrak{T}}) + \log \theta) = \mathbb{P}(\Psi_{T_o} \geq \theta \Psi_{\mathfrak{T}}) \leq \frac{1}{\theta}.$$

Conclude with the choice  $\theta = \sqrt{\log \eta}$ .  $\square$

*Proof of Lemma 10.* Recall from Eq. (21) that  $\log f(\mathcal{W}_t)$  satisfies the following SDE

$$d \log f(\mathcal{W}_t) = \sum_{i=1}^n \left[ w_i dt + \int \log(1 - 2w_i) \mathbf{1}_{0 < z \leq \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}})v_i} N^{[i]}(dt, dz) \right],$$

where  $(v_i, w_i) = (S_i(\mathcal{V}_{t-}), S_i(\mathcal{W}_{t-}))$ . Let  $\psi_i := \log(1 - 2w_i) \mathbf{1}_{0 < z \leq \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}})v_i}$ . Let  $\gamma > 0$ . Introduce the exponentiated process

$$\Psi_t := \exp \left[ \gamma \int_0^t \int \sum_i \psi_i N^{[i]}(ds, dz) - \int_0^t \int \sum_i [\exp(\gamma\psi_i) - 1] dz ds \right].$$

Apply Itô's formula, similar to the calculation in Lemma 9, deduce that  $(\Psi_t)_{t \geq 0}$  is a local martingale. It satisfies  $\mathbb{E}[\Psi_{\mathfrak{T}} | \Psi_0] = \Psi_0 = 1$ . Markov's inequality gives that for any  $\theta > 0$ ,

$$\mathbb{P}(\log \Psi_{\mathfrak{T}} \geq \log \theta) = \mathbb{P}(\Psi_{\mathfrak{T}} \geq \theta) \leq \frac{\mathbb{E}[\Psi_{\mathfrak{T}}]}{\theta} = \frac{1}{\theta}.$$

Take  $\theta = \sqrt{\log \eta}$ ,  $\gamma = 1$ . Notice that

$$\begin{aligned} \int [\exp(\gamma\psi_i) - 1] dz &= (-2w_i) \left( \frac{1}{2} - (1 - \delta_i \mathbf{1}_{t < \mathfrak{T}})v_i \right) \\ &= -w_i + 2(1 - \delta_i \mathbf{1}_{t < \mathfrak{T}})w_i v_i. \end{aligned}$$

Then with probability at least  $1 - \frac{1}{\sqrt{\log \eta}}$ ,

$$\log f(\mathcal{W}_{\mathfrak{T}}) - \log f(\mathcal{W}_0) < \left[ 2 \sum_{i=1}^n \int_0^{\mathfrak{T}} (1 - \delta_i) w_i v_i dt \right] + \frac{1}{2} \log \log \eta.$$

□

*Proof of Lemma 11.* From SDEs (21) for  $\log f(\mathcal{W}_t)$  and  $\log f(\mathcal{V}_t)$ , take difference to obtain

$$d[\log f(\mathcal{W}_t) - \log f(\mathcal{V}_t)] = \sum_{i=1}^n [w_i - v_i] dt + \sum_{i=1}^n \int \psi_i N^{[i]}(dt, dz),$$

where  $\psi_i \equiv \psi_i(\mathcal{V}_{t-}, \mathcal{W}_{t-}, z)$  is defined as follows, with  $I_i := \min \left\{ \frac{1}{2} - v_i, \frac{1}{2} - v_i + \delta_i \mathbf{1}_{t < \mathfrak{T}} v_i \right\}$ ,

$$\psi_i := \begin{cases} [\log(1 - 2w_i) - \log(1 - 2v_i)] \mathbf{1}_{0 < z \leq I_i} + \log(1 - 2w_i) \mathbf{1}_{I_i < z < \frac{1}{2} - v_i + \delta_i \mathbf{1}_{t < \mathfrak{T}} v_i} & \text{if } v_i > 0 \\ [\log(1 - 2w_i) - \log(1 - 2v_i)] \mathbf{1}_{0 < z \leq I_i} - \log(1 - 2v_i) \mathbf{1}_{I_i < z < \frac{1}{2} - v_i} & \text{otherwise.} \end{cases}$$

In words, there are extra jumps on  $\mathcal{W}$  or  $\mathcal{V}$  depending on whether  $v_i > 0$  or not. Let  $\gamma > 0$ . Introduce the exponentiated process

$$\Psi_t := \exp \left[ \gamma \int_0^t \int \sum_i \psi_i N^{[i]}(ds, dz) - \int_0^t \int \sum_i [\exp(\gamma \psi_i) - 1] dz ds \right]. \quad (28)$$

Apply Itô's formula, similar to that in Lemma 9, deduce that  $\Psi_t$  is local martingale. It satisfies  $\mathbb{E}[\Psi_{T_o} | \Psi_0] = \Psi_0 = 1$ . Markov's inequality gives that for any  $\theta > 0$ ,

$$\mathbb{P}(\log \Psi_{T_o} \geq \log \theta) = \mathbb{P}(\Psi_{T_o} \geq \theta) \leq \frac{\mathbb{E}[\Psi_{T_o}]}{\theta} = \frac{1}{\theta}.$$

Take  $\theta = \sqrt{\log \eta}$ ,  $\gamma = 1$ . Notice that

$$\int [\exp(\psi_i) - 1] dz = \begin{cases} -[w_i - v_i] - 2\delta_i \mathbf{1}_{t < \mathfrak{T}} w_i v_i & \text{if } v_i > 0 \\ -[w_i - v_i] - \frac{2\delta_i \mathbf{1}_{t < \mathfrak{T}} w_i v_i}{1 - 2v_i} & \text{otherwise.} \end{cases}$$

Then with probability at least  $1 - \frac{1}{\sqrt{\log \eta}}$ ,

$$\log f(\mathcal{W}_{T_o}) - \log f(\mathcal{V}_{T_o}) < \left[ -2 \sum_{i=1}^n \int_0^{\mathfrak{T}} \delta_i w_i v_i \left( \mathbf{1}_{v_i > 0} + \mathbf{1}_{v_i \leq 0} \frac{1}{1 - 2v_i} \right) dt \right] + \frac{1}{2} \log \log \eta.$$

□

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## A Additional properties of the Boolean hypercube and the reverse heat process

### A.1 Additional proof for biased Fourier analysis

*Proof of Proposition 1.* First, we verify that  $(\phi_S)_{S \in [n]}$  form an orthonormal basis. We have

$$\mathbb{E}_{\mu_p}[\phi_i^2] = p_i \frac{(1-p_i)^2}{p_i(1-p_i)} + (1-p_i) \frac{p_i^2}{p_i(1-p_i)} = 1.$$

As a result, we also have  $\mathbb{E}_{\mu_p}[\phi_S^2] = \mathbb{E}_{\mu_p}[\prod_{i \in S} \phi_i^2] = \prod_{i \in S} \mathbb{E}_{\mu_p}[\phi_i^2] = 1$  because  $\mu_p$  is a product measure and  $\phi_S$  is in a product form. For the orthogonality, we have

$$\mathbb{E}_{\mu_p}[\phi_i(y)\phi_\emptyset] = \mathbb{E}_{\mu_p}[\phi_i(y)] = p_i \frac{1-p_i}{\sqrt{p_i(1-p_i)}} + (1-p_i) \frac{-p_i}{\sqrt{p_i(1-p_i)}} = 0. \quad (29)$$

Then for  $S, R$  two subsets of  $[n]$  and  $S \neq R$ , we have that  $S \cap R$  and  $(S \cup R) \setminus (S \cap R)$  form a partition of  $S \cup R$ , and

$$\begin{aligned} \mathbb{E}_{\mu_p}[\phi_S \phi_R] &= \mathbb{E}_{\mu_p}\left[\prod_{i \in S \cap R} \phi_i^2 \prod_{j \in (S \cup R) \setminus (S \cap R)} \phi_j\right] \\ &\stackrel{(i)}{=} \prod_{i \in S \cap R} \mathbb{E}_{\mu_p}[\phi_i^2] \prod_{j \in (S \cup R) \setminus (S \cap R)} \mathbb{E}_{\mu_p}[\phi_j] \\ &\stackrel{(ii)}{=} 0 \end{aligned}$$

(i) follows because  $\mu_p$  is a product measure. (ii) follows from Eq. (29) and the fact that since  $S \neq R$  the product over  $(S \cup R) \setminus (S \cap R)$  is not empty. Hence,  $(\phi_S)$  are orthogonal to each other and all have norm 1. The cardinality of  $(\phi_S)$  is  $2^n$ , which matches the space of real functions on  $\{-1, 1\}^n$ . We conclude that  $(\phi_S)_{S \in [n]}$  form an orthonormal basis.

Second, given a function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}$ , it can be written as

$$f(x) = \sum_{S \in [n]} \hat{f}_p(S) \phi_S(x), \quad \forall x \in \{-1, 1\}^n \quad (30)$$

where  $\hat{f}_p(S) = \mathbb{E}_{\mu_p}[f \phi_S]$ . The above expression coincides with the unique multilinear expansion of  $f$ , so we can treat  $f$  as a polynomial and take derivatives directly. Let  $\mathfrak{S} = \{i_1, \dots, i_k\} \subseteq [n]$  be a set of indices and  $z \in (-1, 1)^n$ . Note that when  $p = \frac{1+z}{2}$ , then  $z_i = 2p_i - 1$  and

$$\phi_i(z) = \frac{1}{2} \left( \frac{1-2p_i}{\sqrt{p_i(1-p_i)}} + z_i \frac{1}{\sqrt{p_i(1-p_i)}} \right) = 0. \quad (31)$$

When taking derivatives of  $f$  with respect to  $i_1, \dots, i_k$ -th coordinate, any term with  $S$  such that  $\mathfrak{S} \subseteq S$  in Eq. (30) will survive. However, if there are more terms left after taking derivative, say  $j \in (S \setminus \mathfrak{S})$ , then according to Eq. (31) it will be zero. In the end, only  $S = \mathfrak{S}$  remains in the sum. Each derivative with respect to  $i$  gives a factor of  $\frac{1}{2} \frac{1}{\sqrt{p_i(1-p_i)}} = \frac{1}{\sqrt{1-z_i^2}}$ . Finally, we obtain

$$\partial_{i_1} \dots \partial_{i_k} f(z) = \left( \prod_{i \in \mathfrak{S}} \frac{1}{\sqrt{1-z_i^2}} \right) \hat{f}_p(\mathfrak{S}).$$

□

## A.2 Second-order smoothness gained from the heat semigroup

**Lemma 12** (Hessian bound). *For any nonnegative function  $f : \{-1, 1\}^n \rightarrow \mathbb{R}_+$  with  $f \neq 0$ , consider its multilinear expansion. Let  $\rho \in (0, 1)$ . Then for any  $x \in \{-\rho, \rho\}^n$ , we have*

$$\nabla^2 \log f(x) \succeq -\frac{1}{1-\rho} \mathbb{I}_n.$$

Since  $P_\tau f(\cdot) = f(e^{-\tau} \cdot)$ , a direct corollary is  $\nabla^2 \log P_\tau f(x) \succeq -\frac{1}{1-e^{-\tau}} \mathbb{I}_n$  for any  $x \in \{-1, 1\}^n$ . This result is reminiscent of the semi-log-convexity gained from the heat semigroup in the Gaussian space (see Section 1.1 [EL18]).

*Proof of Lemma 12.* Let  $x \in \{-\rho, \rho\}^n$  and  $H := \nabla^2 \log f(x)$ . Then since  $f$  is a multilinear polynomial, we have

$$\begin{aligned} H_{ii} &= -\frac{\partial_i^2 f}{f^2} \\ H_{ij} &= -\frac{\partial_{ij} f - \partial_i f \partial_j f}{f^2}, \quad j \neq i. \end{aligned}$$

Take  $p = \frac{1+x}{2}$ . Using  $p$ -biased Fourier analysis in Proposition 1, we can write derivatives as Fourier coefficients.

$$\begin{aligned} f(x) &= \mathbb{E}_{\mu_p}[f] \\ \partial_i f(x) &= \frac{1}{\sqrt{1-\rho^2}} \hat{f}_p(\{i\}) = \frac{1}{\sqrt{1-\rho^2}} \mathbb{E}_{\mu_p}[f \phi_i] \\ \partial_{ij} f(x) &= \frac{1}{1-\rho^2} \hat{f}_p(\{i, j\}) = \frac{1}{1-\rho^2} \mathbb{E}_{\mu_p}[f \phi_i \phi_j], \end{aligned}$$

where  $\phi_i$  is defined in Eq. (24). Let  $\pi$  be a tilted measure on  $\{-1, 1\}^n$ , such that for any function  $h : \{-1, 1\}^n \rightarrow \mathbb{R}$ ,

$$\int h(x) d\pi(x) := \frac{\int h(x) f(x) d\mu_p(x)}{\int f(x) d\mu_p(x)}.$$

Then we have

$$\begin{aligned} H_{ii} &= -\frac{1}{1-\rho^2} \mathbb{E}_\pi[\phi_i]^2 \\ H_{ij} &= -\frac{1}{1-\rho^2} [\mathbb{E}_\pi[\phi_i]\mathbb{E}_\pi[\phi_j] - \mathbb{E}_\pi[\phi_i\phi_j]], \quad j \neq i. \end{aligned}$$

For any vector  $v \in \mathbb{R}^n$ , let  $R := \sum_i v_i \phi_i$ . From the trivial bound  $0 \leq \text{Var}_\pi(R)$ , we deduce that

$$\begin{aligned} 0 &= \mathbb{E}_\pi R^2 - (\mathbb{E}_\pi R)^2 \\ &= \mathbb{E}_\pi \left[ \sum_{ij} v_i v_j \phi_i \phi_j \right] - \left( \sum_i v_i \mathbb{E}_\pi \phi_i \right)^2 \\ &= \sum_i v_i^2 (\mathbb{E}_\pi[\phi_i^2] - \mathbb{E}_\pi[\phi_i]^2) + \sum_{ij, i \neq j} (1-\rho^2) H_{ij} v_i v_j \\ &= \sum_i v_i^2 \mathbb{E}_\pi[\phi_i^2] + (1-\rho^2) \sum_i H_{ii} + (1-\rho^2) \sum_{ij, i \neq j} H_{ij} v_i v_j. \end{aligned}$$

Rewriting, we obtain

$$v^\top H v \succeq -\frac{1}{1-\rho^2} \sum_{i=1}^n v_i^2 \mathbb{E}_\pi[\phi_i^2]$$

We conclude with the observation that  $\mathbb{E}[\phi_i^2] \leq 1 + \rho, \forall i \in [n]$ .  $\square$

### A.3 Additional properties of the reverse heat process

**Lemma 13** (Score martingale). *For any  $i \in [n]$ ,  $(S_i(\mathcal{V}_t))_{t \geq 0}$  is a martingale. And*

$$dS_i(\mathcal{V}_t) = \sum_{j=1}^n \int \Delta_j S_i(\mathcal{V}_{t-}) \mathbf{1}_{0 \leq z \leq \frac{1}{2} - S_j(\mathcal{V}_{t-})} \tilde{N}^{[j]}(dt, dz).$$

where for  $s_j := S_j(x)$ ,  $r_{ij} = \frac{x_i x_j \partial_{ij} f(x)}{f(x)}$ ,

$$\begin{aligned} \Delta_i S_i(x) &= -\frac{2s_i(1-s_i)}{1-2s_i} \\ \Delta_j S_i(x) &= \frac{2(s_i s_j - r_{ij})}{1-2s_j}, \quad j \neq i. \end{aligned}$$

This property is reminiscent of the fact that Föllmer's drift is a martingale (see e.g., Fact 2.2 [EL18]).

*Proof of Lemma 13.* Recall Itô's formula for a jump process, for a smooth function  $g : [-1, 1]^n \rightarrow \mathbb{R}$ ,

$$dg(\mathcal{V}_t) = \langle \nabla g(\mathcal{V}_{t-}), \mathcal{V}_{t-} \rangle dt + \sum_{j=1}^n \int \Delta_j g(\mathcal{V}_{t-}) \mathbf{1}_{0 < z \leq \frac{1}{2} - S_j(\mathcal{V}_{t-})} N^{[j]}(dt, dz).$$

where the jump increment  $\Delta_j g(x) := g(\varsigma_j(x)) - g(x)$ . We apply Itô's formula to  $S_i$ . First, note that for  $j \in [n]$ ,

$$\partial_j S_i = \begin{cases} \frac{\partial_i f}{f} + x_i \left( -\frac{\partial_i f \partial_i f}{f^2} \right) & j = i \\ x_i \left( \frac{\partial_{ij} f}{f} - \frac{\partial_i f \partial_j f}{f^2} \right) & \text{otherwise.} \end{cases}$$

Hence, the first part in the derivative becomes

$$\begin{aligned} \langle \nabla S_i(x), x \rangle &= S_i(x) + \sum_{j=1}^n R_{ij}(x) - S_i(x) \sum_j S_j(x), \\ &= S_i(x)(1 - S_i(x)) + \sum_{j=1, j \neq i}^n (R_{ij}(x) - S_i(x)S_j(x)) \end{aligned}$$

where  $R_{ij}(x) = \frac{x_i x_j \partial_{ij} f(x)}{f(x)}$  and  $R_{ii} = 0$ .

For the jump increments, using that  $f$  and  $\partial_i f$  are multilinear, we have

$$\begin{aligned} f(x - 2x_j e_j) &= f(x) - 2x_j \partial_j f(x), \\ \partial_i f(x - 2x_j e_j) &= \partial_i f(x) - 2x_j \partial_{ij} f(x), \text{ for } j \neq i \\ \partial_i f(x - 2x_i e_i) &= \partial_i f(x). \end{aligned}$$

Then we deduce that

$$\begin{aligned} \Delta_i S_i(x) &= \frac{-x_i \partial_i f(x)}{f(x - 2x_i e_i)} - \frac{x_i \partial_i f(x)}{f(x)} \\ &= \frac{-S_i(x)}{1 - 2S_i(x)} - S_i(x) \\ &= \frac{-S_i(x)(1 - S_i(x))}{\frac{1}{2}(1 - 2S_i(x))}. \\ \Delta_j S_i(x) &= \frac{x_i (\partial_i f(x) - 2x_j \partial_{ij} f(x))}{f(x) - 2x_j \partial_j f(x)} - S_i(x) \\ &= \frac{S_i(x) - 2R_{ij}(x)}{1 - 2S_j(x)} - S_i(x) \\ &= \frac{S_i(x)S_j(x) - R_{ij}(x)}{\frac{1}{2}(1 - 2S_j(x))}. \end{aligned}$$

Since the jump rate is  $\frac{1}{2}(1 - 2S_i(x))$ , the drift coming from centering the jumps cancel exactly with  $\langle \nabla S_i(x), x \rangle$ . We obtain that

$$dS_i(\mathcal{V}_t) = \sum_{j=1}^n \int \Delta_j S_i(\mathcal{V}_{t-}) \mathbf{1}_{0 < z \leq \frac{1}{2}(1 - 2S_j(\mathcal{V}_{t-}))} \tilde{N}^{[j]}(dt, dz).$$

Hence,  $S_i(\mathcal{V}_t)$  is a local martingale. Since  $S_i(\mathcal{V}_t)$  is also bounded by Lemma 4, it is a martingale.  $\square$