SECOND ORDER BISMUT FORMULAE AND APPLICATIONS TO NEUMANN SEMIGROUPS ON MANIFOLDS

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Dedicated to the memory of Professor Giuseppe Da Prato

ABSTRACT. Let M be a complete connected Riemannian manifold with boundary ∂M, and let P_t be the Neumann semigroup generated by $\frac{1}{2}L$ where $L = \Delta + Z$ for a C^1-vector field Z on M. We establish Bismut type formulae for LP_tf and Hess_{P_tf} and present estimates of these quantities under suitable curvature conditions. When P_t is symmetric in $L^2(\mu)$ for some probability measure μ, a new type of log-Sobolev inequality is established which links the relative entropy H, the Stein discrepancy S, and relative Fisher information I, generalizing the corresponding result of [9] in the case without boundary.

1. Introduction

Consider a d-dimensional complete Riemannian manifold M, possibly with non-empty boundary ∂M, and let X_t be the reflecting diffusion process on M generated by $\frac{1}{2}L$ where $L = \Delta + Z$; here Δ is the Laplace-Beltrami operator and Z a smooth vector field on M. According to [12, 13, 27], the reflecting diffusion process X_t^x starting at x can be constructed as solution to the following SDE on M with reflection:

$$\mathrm{d}X_t^x = //_t \circ \mathrm{d}B_t + \frac{1}{2}Z(X_t^x)\,\mathrm{d}t + \frac{1}{2}N(X_t^x)\,\mathrm{d}l_t^x, \quad X_0^x = x, \tag{1.1}$$

where B_t is a standard Brownian motion on the tangent space $T_xM \equiv \mathbb{R}^d$, $//_t\colon T_xM \to T_{X_t^x}M$ the stochastic parallel transport along X_t^x, N the inward normal unit vector field on ∂M, and l_t^x the local time of X_t^x on ∂M. Throughout this paper, we assume that SDE (1.1) is non-explosive. Then the Neumann semigroup P_t generated by $\frac{1}{2}L$ is given by

$$P_tf(x) = \mathbb{E}\left[f(X_t^x)\right], \quad t \geq 0,\ x \in M,\ f \in \mathcal{B}_b(M)$$

where $\mathcal{B}_b(M)$ denotes the set of bounded measurable functions on M.

2010 *Mathematics Subject Classification.* 58J65, 58J35, 60J60.

Key words and phrases. Diffusion semigroup; Neumann boundary conditions; Bismut formula; Hessian formula; Hessian estimate; Stein's method.

Supported by National Natural Science Foundation of China (Grant No. 11831014, 11921001, 12471137).

To study the regularity of diffusion semigroups using tools from stochastic analysis, Bismut [4] introduced his famous probabilistic formula for the gradient of heat semigroups on Riemannian manifolds without boundary. This type of formulae has been studied in [10, 11, 21] using martingale arguments, and been extended to second order derivatives in [1, 11, 15, 16, 18, 19, 21, 24].

In the case the boundary of M is non-empty, Bismut type formulae have been derived in [27, 8] for the gradient of the Neumann semigroup P_t, see also [17, 12, 29] for gradient estimates. In this paper, we aim at establishing Bismut type formulae for second order derivatives of the Neumann semigroup, along with some geometric applications.

Let $\mathrm{Ric}_Z := \mathrm{Ric} - \nabla Z$ where Ric is the Ricci curvature tensor, and let II be the second fundamental form of the boundary:

$$\mathrm{II}(X,Y) = -\langle \nabla_X N, Y\rangle, \quad X,Y \in T_x\partial M,\ x\in\partial M.$$

A derivative formula for P_tf is given in [12, 27] by constructing an appropriate multiplicative functional. Throughout the paper, we assume that the reflecting diffusion process generated by L is non-explosive, and that there exist functions $K\in C(M)$ and $\sigma\in C(\partial M)$ such that

$$\mathrm{Ric}_Z := \mathrm{Ric} - \nabla Z \geq K, \qquad \mathrm{II}\geq \sigma, \tag{1.2}$$

i.e. $\mathrm{Ric}_Z(X,X)\geq K(x)|X|^2$ for $x\in M,\ X\in T_xM$, and $\mathrm{II}(X,X)\geq \sigma(x)|X|^2$ for $x\in\partial M,\ X\in T_x\partial M$. Under the assumption that

(A) the functions K and σ in (1.2) are constant, $\mathbb{E}[\mathrm{e}^{\sigma^- l_t}]<\infty$ for any $t\geq 0$,

a Bismut type formula for ∇P_tf has been established in [27] for $f\in\mathcal{B}_b(M)$ such that $\nabla P_\cdot f$ is bounded on $[0,t]\times M$. More precisely, there exists a family of random homomorphisms $Q_t\colon T_xM\to T_{X_t^x}M$ with the property that

$$|Q_t|\leq \mathrm{e}^{-Kt/2-\sigma l_t/2} \quad\text{and}\quad \langle N(X_t^x), Q_t(v)\rangle \mathbf{1}_{\{X_t^x\in\partial M\}}=0, \quad v\in T_xM,$$

such that for $f\in C_b^1(M)$ satisfying the boundedness condition of $\nabla P_\cdot f$ on $[0,t]\times M$, one has

$$\nabla P_tf(v) = \mathbb{E}\left[\langle \nabla f(X_t^x), Q_t(v)\rangle\right], \quad v\in T_xM, \tag{1.3}$$

and

$$\nabla P_tf(v) = \mathbb{E}\left[f(X_t^x)\int_0^t \langle h'(s)Q_s(v), /\!/_s \mathrm{d}B_s\rangle\right], \quad v\in T_xM \tag{1.4}$$

for any choice of a non-negative $h\in C_b^1([0,t])$ such that $h(0)=0,\ h(t)=1$. When Ric_Z and II are bounded from below, the second part of condition **(A)** holds if the following condition **(B)** holds, see [27, Section 3.2]. Moreover, it also implies that $|\nabla P_\cdot f|$ is bounded on $[0,t]\times M$ for $f\in\mathcal{B}_b(M)$, see Remark 2.5 in the next section for explanation.

(B) The boundary ∂M is convex or there exists a non-negative constant θ such that $\mathrm{II} \le \theta$ and a positive constant r_0 such that on $\partial_{r_0} D := \{x \in D : \rho_{\partial D}(x) \le r_0\}$ the distance function $\rho_{\partial D}$ to the boundary ∂D is smooth, the sectional curvature of M being bounded above and $|Z|$ bounded.

Therefore, the first part of condition **(A)** and the condition (**B**) imply the Bismut type formula (1.4) for any $f \in \mathcal{B}_b(M)$.

The aim of this paper is to extend (1.3) and (1.4) to second order derivatives and to establish Bismut type formulae for LP_tf and $\mathrm{Hess}_{P_tf} := \nabla \mathbf{d} P_t f$, along with some applications. When compared to the case without boundary as in [1], the present study faces an essential new difficulty. Indeed, by formal calculations, the Bismut formula for second derivatives of P_tf includes a stochastic integral of Q_t^{-1}, the inverse of the above mentioned multiplicative functional Q_t. However, in the present setting Q_t is singular near the boundary so that existence of the desired stochastic integral poses a problem. To avoid the discussion concerning well-definedness of Q_t^{-1}, we introduce a sequence of martingales $M_t^{(h,n)}$ in the following section and using the limit of these martingales in L^p sense, we derive a Bismut type formula for LP_tf in terms of the multiplicative functional Q_t, which provides as consequence an upper estimate depending on the lower bounds of Ric_Z and II, more precisely, condition (**A**) and $\|Z\|_\infty < \infty$. Let $x \in M$ and $T > 0$. For $f \in \mathcal{B}_b(M)$ such that $|\nabla P_\cdot f|$ is bounded on $[0,T] \times M$,

$$|L(P_Tf)|(x) \le 2\|f\|_\infty \left(\frac{\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{(3+\sqrt{10})\big(\mathbb{E}^x[\mathrm{e}^{\sigma^- l_T}]\big)^{1/2}\,\mathrm{e}^{K^- T/2}}{T} \right).$$

If the boundary is convex, i.e. $\sigma \ge 0$, we have the following corollary,

$$|L(P_Tf)|(x) \le (P_Tf^2)^{1/2}(x) \left(\frac{2\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{\sqrt{2}\,\mathrm{e}^{K^- T/2}}{T} \right)$$

for $f \in \mathcal{B}_b(M)$, here $|\nabla P_\cdot f|$ is bounded on $[0,t] \times M$ since the local time can be estimated when the boundary is convex. Compared with the formula for $L(P_Tf)$ in [24], our Bismut type formula for LP_tf contains only one test function h (see Theorem 2.2 below), as consequence, the estimate of $|L(P_Tf)|$ are new even in the case without boundary where the existing estimate in [24] depends on the uniform norm of Ric_Z. It is worthy to mention that under condition **(B)** with $\mathrm{Sect} \le k$ for some $k \in \mathbb{R}$, the term $\mathbb{E}[\mathrm{e}^{\sigma^- l_t}]$ can be further estimated and the upper bound of $|LP_Tf|$ can be written explicitly:

$$|L(P_Tf)|(x) \le 2\|f\|_\infty \left(\frac{\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{(3+\sqrt{10})\,\mathrm{e}^{\frac{d\sigma^- r_1}{2} + \frac{d\sigma^-}{r_1} + 2(\sigma^-)^2 + \frac{K^- T}{2}}}{T} \right),$$

for some $r_1 = r_0 \wedge \ell^{-1}(0)$ where ℓ is given in (5.5) below.

In Section 3, we establish a Bismut type formula for $\mathrm{Hess}_{P_t f}$ and use it for Hessian estimates of $P_t f$. Establishing formulas for the Hessian naturally requires more knowledge on the curvature of the manifold. Note that in [1, 24, 16, 19], the authors used information related to curvature and its derivative to establish a Hessian formula and deduced estimates in terms of these curvature conditions. When it comes to manifolds with boundary, it seems unavoidable to exploit geometric information concerning the boundary as well. Before going into the details, let us remark that the multiplicative functional Q_t in the derivative formula (1.3) satisfies

$$\langle N(X_t), Q_t(v)\rangle \mathbf{1}_{\{X_t\in\partial M\}} = 0$$

which is reasonable since

$$\langle \nabla P_{T-t} f(X_t),\ N(X_t)\rangle \mathbf{1}_{\{X_t\in\partial M\}} = 0.$$

It follows that to express $\nabla P_t f$ on the boundary, information on the second fundamental form

$$\mathrm{II}^\sharp(P_\partial(v)) = -(\nabla_{P_\partial(v)} N)^\sharp$$

is sufficient. However, when it comes to the second order derivative of $P_t f$ on the boundary, no condition like

$$\mathrm{Hess}_{P_{T-t} f}(N(X_t), \boldsymbol{\cdot})\mathbf{1}_{\{X_t\in\partial M\}} = 0$$

is satisfied, which naturally demands for full information on ∇N. This indicates that one needs to control the negative part of the lower bound of II. For this reason, in Section 3, two new functional $\tilde{Q}_t$ and W_t are introduced in (3.3) and (3.12) respectively, which our Bismut formula for $\mathrm{Hess}_{P_t f}$ will be based on and which then allow to derive upper bounds under the following condition: assume that the functions K and σ in (1.2) are constant, and there exist three non-negative constants α, β and γ, such that for $x \in M$,

$$|R|_{\mathrm{HS}}(x) \le \alpha, \quad |\mathbf{d}^* R + \nabla \mathrm{Ric}_Z^\sharp - R(Z)|(x) < \beta, \quad |\nabla(\nabla N)^\sharp + R(N)|(x) < \gamma,$$

where for $v_1, v_2 \in T_x M$,

$$|R|_{\mathrm{HS}}(x) = \sup\left\{ |R^{\sharp,\sharp}(v_1,v_2)|_{\mathrm{HS}}(x) : v_1, v_2 \in T_x M,\ |v_1| \le 1,\ |v_2| \le 1 \right\}.$$

If $|\nabla P_\cdot f|$ and $|\mathrm{Hess}_{P_\cdot f}|$ are bounded on $[\delta, T]\times M$ for $f \in \mathcal{B}_b(M)$ and any $\delta > 0$, and $\mathbb{E}^x[\mathrm{e}^{(\sigma^- + \varepsilon) l_t}] < \infty$ for any $t \ge 0$ and some $\varepsilon > 0$, then

$$\begin{aligned}|\mathrm{Hess}_{P_T f}|(x) \le{}& \left(\alpha + \frac{\beta}{2}\sqrt{T} + \frac{2}{T}\right) \mathrm{e}^{K^- T}\, \mathbb{E}^x[\mathrm{e}^{\sigma^- l_T}] (P_T f^2)^{1/2} \\ &+ \frac{\gamma}{2\sqrt{T}}\, \mathrm{e}^{K^- T}\, \mathbb{E}^x\left[\mathrm{e}^{\sigma^- l_T}\right]^{1/2} \left[\mathbb{E}^x\left(\int_0^T \mathrm{e}^{\frac{1}{2}\sigma^- l_s}\, \mathrm{d} l_s\right)^2\right]^{1/2} (P_T f^2)^{1/2}\end{aligned}$$

for $f \in \mathcal{B}_b(M)$. On the other hand, if condition (**B**) also holds, one can construct a function ϕ satisfying the condition (**C**) (see Remark 5.3 in Appendix), which is shown up in Subsection 3.2. This further implies that $|\nabla P_\cdot f|$ and $|\mathrm{Hess}_{P_\cdot f}|$ are bounded on $[\delta, T]\times M$ for any $\delta > 0$ and $f \in \mathcal{B}_b(M)$, and $\mathbb{E}^x[\mathrm{e}^{(\sigma^-+\varepsilon)l_t}] < \infty$ for any $t \geq 0$ and some $\varepsilon > 0$ as well. Note that $\mathbb{E}^x[\mathrm{e}^{(\sigma^-+\varepsilon)l_t}] < \infty$ can be further estimated (see Remark 5.2 in Appendix) and the upper bound of $|\mathrm{Hess}_{P_T f}|$ can be specified explicitly.

We also present a Hessian formula for P_t with gradient terms under condition (**C**) in Subsection 3.2, see Theorem 3.7 and Corollary 3.8. As an application, in Section 4, we apply this Hessian estimates of $P_t f$ to prove inequalities connecting the relative entropy H, the Stein discrepancy S and the relative Fisher information I, which extend the corresponding results derived in our recent work [9] for $\partial M = \emptyset$ to the case with boundary; see Ledoux, Nourdin and Peccati [14] for the earlier study in the Euclidean case $M = \mathbb{R}^d$.

2. Bismut formula and estimate for $LP_t f$

To state the main result, we first recall the construction of the multiplicative functional Q_t appearing in the Bismut formula, see [24] for the case without boundary.

For $t \geq 0$, let $/\!/_{0\to t} : T_{X_0}M \to T_{X_t}M$ denote stochastic parallel transport along the paths of the reflecting diffusion process X. The covariant differential D in $t \geq 0$ is defined as $\mathrm{D} := /\!/_{0\to t}\, \mathrm{d}\, /\!/_{t\to 0}$ where d is the usual Itô stochastic differential in $t \geq 0$. For a process $v_t \in T_{X_t}M$ we then have

$$\mathrm{D}v_t = /\!/_{0\to t}\, \mathrm{d}\, /\!/_{t\to 0}\, v_t, \quad t \geq 0.$$

For $n \in \mathbb{N}$ and $t \geq 0$, let $Q_t^{(n)} : T_{X_0}M \to T_{X_t}M$ solve the covariant differential equation: for $t \geq 0$,

(2.1)
$$\mathrm{D}Q_t^{(n)} = -\frac{1}{2}\left\{\mathrm{Ric}_Z^\sharp(Q_t^{(n)})\,\mathrm{d}t + \mathrm{II}^\sharp(Q_t^{(n)})\,\mathrm{d}l_t + nP_N(Q_t^{(n)})\,\mathrm{d}l_t\right\}, \quad Q_0^{(n)} = \mathrm{id},$$

where id is the identity map on $T_{X_0}M$ and P_N the projection operator onto the normal direction N of ∂M such that when $X_t \in \partial D$,

$$P_N(Q_t^{(n)}v) = \langle Q_t^{(n)}v, N(X_t)\rangle\, N(X_t), \quad v \in T_{X_0}M.$$

Furthermore for $P_\partial : T_xM \to T_x\partial M$ being the projection operator for $x \in \partial M$, let

$$\langle \mathrm{II}^\sharp(Q_t^{(n)})v_1, v_2\rangle := \mathrm{II}(P_\partial Q_t^{(n)}v_1, P_\partial v_2), \quad v_1, v_2 \in T_{X_t}M,\ X_t \in \partial M.$$

By the curvature conditions (1.2), we then have

$$\sup_{n\geq 1}|Q_t^{(n)}| \leq \mathrm{e}^{-\frac{1}{2}\int_0^t K(X_s)\,\mathrm{d}s - \frac{1}{2}\int_0^t \sigma(X_s)\,\mathrm{d}l_s}, \quad t \geq 0, \tag{2.2}$$

and

$$\int_0^t |P_N(Q_s^{(n)})|^2\,\mathrm{d}l_s \leq \frac{1}{n}\int_0^t |Q_s^{(n)}|^2\big\{K^-(X_s)\,\mathrm{d}s + \sigma^-(X_s)\,\mathrm{d}l_s\big\} \to 0 \tag{2.3}$$

as $n \to \infty$. Define

$$\{Q_t^{(n)}\}^{-1} := /\!/_{t\to 0}\{Q_t^{(n)} /\!/_{t\to 0}\}^{-1} : T_{X_t}M \to T_xM \tag{2.4}$$

where $\{Q_t^{(n)}//_{t\to 0}\}^{-1}$ is the inverse of the operator

$$Q_t^{(n)}//_{t\to 0}:\ T_{X_t}M \to T_{X_t}M.$$

To show that $\{Q_t^{(n)}\}^{-1}$ exists, let

$$\tau_k := \inf\big\{t \geq 0:\ \rho_o(X_t) \geq k\big\},\quad k \geq 1,$$

where ρ_o is the Riemannian distance to a reference point $o \in M$. Fix $T > 0$. By [27, Lemma 3.1.2], we have

$$\mathbb{E}[\mathrm{e}^{\lambda l_{T\wedge\tau_k}}] < \infty,\quad \lambda > 0. \tag{2.5}$$

Since Ric_Z and II are locally bounded, (2.1) and (2.5) imply that $Q_t^{(n)}//_{t\to 0}$ is invertible with

$$\mathbb{E}\left[\sup_{t\in[0,T\wedge\tau_k]} \big|\{Q_t^{(n)}\}^{-1}\big|^p\right] = \mathbb{E}\left[\sup_{t\in[0,T\wedge\tau_k]} \big|\{Q_t^{(n)}//_{t\to 0}\}^{-1}\big|^p\right] < \infty,\quad p,k \geq 1.$$

To derive a Bismut formula for LP_tf, we need to estimate the martingales

$$M_t^{(h,n)} := \int_0^t \left\langle h_s Q_s^{(n)} \int_0^s h_r\{Q_r^{(n)}\}^{-1}//_r\mathrm{d}B_r,\ //_s\mathrm{d}B_s\right\rangle,\quad n \geq 1, \tag{2.6}$$

for a reference adapted real process h. When M is compact, [12, Theorem 3.4] implies that as $n \to \infty$ the process $Q_t^{(n)}$ converges in $L^2(\mathbb{P})$ to an adapted right-continuous process Q_t with left-limits such that $P_NQ_t = 0$ if $X_t \in \partial M$. This construction has been extended in [27, Proof of Theorem 3.2.1] to non-compact manifolds. However, although $\{Q_t^{(n)}\}^{-1}$ exists for every $n \geq 1$, Q_t is not invertible on the boundary since $P_NQ_t = 0$. Hence a priori, existence of the stochastic integral

$$\int_0^t \left\langle h_sQ_s \int_0^s h_rQ_r^{-1}//_r\mathrm{d}B_r,\ //_s\mathrm{d}B_s\right\rangle$$

is not obvious.

Lemma 2.1. *Let $K \in C(M)$ and $\sigma \in C(\partial M)$ such that* (1.2) *holds. Then for any adapted real process $(h_t)_{t\in[0,T]}$ with*

$$C(h) := \mathbb{E}\left[\int_0^T h_s^2\, \mathrm{e}^{\int_0^s K^-(X_r)\mathrm{d}r + \int_0^s \sigma^-(X_r)\mathrm{d}l_r}\,\mathrm{d}s\right] < \infty, \tag{2.7}$$

the martingales $M_t^{(h,n)}$ in (2.6) *satisfy*

$$\sup_{n\geq 1}\mathbb{E}\left[\sup_{t\in[0,T]}\big|M_t^{(h,n)}\big|\right] \leq 3\Big(3+\sqrt{10}\Big)\left(C(h)\,\mathbb{E}\int_0^T h_s^2\,\mathrm{d}s\right)^{1/2} < \infty. \tag{2.8}$$

In addition, if there is a constant $\alpha > 1$ such that

$$\mathbb{E}\left[\left(\int_0^T h_s^2\mathrm{d}s\right)^{\alpha}\right] < \infty, \tag{2.9}$$

then there exists a real random variable M_T^h *with* $\mathbb{E}\big[|M_T^h|^{\frac{2\alpha}{1+\alpha}}\big]<\infty$, *and a subsequence* $n_m\to\infty$ *as* $m\to\infty$, *such that*

$$\lim_{m\to\infty}\mathbb{E}\big[\eta M_T^{(h,n_m)}\big]=\mathbb{E}\big[\eta M_T^h\big],\quad \eta\in L^{\frac{2\alpha}{\alpha-1}}(\mathbb{P}).$$

In case (2.9) *holds for* $\alpha=1$ *as well, one has*

$$\mathbb{E}\big[|M_T^h|\big]\le 3\Big(3+\sqrt{10}\Big)\,\left(C(h)\,\mathbb{E}\left[\int_0^T h_s^2\,\mathrm{d}s\right]\right)^{1/2}.$$

Proof. (a) We first prove (2.8). By Fatou's lemma, it suffices to show

$$\begin{aligned}I_{k,n}&:=\mathbb{E}\left[\sup_{t\in[0,T\wedge\tau_k]}\left|\int_0^t\left\langle h_sQ_s^{(n)}\int_0^s h_r\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r,\,/\!/_s\mathrm{d}B_s\right\rangle\right|\right]\\&\le 3\left(3+\sqrt{10}\right)\sqrt{C(h)}\,\left(\mathbb{E}\int_0^T h_s^2\,\mathrm{d}s\right)^{1/2},\quad k,n\ge 1.\end{aligned}\tag{2.10}$$

For fixed $n\ge1$ let

$$\xi_s:=Q_s^{(n)}\int_0^s h_r\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r,\quad s\ge 0.$$

By Lenglart's inequality (see [3, Proposition 5.69]) and Schwarz's inequality, it follows that

$$\begin{aligned}I_{k,n}&\le 3\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k}|\xi_s|^2h_s^2\mathrm{d}s\right)^{1/2}\right]\\&\le 3\mathbb{E}\Bigg[\sup_{s\in[0,T\wedge\tau_k]}|\xi_s|\,\mathrm{e}^{-\frac12\int_0^s K^-(X_r)\mathrm{d}r-\frac12\int_0^s\sigma^-(X_r)\mathrm{d}l_r}\\&\qquad\times\left(\int_0^{T\wedge\tau_k}h_s^2\,\mathrm{e}^{\int_0^s K^-(X_r)\mathrm{d}r+\int_0^s\sigma^-(X_r)\mathrm{d}l_r}\,\mathrm{d}s\right)^{1/2}\Bigg]\\&\le 3\left\{\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]}|\xi_s|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\mathrm{d}r-\int_0^s\sigma^-(X_r)\mathrm{d}l_r}\right]C(h)\right\}^{1/2}.\end{aligned}\tag{2.11}$$

Furthermore, by Itô's formula we have

$$\begin{aligned}\mathrm{d}|\xi_s|^2&=2\langle\xi_s,h_s/\!/_s\mathrm{d}B_s\rangle-\big\{\mathrm{Ric}_Z(\xi_s,\xi_s)\mathrm{d}s+\mathrm{II}(\xi_s,\xi_s)\mathrm{d}l_s\big\}\\&\qquad-n|P_N\xi_s|^2\mathrm{d}l_s+\mathrm{d}[\xi,\xi]_s\\&\le 2\langle\xi_s,h_s/\!/_s\mathrm{d}B_s\rangle-K(X_s)|\xi_s|^2\mathrm{d}s-\sigma(X_s)|\xi_s|^2\mathrm{d}l_s+h_s^2\mathrm{d}s,\quad 0\le s<\tau_k,\end{aligned}$$

which implies

$$\begin{aligned}&\mathrm{d}\Big\{|\xi_s|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\mathrm{d}r-\int_0^s\sigma^-(X_r)\mathrm{d}l_r}\Big\}\\&\le\mathrm{e}^{-\int_0^s K^-(X_r)\mathrm{d}r-\int_0^s\sigma^-(X_r)\mathrm{d}l_r}\big\{2\langle\xi_s,h_s/\!/_s\mathrm{d}B_s\rangle+h_s^2\mathrm{d}s\big\},\end{aligned}\tag{2.12}$$

for $0 \le s < \tau_k$. By the condition $\xi_0 = 0$ and Lenglart's inequality, we have

$$\begin{aligned}
&\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} |\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right] \\
&\quad\le \mathbb{E}\left[\int_0^T h_s^2\,\mathrm{d}s + 6\bigg(\int_0^{T\wedge\tau_k} |\xi_s|^2 h_s^2\, \mathrm{e}^{-2\int_0^s K^-(X_r)\,\mathrm{d}r - 2\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\bigg)^{1/2}\right] \\
&\quad\le \mathbb{E}\Bigg[\int_0^T h_s^2\,\mathrm{d}s + 6\bigg(\sup_{s\in[0,T\wedge\tau_k]} |\xi_s|\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\bigg) \\
&\qquad\qquad\qquad\qquad\qquad\qquad \times \bigg(\int_0^{T\wedge\tau_k} h_s^2\,\mathrm{d}s\bigg)^{1/2}\Bigg] \\
&\quad\le \frac{1}{2\delta}\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} |\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right] \\
&\qquad + (18\delta + 1)\mathbb{E}\left[\int_0^T h_s^2\,\mathrm{d}s\right],
\end{aligned}$$

for any $\delta > 0$. Taking the optimal choice $\delta = \frac{1}{6}\big(3 + \sqrt{10}\big)$, we obtain

$$\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} |\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right] \le \big(3+\sqrt{10}\big)^2\mathbb{E}\left[\int_0^T h_s^2\,\mathrm{d}s\right].$$

Combining this with (2.11), estimate (2.10) follows by letting k tend to ∞.

(b) Assume that (2.9) holds for some $\alpha > 1$. By estimate (2.12) and the Burkholder-Davis-Gundy inequality, we can find constants $c_1, c_2 > 0$ such that

$$\begin{aligned}
&\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} \Big(|\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\Big)^{\alpha}\right] \\
&\le c_1\mathbb{E}\left[\bigg(\int_0^{T\wedge\tau_k} |\xi_s|^2 h_s^2\, \mathrm{e}^{-2\int_0^s K^-(X_r)\,\mathrm{d}r - 2\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\bigg)^{\alpha/2} + \bigg(\int_0^T h_s^2\,\mathrm{d}s\bigg)^{\alpha}\right] \\
&\le c_1\mathbb{E}\left[\bigg(\sup_{s\in[0,T\wedge\tau_k]} |\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\bigg)^{\alpha/2}\bigg(\int_0^{T\wedge\tau_k} h_s^2\,\mathrm{d}s\bigg)^{\alpha/2}\right] \\
&\qquad + c_1\mathbb{E}\left[\bigg(\int_0^T h_s^2\,\mathrm{d}s\bigg)^{\alpha}\right] \\
&\le \frac{1}{2}\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} \Big(|\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\Big)^{\alpha}\right] + c_2\mathbb{E}\bigg(\int_0^T h_s^2\,\mathrm{d}s\bigg)^{\alpha}.
\end{aligned}$$

Together with (2.9) this implies

$$G := \mathbb{E}\left[\sup_{s\in[0,T]} \Big(|\xi_s|^2\, \mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\Big)^{\alpha}\right] < \infty.$$

On the other hand, by Burkholder-Davis-Gundy's inequality, there exists a constant $c_3 > 0$ such that

$$\begin{aligned}&\mathbb{E}\left[\left|M_T^{(h,n)}\right|^{\frac{2\alpha}{1+\alpha}}\right]\\&\le c_3\,\mathbb{E}\left[\bigg(\int_0^T |\xi_s|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r-\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right.\\&\qquad\qquad\left.\times h_s^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\bigg)^{\frac{\alpha}{1+\alpha}}\right]\\&\le c_3\,G^{\frac{1}{1+\alpha}}\left(\mathbb{E}\int_0^T h_s^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\right)^{\frac{\alpha}{1+\alpha}}<\infty,\quad n\ge 1.\end{aligned}$$

Thus $\{M_T^{(h,n)}\}_{n\ge 1}$ is bounded in $L^{\frac{2\alpha}{1+\alpha}}(\mathbb{P})$, and hence has a subsequence converging weakly to a random variable M_T^h in $L^{\frac{2\alpha}{\alpha-1}}(\mathbb{P})$. □

Theorem 2.2. *Let $K \in C(M)$ and $\sigma \in C(\partial M)$ such that* (1.2) *holds. For $T > 0$ and $f \in \mathcal{B}_b(M)$, let $|\nabla P_\cdot f|$ be bounded on $[0,T]\times M$ and let h_t be an adapted real process such that $\int_0^T h_s\,\mathrm{d}s = -1$ and*

$$\mathbb{E}\left[\int_0^T h_s^2\left(\mathrm{e}^{\int_0^s K^-(X_r^x)\,\mathrm{d}r+\int_0^s \sigma^-(X_r^x)\,\mathrm{d}l_r}+|Z(X_s^x)|^2\right)\,\mathrm{d}s\right]<\infty. \tag{2.13}$$

Then for any $f \in \mathcal{B}_b(M)$,

$$L(P_Tf)(x) = 2\,\mathbb{E}\left[f(X_T^x)\left(M_T^h+\int_0^T\left\langle \tilde{h}_s h_s Z(X_s^x),\, //_s\mathrm{d}B_s\right\rangle\right)\right], \tag{2.14}$$

where $\tilde{h}_t := 1+\int_0^t h_s\,\mathrm{d}s$. Consequently,

$$\begin{aligned}|L(P_Tf)(x)| \le 6\,\|f\|_\infty\Bigg\{&\mathbb{E}\left[\left(\int_0^T |\tilde{h}_s h_s Z(X_s^x)|^2\,\mathrm{d}s\right)^{1/2}\right]\\&+\left(3+\sqrt{10}\right)\left(C(h)\,\mathbb{E}\int_0^T h_s^2\,\mathrm{d}s\right)^{1/2}\Bigg\}.\end{aligned} \tag{2.15}$$

Proof. (1) We first assume $f \in \mathcal{C}_N^\infty(L)$, the class of functions $f \in C^\infty(M)$ such that $Nf|_{\partial M} = 0$ and $\|Lf\|_\infty < \infty$. In this case, we have the Kolmogorov equations (see [27, Theorem 3.1.3]),

$$\partial_t P_{T-t}f = -LP_{T-t}f = -P_{T-t}Lf,\quad NP_tf|_{\partial M} = 0,\quad t\in[0,T]. \tag{2.16}$$

In the sequel, we write for simplicity

$$X_t = X_t^x,\quad N_t = N(X_t),\quad Z_t = Z(X_t),\quad M_t := LP_{T-t}f(X_t),\quad t\in[0,T].$$

Furthermore, we write $A_t \overset{\mathrm{m}}{=} B_t$ for two processes A_t and B_t if the difference $A_t - B_t$ is a local martingale. By Itô's formula and (2.16), we obtain

$$\mathrm{d}M_t = \langle \nabla(LP_{T-t}f)(X_t), //_t\,\mathrm{d}B_t\rangle + \partial_t(LP_{T-t}f)(X_t)\,\mathrm{d}t$$

$$
\begin{aligned}
&+\frac{1}{2}L(LP_{T-t}f)(X_t)\,\mathrm{d}t+\frac{1}{2}N(LP_{T-t}f)(X_t)\,\mathrm{d}l_t\\
&=\langle\nabla(LP_{T-t}f)(X_t), /\!/_t\,\mathrm{d}B_t\rangle+\frac{1}{2}N(P_{T-t}Lf)(X_t)\,\mathrm{d}l_t\\
&=\langle\nabla(LP_{T-t}f)(X_t), /\!/_t\,\mathrm{d}B_t\rangle,\quad t\in[0,T].
\end{aligned}
$$

Then

$$
\mathrm{d}(M_t\tilde{h}_t^2)=\tilde{h}_t^2\,\mathrm{d}M_t+2\tilde{h}_t(\tilde{h}_t)'M_t\,\mathrm{d}t=\tilde{h}_t^2\,\mathrm{d}M_t+2\tilde{h}_th_tM_t\,\mathrm{d}t,
$$

which together with $\tilde{h}_0=1$ implies

$$
(LP_{T-t}f)(X_t)\,\tilde{h}_t^2-LP_Tf(x)\overset{\mathrm{m}}{=}2\int_0^t LP_{T-s}f(X_s)\tilde{h}_sh_s\mathrm{d}s. \tag{2.17}
$$

With $\Delta=-\mathbf{d}^*\mathbf{d}$ and $L=\Delta+Z$, we have

$$
-(LP_{T-t}f)(X_t)=\{\mathbf{d}^*(\mathbf{d}P_{T-t}f)-(\mathbf{d}P_{T-t}f)(Z)\}\,(X_t). \tag{2.18}
$$

Combined with (2.17) this further yields

$$
\begin{aligned}
&(LP_{T-t}f)(X_t)\tilde{h}_t^2-LP_Tf(x)\\
&\overset{\mathrm{m}}{=}2\int_0^t LP_{T-s}f(X_s)\tilde{h}_sh_s\,\mathrm{d}s\\
&=-2\int_0^t\mathbf{d}^*(\mathbf{d}P_{T-s}f)\tilde{h}_sh_s\,\mathrm{d}s+2\int_0^t(\mathbf{d}P_{T-s}f)(Z)\tilde{h}_sh_s\,\mathrm{d}s. \qquad (2.19)
\end{aligned}
$$

Let $Q_t^{(n)*}\colon T_{X_t}M\to T_xM$ be the adjoint operator to $Q_t^{(n)}$. By Itô's formula and the Weitzenböck formula, we obtain

$$
\begin{aligned}
\mathrm{d}\left\{(\mathbf{d}P_{T-t}f)(X_t)Q_t^{(n)}\right\}&=\big(\nabla_{/\!/_t\mathrm{d}B_t}\mathbf{d}P_{T-t}f(X_t)\big)(Q_t^{(n)})\\
&\quad+\left\{\mathrm{Hess}_{P_{T-t}f}(N_t,N_t)\,Q_t^{(n)*}N_t\right\}(X_t)\,\mathrm{d}l_t.
\end{aligned}
$$

Combining this with

$$
\mathbf{d}^*(\mathbf{d}P_{T-t}f)\tilde{h}_th_t\,\mathrm{d}t=-\left\{(\nabla_{/\!/_t\,\mathrm{d}B_t}\mathbf{d}P_{T-t}f)(Q_t^{(n)}\tilde{h}_th_t(Q_t^{(n)})^{-1}/\!/_t\,\mathrm{d}B_t)\right\}(X_t),
$$

and using Itô's formula, we derive

$$
\begin{aligned}
&\int_0^t\mathbf{d}^*(\mathbf{d}P_{T-s}f)\tilde{h}_sh_s\,\mathrm{d}s\\
&\quad\overset{\mathrm{m}}{=}-\big(\mathbf{d}P_{T-t}f\big)\bigg(Q_t^{(n)}\tilde{h}_t\int_0^t h_s(Q_s^{(n)})^{-1}/\!/_s\,\mathrm{d}B_s\bigg)\\
&\qquad+\int_0^t\mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\Big\langle N_s,\ \tilde{h}_sQ_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\,\mathrm{d}B_r\Big\rangle\,\mathrm{d}l_s\\
&\qquad+\int_0^t(\mathbf{d}P_{T-s}f)\Big(h_sQ_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\,\mathrm{d}B_r\Big)\,\mathrm{d}s. \qquad (2.20)
\end{aligned}
$$

To deal with the last term of the above equation and the second term on the right-hand side of (2.19), we observe that by Itô's formula

$$\mathrm{d}P_{T-s}f(X_s) = \langle \nabla P_{T-s}f(X_s),\ //_s\,\mathrm{d}B_s\rangle = (\mathbf{d}P_{T-s}f)(//_s\,\mathrm{d}B_s),$$

so that

$$\begin{aligned}
&\int_0^t \big(\mathbf{d}P_{T-s}f\big)(Z_s)\tilde h_s h_s\,\mathrm{d}s \overset{\mathrm{m}}{=} P_{T-t}f(X_t)\int_0^t \langle \tilde h_s h_s Z_s,\ //_s \mathrm{d}B_s\rangle,\\
&\int_0^t (\mathbf{d}P_{T-s}f)\Big(Q_s^{(n)}h_s\int_0^s h_r\{Q_r^{(n)}\}^{-1}//_r\,\mathrm{d}B_r\Big)\,\mathrm{d}s\\
&\overset{\mathrm{m}}{=} P_{T-t}f(X_t)\int_0^t \Big\langle h_s Q_s^{(n)}\int_0^s h_r\{Q_r^{(n)}\}^{-1}//_r\,\mathrm{d}B_r, //_s\mathrm{d}B_s\Big\rangle.
\end{aligned}$$

Combining these equations with (2.20) and (2.18), we obtain

$$\begin{aligned}
&\int_0^t (LP_{T-s}f)(X_s)\tilde h_s h_s\,\mathrm{d}s - \mathbf{d}P_{T-t}f\left(Q_t^{(n)}\tilde h_t\int_0^t h_s(Q_s^{(n)})^{-1}//_s\mathrm{d}B_s\right)(X_t)\\
&\quad+\int_0^t \mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\Big\langle N_s,\ Q_s^{(n)}\tilde h_s\int_0^s h_r(Q_r^{(n)})^{-1}//_r\mathrm{d}B_r\Big\rangle\,\mathrm{d}l_s\\
&\quad+P_{T-t}f(X_t)\int_0^t \tilde h_s\langle h_s Z_s, //_s\mathrm{d}B_s\rangle\\
&\quad+P_{T-t}f(X_t)\int_0^t\Big\langle Q_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}//_r\,\mathrm{d}B_r,\ h_s//_s\mathrm{d}B_s\Big\rangle \overset{\mathrm{m}}{=} 0.
\end{aligned}$$

The last equation and Eq. (2.17) yield

(2.21)

$$\begin{aligned}
&(LP_{T-t}f)(X_t)\tilde h_t^2 - LP_Tf(x) - 2\mathbf{d}P_{T-t}f\left(Q_t^{(n)}\tilde h_t\int_0^t h_s(Q_s^{(n)})^{-1}//_s\mathrm{d}B_s\right)\\
&\quad+2\int_0^t \mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\Big\langle N_s,\ Q_s^{(n)}\tilde h_s\int_0^s h_r(Q_r^{(n)})^{-1}//_r\mathrm{d}B_r\Big\rangle\,\mathrm{d}l_s\\
&\quad+2P_{T-t}f(X_t)\int_0^t \tilde h_s\langle h_s Z_s, //_s\mathrm{d}B_s\rangle\\
&\quad+2P_{T-t}f(X_t)\int_0^t\Big\langle Q_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}//_r\,\mathrm{d}B_r,\ h_s//_s\mathrm{d}B_s\Big\rangle \overset{\mathrm{m}}{=} 0.
\end{aligned}$$

To get rid of the local martingales in the above calculations, we consider the diffusion process up to exit times from bounded balls. Since $\mathrm{Hess}_{P_\cdot f}$ is locally bounded, for any $k\geq 1$ we find a constant $c_k>0$ such that

$$\begin{aligned}
&\left|\mathbb{E}\left[\int_0^{T\wedge\tau_k}\mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\left\langle N_s,\ Q_s^{(n)}\tilde h_s\int_0^s h_r(Q_r^{(n)})^{-1}//_r\mathrm{d}B_r\right\rangle\mathrm{d}l_s\right]\right|\\
&\leq c_k\left(\mathbb{E}\int_0^{T\wedge\tau_k}|(Q_s^{(n)})^*N_s|^2\,\mathrm{d}l_s\right)^{1/2}\left(\mathbb{E}\int_0^{T\wedge\tau_k}\left|\int_0^s h_r(Q_r^{(n)})^{-1}//_r\mathrm{d}B_r\right|^2\mathrm{d}l_s\right)^{1/2}.
\end{aligned}$$

(2.22)

Next we observe from (2.2), (2.3) and (2.5) that

$$\lim_{n\to\infty}\mathbb{E}\left[\int_0^{T\wedge\tau_k}|(Q_s^{(n)})^*N|^2\,\mathrm{d}l_s\right]=\lim_{n\to\infty}\mathbb{E}\int_0^{T\wedge\tau_k}\left|P_NQ_s^{(n)}(Q_s^{(n)})^*N\right|^2\mathrm{d}l_s$$
$$\leq\lim_{n\to\infty}\mathbb{E}\Bigg[\sup_{t\in[0,T\wedge\tau_k]}|Q_t^{(n)}|^2\int_0^{T\wedge\tau_k}\left|P_NQ_s^{(n)}\right|^2\mathrm{d}s\Bigg]=0,$$

and by Burkholder-Davis-Gundy's inequality,

$$\mathbb{E}\left[\int_0^{T\wedge\tau_k}\left|\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\mathrm{d}B_r\right|^2\mathrm{d}l_s\right]$$
$$\leq\mathbb{E}\Bigg[l_{T\wedge\tau_k}\sup_{s\in[0,T\wedge\tau_k]}\left|\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\mathrm{d}B_r\right|^2\Bigg]<\infty.$$

Using these estimates and taking the upper bound of (2.22), we arrive at (2.23)

$$\lim_{n\to\infty}\mathbb{E}\left[\int_0^{T\wedge\tau_k}\mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\left\langle N_s,\,Q_s^{(n)}\tilde{h}_s\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\mathrm{d}B_r\right\rangle\mathrm{d}l_s\right]=0.$$

On the other hand, since the process in (2.21) is a martingale up to time $T\wedge\tau_k$, its expectation at time $T\wedge\tau_k$ vanishes, so that

$$L(P_Tf)(x)-\mathbb{E}\Bigg[\tilde{h}^2_{T\wedge\tau_k}LP_{T-T\wedge\tau_k}f(X_{T\wedge\tau_k})$$
$$-2\mathbf{d}P_{T-T\wedge\tau_k}f\Big(Q_t^{(n)}\tilde{h}_{T\wedge\tau_k}\int_0^{T\wedge\tau_k}h_s(Q_s^{(n)})^{-1}/\!/_s\mathrm{d}B_s\Big)\Bigg]$$
$$=2\mathbb{E}\left[f(X_T)\int_0^{T\wedge\tau_k}\Big\langle Q_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\mathrm{d}B_r,h_s/\!/_s\mathrm{d}B_s\Big\rangle\right]$$
$$+2\mathbb{E}\left[f(X_T)\int_0^{T\wedge\tau_k}\langle\tilde{h}_sh_sZ_s,/\!/_s\mathrm{d}B_s\rangle\right]$$
$$+2\mathbb{E}\left[\int_0^{T\wedge\tau_k}\mathrm{Hess}_{P_{T-s}f}(N_s,N_s)\left\langle N_s,\;\tilde{h}_sQ_s^{(n)}\int_0^s h_r(Q_r^{(n)})^{-1}/\!/_r\,\mathrm{d}B_r\right\rangle\mathrm{d}l_s\right].$$

By $\tilde{h}_T=0$, Lemma 2.1, (2.23), (2.13) and the boundedness of $|\mathbf{d}P_\cdot f|$ on $[0,T]\times M$, we may first choose a subsequence $n_m\to\infty$ and then take the limit as $k\to\infty$ to derive (2.14) for $f\in C_N^\infty(L)$.

(2) To extend the formula to $f\in\mathcal{B}_b(M)$, we let $h_t=0$ for $t\geq T$ and define finite signed measures μ_ε on M as

$$\mu_\varepsilon(A):=2\,\mathbb{E}\left[\mathbf{1}_A(X^x_{T+\varepsilon})\left(M_T^h+\int_0^T\left\langle\tilde{h}_sh_sZ(X_s^x),\,/\!/_s\mathrm{d}B_s\right\rangle\right)\right],\quad\varepsilon\geq0,$$

for measurable subsets $A\subset M$. By step (1) and (2.16), we have

$$\frac{P_{T+\varepsilon}f(x)-P_Tf(x)}{\varepsilon}=\frac{1}{\varepsilon}\int_0^\varepsilon LP_{r+T}f(x)\,\mathrm{d}r$$

$$= \frac{1}{\varepsilon}\int_0^\varepsilon \mathrm{d}r \int_M f\,\mathrm{d}\mu_r = \int_M f\,\mathrm{d}\mu^{(\varepsilon)},$$

for $f \in \mathcal{C}_N^\infty(L)$, $\varepsilon > 0$, where $\mu^{(\varepsilon)} := \frac{1}{\varepsilon}\int_0^\varepsilon \mu_r\,\mathrm{d}r$ is a finite signed measure on M. Since functions in $\mathcal{C}_N^\infty(L)$ determine finite measures, according to Lemma 2.1 and condition (2.16), μ_ε is a finite measure, and this implies (we have in particular $M^h_{T+r} = M^h_T$ since $h_t = 0$ for $t \geq T$),

$$\frac{P_{T+\varepsilon}f(x) - P_T f(x)}{\varepsilon} = \int_M f\,\mathrm{d}\mu^{(\varepsilon)}$$
$$= \frac{1}{\varepsilon}\int_0^\varepsilon 2\mathbb{E}\left[f(X_{T+r})\bigg(M_T^h + \int_0^T \Big\langle \tilde h_s h_s Z_s,\ //_s \mathrm{d}B_s\Big\rangle\bigg)\right]\mathrm{d}r, \quad f \in \mathcal{B}_b(M), \varepsilon > 0.$$

Since the law of X_T is absolutely continuous and $P_r f \to f$ a.e. as $r \downarrow 0$, we get by the strong Markov property $\mathbb{E}^{\mathcal{F}_T} f(X_{T+r}) = P_r f(X_T) \to f(X_T)$ a.s. as $r \downarrow 0$. By the dominated convergence theorem we may let $\varepsilon \downarrow 0$ to arrive at

(2.24)
$$\frac{\mathrm{d}P_t f(x)}{\mathrm{d}t}\Big|_{t=T} = 2\mathbb{E}\left[f(X_T)\bigg(M_T^h + \int_0^T \Big\langle \tilde h_s h_s Z_s,\ //_s \mathrm{d}B_s\Big\rangle\bigg)\right], \quad f \in \mathcal{B}_b(M).$$

On the other hand, for any $f \in \mathcal{B}_b(M)$ and $\varepsilon > 0$, $P_{t+\varepsilon} f(x)$ is C^1 in $t \geq 0$ and C^2 in x with $NP_{t+\varepsilon} f|_{\partial M} = 0$. Hence, by Itô's formula applied to the process $(\phi P_T f)(X_t)$ for some cut-off function ϕ at x, the proof of (3.1.5) in [27] gives

$$LP_t f(x) = \frac{\mathrm{d}}{\mathrm{d}t} P_t f(x), \quad t > 0,\ f \in \mathcal{B}_b(M). \tag{2.25}$$

Combining (2.24) and (2.25), we prove (2.14) for all $f \in \mathcal{B}_b(M)$. □

Remark 2.3. When reduced to the case without boundary, our estimate still improves the result in [24]. Moreover, compared to the estimate in [24], Theorem 2.2 only uses the lower bound of Ric_Z instead of boundedness of Ric_Z.

Under curvature condition (**A**), with the particular choice $h_s := -1/T$ for $s \in [0, T]$, we obtain

Corollary 2.4. *Assume that condition* (**A**) *holds,* $\|Z\|_\infty < \infty$ *and* $|\nabla P_\cdot f|$ *is bounded on* $[0, T] \times M$ *for* $f \in \mathcal{B}_b(M)$. *Let* $x \in M$ *and* $T > 0$. *Then*

$$|L(P_T f)|(x) \leq 2\|f\|_\infty \left(\frac{\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{(3+\sqrt{10})\big(\mathbb{E}^x[\mathrm{e}^{\sigma^- l_T}]\big)^{1/2}\,\mathrm{e}^{K^- T/2}}{T}\right),$$

for $f \in \mathcal{B}_b(M)$. *If* $\sigma \geq 0$, *then for* $f \in \mathcal{B}_b(M)$,

$$|L(P_T f)|(x) \leq (P_T f^2)^{1/2}(x)\left(\frac{2\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{\sqrt{2}\,\mathrm{e}^{K^- T/2}}{T}\right). \tag{2.26}$$

Proof. The first assertion is a direct consequence of inequality (2.15). It hence suffices to show inequality (2.26). Note that

$$\left|\mathbb{E}^x\left[f(X_T^x)M_T^{(h,n)}\right]\right| \le (P_T f^2)^{1/2}(x)\left[\mathbb{E}\left|M_T^{(h,n)}\right|^2\right]^{1/2}, \tag{2.27}$$

where $M^{(h,n)}$ is defined as in (2.6). Let $h_s = -1/T$. Then,

$$\left[\mathbb{E}\left|M_{T\wedge\tau_k}^{(h,n)}\right|^2\right]^{1/2} \le \frac{1}{T^2}\left[\int_0^T \mathbb{E}\left|Q_{s\wedge\tau_k}^{(n)}\int_0^{s\wedge\tau_k}\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r\right|^2\mathrm{d}s\right]^{1/2}.$$

By Itô's formula, we see that

$$\begin{aligned}&\mathrm{d}\left(\mathrm{e}^{-K^- s}\left|Q_s^{(n)}\int_0^s (Q_r^{(n)})^{-1}/\!/_r\mathrm{d}B_r\right|^2\right)\\ &\le 2\,\mathrm{e}^{-K^- s}\left\langle Q_s^{(n)}\int_0^s\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r,\ /\!/_s\mathrm{d}B_s\right\rangle + \mathrm{d}s.\end{aligned} \tag{2.28}$$

For $0 < s \le \tau_k$, this implies that

$$\mathbb{E}\left[\mathrm{e}^{-K^- s\wedge\tau_k}\left|Q_{s\wedge\tau_k}^{(n)}\int_0^{s\wedge\tau_k}\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r\right|^2\right] \le s.$$

Letting k tend to ∞ yields

$$\mathbb{E}\left[\left|Q_{s\wedge\tau_k}^{(n)}\int_0^{s\wedge\tau_k}\{Q_r^{(n)}\}^{-1}/\!/_r\mathrm{d}B_r\right|^2\right] \le s\,\mathrm{e}^{K^- s}.$$

Combining this with (2.28) and (2.27), we see that $\{M_T^{(h,n)}\}_{n\ge1}$ is bounded in $L^2(\mathbb{P})$, and thus obtain a subsequence converging weakly to a random variable M_T^h in $L^2(\mathbb{P})$ and satisfying

$$\mathbb{E}\left[|M_T^h|^2\right] \le \frac{\mathrm{e}^{K^- T}}{2T^2}.$$

By this and the Bismut formula (2.14), the second assertion (2.26) holds. □

Remark 2.5. Let

$$\mathcal{D} := \{\phi \in C_b^2(M):\ \inf\phi = 1,\ N\log\phi \ge \sigma\}.$$

(A') The functions K, σ in (3.1) are constant, and there exists $\phi \in \mathcal{D}$ such that

$$K_\phi = \sup_{x\in M}\big\{-L\log\phi + 2|\nabla\log\phi|^2\big\} < \infty.$$

By [27, Section 3.2], such ϕ can be constructed if ∂M has strictly positive injectivity radius, the sectional curvature of M being bounded above and Z bounded. In particular, if the manifold is compact, these conditions are met automatically. By [6, Theorem 2.2], if

$$\mathrm{Ric}_Z + L\log\phi - 2|\nabla\log\phi|^2 \ge K - K_\phi,$$

we then obtain

$$\|\nabla P_t f\|_\infty \le \|\phi\|_\infty \|\nabla f\|_\infty \,\mathrm{e}^{-(K-K_\phi)t}, \quad t>0, \tag{2.29}$$

which implies that $|\nabla P_\cdot f|$ is bounded on $[0,T]\times M$ for $f\in C_b^1(M)$.

Corollary 2.6. *Assume that condition* $(\mathbf{A}')$ *holds. Let* $x\in M$ *and* $T>0$. *Then*

$$|L(P_T f)|(x) \le 2\|f\|_\infty \left(\frac{\sqrt{3}\|Z\|_\infty}{3\sqrt{T}} + \frac{(3+\sqrt{10})\|\phi\|_\infty \,\mathrm{e}^{\frac{1}{2}(K_\phi+K^-)T}}{T} \right),$$

for $f\in \mathcal{B}_b(M)$.

Remark 2.7. In the Appendix, we recall the method from [27] to construct ϕ under condition $(\mathbf{B})$. From this condition, $\|\phi\|_\infty$ and K_ϕ can be estimated as presented in Remark 5.3.

3. Bismut type Hessian formula for Neumann semigroup

To state the main result of this section, we first introduce some curvature conditions. For $x\in M$ and $v_1\in T_xM$, let $\mathrm{Ric}_Z^\sharp(v_1)\in T_xM$ be given by

$$\langle \mathrm{Ric}_Z^\sharp(v_1), v_2\rangle := \mathrm{Ric}_Z(v_1,v_2) = \mathrm{Ric}(v_1,v_2) - \langle \nabla_{v_1} Z, v_2\rangle, \quad v_2\in T_xM.$$

Let R denote the Riemann curvature tensor. Then $\mathbf{d}^*R(v_1)$ is the linear operator on T_xM determined by

$$\langle \mathbf{d}^*R(v_1,v_2), v_3\rangle = \langle (\nabla_{v_3}\mathrm{Ric}^\sharp)(v_1), v_2\rangle - \langle (\nabla_{v_2}\mathrm{Ric}^\sharp)(v_3), v_1\rangle, \quad v_3\in T_xM,$$

where we write $\mathbf{d}^*R(v_1,v_2)\equiv \mathbf{d}^*R(v_1)v_2$. Moreover, let $R(v_1): T_xM\otimes T_xM\to T_xM$ be given by

$$\langle R(v_1)(v_2,v_3), v_4\rangle := \langle R(v_1,v_2)v_3, v_4\rangle, \quad v_2,v_3,v_4\in T_xM.$$

Finally, let $|\cdot|$ be the operator norm on tensors, and $\|\cdot\|_\infty$ be the uniform norm of $|\cdot|$ over M.

Assume that there exist two functions $K\in C(M)$ and $\sigma\in C(\partial M)$ such that

$$\mathrm{Ric}_Z := \mathrm{Ric} - \nabla Z \ge K, \qquad \mathrm{II}\ge \sigma, \tag{3.1}$$

where the second condition means $-\langle \nabla_X N, X\rangle \ge -\sigma(x)^-|X|^2$ for $x\in\partial M$ and $X\in T_xM$. Moreover, assume that there exist three non-negative functions α, β and γ, such that

$$\begin{aligned} &|R|_{\mathrm{HS}}(x)\le \alpha(x),\ \ |\mathbf{d}^*R + \nabla \mathrm{Ric}_Z^\sharp - R(Z)|(x) < \beta(x),\\ &|\nabla(\nabla N)^\sharp + R(N)|(x) < \gamma(x), \end{aligned} \tag{3.2}$$

where for $x\in M$ and $v_1,v_2\in T_xM$,

$$|R|_{\mathrm{HS}}(x) = \sup\left\{ |R^{\sharp,\sharp}(v_1,v_2)|_{\mathrm{HS}}(x) : v_1,v_2\in T_xM,\ |v_1|\le 1,\ |v_2|\le 1\right\}.$$

To establish a Hessian formula for $P_t f$, we first introduce an operator $\tilde{Q}_t : T_xM \to T_{X_t}M$ defined by

$$\mathrm{D}\tilde{Q}_t = -\frac{1}{2}\mathrm{Ric}^\sharp_Z(\tilde{Q}_t)\,\mathrm{d}t + \frac{1}{2}(\nabla N)^\sharp(\tilde{Q}_t)\,\mathrm{d}l_t, \quad \tilde{Q}_0 = \mathrm{id}. \tag{3.3}$$

Then let the operator-valued process $W^{\tilde{h}}_t : T_xM \otimes T_xM \to T_{X_t(x)}M$ be defined as solutions to the following covariant Itô equation

$$\begin{aligned}\mathrm{D}W^{\tilde{h}}_t(v,v) = {}& R(//_t\mathrm{d}B_t, \tilde{Q}_t(\tilde{h}_t v))\tilde{Q}_t(v)\\ &- \frac{1}{2}(\mathbf{d}^*R - R(Z) + \nabla\mathrm{Ric}_Z)^\sharp(\tilde{Q}_t(\tilde{h}_t v), \tilde{Q}_t(v))\,\mathrm{d}t\\ &- \frac{1}{2}(\nabla^2 N - R(N))^\sharp(\tilde{Q}_t(\tilde{h}_t v), \tilde{Q}_t(v))\,\mathrm{d}l_t\\ &- \frac{1}{2}\mathrm{Ric}^\sharp_Z(W^{\tilde{h}}_t(v,v))\,\mathrm{d}t + \frac{1}{2}(\nabla N)^\sharp(W^{\tilde{h}}_t(v,v))\,\mathrm{d}l_t\end{aligned}$$

with initial condition $W^{\tilde{h}}_0(v,v) = 0$.

In this section, we first introduce the local version of the Bismut type Hessian formula for P_t and then introduce some proper global curvature conditions to establish the global version of it.

3.1. **Local Bismut type Hessian formula for Neumann semigroup.** The following is our main result in this subsection.

Theorem 3.1. *Let D be an open relatively compact subset of M, $T > 0$ and $x \in D$. Suppose that (3.1) and (3.2) hold. Let $h(\cdot)$ be an adapted and bounded real process such that $\int_0^t h_s\,\mathrm{d}s = -1$ for $t \geq T \wedge \tau_D$, and such that*

$$\begin{aligned}\mathbb{E}\Bigg[&\int_0^{T\wedge\tau_D} \Big(h_s^2 + \tilde{h}_s^2(\alpha^2(X_s) + \beta^2(X_s))\Big)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\\ &+ \int_0^{T\wedge\tau_D} \tilde{h}_s^2\gamma^2(X_s)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}l_s\Bigg] < \infty\end{aligned} \tag{3.4}$$

where $\tilde{h}_t = 1 + \int_0^t h_s\,\mathrm{d}s$. Then for $f \in \mathcal{B}_b(M)$ and $v \in T_xM$,

$$\begin{aligned}&\mathrm{Hess}_{P_T f}(v,v)(x)\\ &= -\mathbb{E}^x\left[f(X_{T\wedge\tau_D})\int_0^T \langle W^{\tilde{h}}_s(v, h_s v), //_s\mathrm{d}B_s\rangle\right]\\ &\quad + \mathbb{E}^x\left[f(X_{T\wedge\tau_D})\left(\left(\int_0^T \langle \tilde{Q}_s(h_s v), //_s\mathrm{d}B_s\rangle\right)^2 - \int_0^T |\tilde{Q}_s(h_s v)|^2\,\mathrm{d}s\right)\right].\end{aligned}$$

Moreover,

$$|\mathrm{Hess}_{P_T f}| \leq 3\|f\|_D C(h)^{1/2}$$

$$\times\left\{\frac{1}{2}\left[\mathbb{E}\left(\int_0^{T\wedge\tau_D}\beta^2(X_s)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde{h}_s^2\,\mathrm{d}s\right)\right]^{1/2}\right.$$
$$+(3+\sqrt{10})\left[\mathbb{E}\left(\int_0^{T\wedge\tau_D}\alpha^2(X_s)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde{h}_s^2\,\mathrm{d}s\right)\right]^{\frac{1}{2}}$$
$$\left.+\frac{1}{2}\left[\mathbb{E}\left(\int_0^{T\wedge\tau_D}\gamma^2(X_s)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde{h}_s^2\,\mathrm{d}l_s\right)\right]^{\frac{1}{2}}+\frac{2}{3}C(h)^{\frac{1}{2}}\right\},\tag{3.5}$$

where $C(h)$ is defined as in (2.7)*.*

Remarks 3.2. 1) The original idea of the proof for the Hessian formula comes from Elworthy-Li [11] and Thalmaier [1]. Our form of the formula is consistent with [5] with the choice of one random test function h only. The main difficulty here is to deal with the impact of the boundary and to weaken the conditions on the curvature and the process h. Theorem 3.1 also improves the results in [1, 5] and gives a new estimate even when the boundary is empty.

2) Let D be an open relatively compact subset of M. Assume that h is an adapted and non-positive process with $h_s = 0$ for $s \geq T\wedge\tau_D$ and $\int_0^T h_s\,\mathrm{d}s = -1$, which imply $\tilde{h}_s = 0$ for $s \geq T\wedge\tau_D$. Then the functions K, σ, α, β and γ are all bounded on D and $|\tilde{h}_s| \leq 1$. Moreover, condition (3.4) can be simplified to

$$\mathbb{E}\left[\int_0^T h_s^2\,\mathrm{e}^{\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\right]<\infty.$$

The corresponding result is then the local version of the Hessian formula for the heat semigroup.

3) As $-\langle\nabla_N N, N\rangle = 0$, we know that $-\nabla N \geq \sigma$ implies $\sigma \leq 0$.

4) Assume $\mathrm{II} \geq \sigma$. Then for $X \in T_xM$ and $x \in \partial M$, $X = X_1 + X_2$ such that $X_1 \in T_x\partial M$ and $X_2 = \langle X, N\rangle N$,

$$\begin{aligned}-\langle\nabla_X N, X\rangle &= -\langle\nabla_{X_1}N, X_1\rangle - \langle X, N\rangle^2\langle\nabla_N N, N\rangle\\ &\quad - \langle X, N\rangle\langle\nabla_{X_1}N, N\rangle - \langle X, N\rangle\langle\nabla_N N, X_1\rangle\\ &= -\langle\nabla_{X_1}N, X_1\rangle - \langle X, N\rangle\langle\nabla_N N, X_1\rangle\\ &\geq \sigma|X_1|^2 \geq -\sigma^-|X|^2.\end{aligned}$$

5) One might naturally try to work with Q_t instead of $\tilde{Q}_t$ to define $M_t(v,v)$, in order to avoid the term ∇N. But we have already seen that Q_t is the limit of $Q_t^{(n)}$, see the proof of [27, Theorem 3.2.1], which satisfy the covariant Itô equation (2.1). We have

$$\begin{aligned}&\mathrm{d}\Big(\nabla\mathbf{d}P_{T-t}f(Q_t^{(n)}(v), Q_t^{(n)}(v))(X_t)\Big)\\ &= \left(\nabla_{//_t\,\mathrm{d}B_t}\nabla\mathbf{d}P_{T-t}f\right)\left(Q_t^{(n)}(v), Q_t^{(n)}(v)\right)\end{aligned}$$

$$
\begin{aligned}
&- (\nabla \mathbf{d} P_{T-t} f)\left(\mathrm{Ric}_Z^\sharp(Q_t^{(n)}(v)), Q_t^{(n)}(v)\right) \mathrm{d}t \\
&- (\nabla \mathbf{d} P_{T-t} f)\left(Q_t^{(n)}(v), \mathrm{II}^\sharp(Q_t^{(n)}(v))\right) \mathrm{d}l_t \\
&+ \partial_t (\nabla \mathbf{d} P_{T-t} f)(Q_t^{(n)}(v), Q_t^{(n)}(v))\, \mathrm{d}t \\
&+ \frac{1}{2}\nabla_N (\nabla \mathbf{d} P_{T-t} f)(Q_t^{(n)}(v), Q_t^{(n)}(v))\, \mathrm{d}l_t \\
&+ \frac{1}{2}(\mathrm{tr}\,\nabla^2 + \nabla_Z)(\nabla \mathbf{d} P_{T-t} f)(Q_t^{(n)}(v), Q_t^{(n)}(v))\, \mathrm{d}t \\
&- n\langle Q_t^{(n)}(v)), N(X_t)\rangle \nabla \mathbf{d} P_{T-t} f(N(X_t), Q_t^{(n)}(v))\, \mathrm{d}l_t \\
\overset{\mathrm{m}}{=}\, & -n\langle Q_t^{(n)}(v)), N(X_t)\rangle\, \nabla \mathbf{d} P_{T-t} f(Q_t^{(n)}(v), N(X_t))\, \mathrm{d}l_t \\
&+ \frac{1}{2}(\mathbf{d} P_{T-t} f)((\nabla(\nabla N)^\sharp + R(N))(Q_t^{(n)}(v), Q_t^{(n)}(v)))\, \mathrm{d}l_t \\
&+ \frac{1}{2}(\mathbf{d} P_{T-t} f)\big((\mathbf{d}^* R - R(Z) + \nabla \mathrm{Ric}_Z^\sharp)(Q_t^{(n)}(v), Q_t^{(n)}(v))\big)\, \mathrm{d}t \\
&- \nabla \mathbf{d} P_{T-t} f(R^{\sharp,\sharp}(Q_t^{(n)}(v), Q_t^{(n)}(v)))\, \mathrm{d}t. \qquad (3.6)
\end{aligned}
$$

The main difficulty is to clarify the limit of

$$n\langle Q_t^{(n)}(v)), N(X_t)\rangle\, \nabla \mathbf{d} P_{T-t} f(Q_t^{(n)}(v), N),$$

as n tends to ∞. To this end, we even need information concerning ∇N on the full vector bundle of the boundary if we use Q_t in the definition of $M_t(v,v)$ in the above proof, and then it is still non-trivial to check the martingale property. In this respect, working with the functional $\tilde{Q}_t$ instead of Q_t not only simplifies the calculation, it also doesn't require additional conditions.

To prove Theorem 3.1, we need the following two lemmata.

Lemma 3.3. *Keeping the assumptions as in Theorem 3.1, we have*

$$
\begin{aligned}
&\mathbb{E}\left[\sup_{t\in[0,T]} \Big|\int_0^t h_s \langle W_s^{\tilde{h}}(v,v),\ //_s \mathrm{d}B_s\rangle\Big|\right] \\
&\le 3C(h)^{1/2}\Bigg\{(3+\sqrt{10})\left(\mathbb{E}\int_0^T \alpha^2(X_s)\, \mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\, \tilde{h}_s^2\, \mathrm{d}s\right)^{1/2} \\
&\quad + \frac{1}{2}\left(\mathbb{E}\int_0^T \beta^2(X_s)\, \mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}r}\, \tilde{h}_s^2\, \mathrm{d}s\right)^{1/2} \\
&\quad + \frac{1}{2}\left(\mathbb{E}\int_0^T \gamma^2(X_s)\, \mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\, \tilde{h}_s^2\, \mathrm{d}l_s\right)^{1/2}\Bigg\}.
\end{aligned}
$$

Proof. By the Lenglart inequality and the Minkowski inequality, we have

$$\mathbb{E}\left[\sup_{t\in[0,T]} \Big|\int_0^{t\wedge\tau_k} h_s \langle W_s^{\tilde{h}}(v,v),\ //_s \mathrm{d}B_s\rangle\Big|\right]$$

$$\le 3\mathbb{E}\left[\int_0^{T\wedge\tau_k} h_s^2 |W_s^{\tilde h}(v,v)|^2\,\mathrm{d}s\right]^{1/2}$$

$$\le 3\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k} h_s^2\big|\xi_s^{(1)}\big|^2\,\mathrm{d}s\right)^{1/2}\right] + \frac{3}{2}\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k} h_s^2\big|\xi_s^{(2)}\big|^2\,\mathrm{d}s\right)^{1/2}\right]$$

$$+\frac{3}{2}\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k} h_s^2\big|\xi_s^{(3)}\big|^2\,\mathrm{d}s\right)^{1/2}\right], \tag{3.7}$$

where

$$\xi_s^{(1)} = \tilde Q_s \int_0^s \tilde Q_r^{-1} R(/\!/_r \mathrm{d}B_r, \tilde Q_r(\tilde h(r)v))\tilde Q_r(v);$$

$$\xi_s^{(2)} = \tilde Q_s \int_0^s \tilde Q_r^{-1} (\mathbf{d}^* R - R(Z) + \nabla \mathrm{Ric}_Z)^\sharp(\tilde Q_r(\tilde h(r)v), \tilde Q_r(v))\,\mathrm{d}r;$$

$$\xi_s^{(3)} = \tilde Q_s \int_0^s \tilde Q_r^{-1} (\nabla^2 N - R(N))^\sharp(\tilde Q_r(\tilde h(r)v), \tilde Q_r(v))\,\mathrm{d}l_r.$$

Then we have

$$\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k} h_s^2|\xi_s^{(1)}|^2\,\mathrm{d}s\right)^{1/2}\right]$$

$$\le \mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} |\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right]^{1/2}$$

$$\times\,\mathbb{E}\left[\int_0^{T\wedge\tau_k} h_s^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\right]^{1/2}, \tag{3.8}$$

and

$$\mathrm{d}\Big|\mathrm{e}^{-\frac12\int_0^s K^-(X_r)\,\mathrm{d}r - \frac12\int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\xi_s^{(1)}\Big|^2$$

$$\le 2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\left\langle R(/\!/_s\mathrm{d}B_s, \tilde Q_s(\tilde h_s v))\tilde Q_s(v), \xi_s^{(1)}\right\rangle$$

$$+\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\left|R^{\sharp,\sharp}(\tilde Q_s(\tilde h_s v), \tilde Q_s(v))\right|_{\mathrm{HS}}^2\,\mathrm{d}s$$

$$\le 2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\left\langle R(/\!/_s\mathrm{d}B_s, \tilde Q_s(\tilde h_s v))\tilde Q_s(v), \xi_s^{(1)}\right\rangle$$

$$+\,\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s,\quad s<\tau_k, \tag{3.9}$$

which implies

$$\mathbb{E}\left[\sup_{s\in[0,T\wedge\tau_k]} |\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r - \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\right]$$

$$\le 6\,\mathbb{E}\left[\left(\int_0^{T\wedge\tau_k} |\xi_s^{(1)}|^2\alpha(X_s)^2\tilde h_s^2\,\mathrm{d}s\right)^{1/2}\right]$$

$$+\,\mathbb{E}\left[\int_0^{T\wedge\tau_k}\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r + \int_0^s \sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\right]$$

$$\begin{aligned}
&\le 6\,\mathbb{E}\Bigg[\bigg(\sup_{s\in[0,T\wedge\tau_k]}|\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r-\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\bigg)^{1/2}\\
&\qquad\times\bigg(\int_0^{T\wedge\tau_k}\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\bigg)^{1/2}\Bigg]\\
&\quad+\mathbb{E}\bigg[\int_0^{T\wedge\tau_k}\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\bigg]\\
&\le\frac{1}{2\delta}\mathbb{E}\bigg[\sup_{s\in[0,T\wedge\tau_k]}|\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r-\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\bigg]\\
&\quad+(1+18\delta)\mathbb{E}\bigg[\int_0^{T\wedge\tau_k}\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\bigg],\quad \delta>0.
\end{aligned}$$

Substituting the optimal choice $\delta=\frac{1}{6}\big(3+\sqrt{10}\big)$, we get

$$\begin{aligned}
&\mathbb{E}\bigg[\sup_{s\in[0,T\wedge\tau_k]}|\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r-\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\bigg]\\
&\quad\le(3+\sqrt{10})^2\mathbb{E}\bigg[\int_0^{T\wedge\tau_k}\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\bigg].
\end{aligned}$$

Combining this with (3.8) and letting k tend to ∞ yields

$$\begin{aligned}
&\mathbb{E}\left(\bigg[\int_0^T h_s^2|\xi_s^{(1)}|^2\,\mathrm{d}s\bigg]^{1/2}\right)\\
&\le\mathbb{E}\bigg[\sup_{s\in[0,T]}|\xi_s^{(1)}|^2\,\mathrm{e}^{-\int_0^s K^-(X_r)\,\mathrm{d}r-\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\bigg]^{1/2}\\
&\qquad\times\mathbb{E}\bigg[\int_0^T h_s^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\mathrm{d}s\bigg]^{1/2}\\
&\le\Big(3+\sqrt{10}\Big)\mathbb{E}\bigg[\int_0^T\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\bigg]^{1/2}C(h)^{1/2}.
\end{aligned}$$

Moreover, for any $\varepsilon>0$,

$$\begin{aligned}
&\mathrm{d}\left(\Big|\mathrm{e}^{-\frac12\int_0^t K^-(X_s)\,\mathrm{d}t-\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\xi_t^{(2)}\Big|^2+\varepsilon\right)^{1/2}\\
&=\frac{\mathrm{d}\Big|\mathrm{e}^{-\frac12\int_0^t K^-(X_s)\,\mathrm{d}t-\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\xi_t^{(2)}\Big|^2}{2\left(\Big|\mathrm{e}^{-\frac12\int_0^t K^-(X_s)\,\mathrm{d}t-\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\xi_t^{(2)}\Big|^2+\varepsilon\right)^{1/2}}\\
&=\mathrm{e}^{-\int_0^t K^-(X_s)\,\mathrm{d}t-\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\left(\Big|\mathrm{e}^{-\frac12\int_0^t K^-(X_s)\,\mathrm{d}t-\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\xi_t^{(2)}\Big|^2+\varepsilon\right)^{-1/2}
\end{aligned}$$

$$\times\Bigg[-(\mathrm{Ric}_Z+K^-(X_t)g)\Big(\xi_t^{(2)},\xi_t^{(2)}\Big)\,\mathrm{d}t+(\nabla N-\sigma^-(X_t)g)\Big(\xi_t^{(2)},\xi_t^{(2)}\Big)\,\mathrm{d}l_t$$

$$+\Big\langle(\mathbf{d}^*R-R(Z)+\nabla\mathrm{Ric}_Z)^\sharp(\tilde Q_t(\tilde h_t v),\tilde Q_t(v)),\xi_t^{(2)}\Big\rangle\,\mathrm{d}t\Bigg]$$

$$\le \mathrm{e}^{-\int_0^t K^-(X_s)\,\mathrm{d}t-\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\left(\Big|\mathrm{e}^{-\frac12\int_0^t K^-(X_s)\,\mathrm{d}s-\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\xi_t^{(2)}\Big|^2+\varepsilon\right)^{-1/2}$$

$$\times\Big\langle(\mathbf{d}^*R-R(Z)+\nabla\mathrm{Ric}_Z)^\sharp(\tilde Q_t(\tilde h_t v),\tilde Q_t(v)),\xi_t^{(2)}\Big\rangle\,\mathrm{d}t$$

$$\le\beta(X_t)\,\mathrm{e}^{\frac12\int_0^t K^-(X_s)\,\mathrm{d}t+\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\,\tilde h_t\,\mathrm{d}t,\quad t<\tau_k.$$

Taking the integral on both sides, and letting ε tend to 0 and k tend to ∞, we then conclude that

$$\Big|\xi_t^{(2)}\Big|\le\mathrm{e}^{\frac12\int_0^t K^-(X_s)\,\mathrm{d}s+\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\times\int_0^t\beta(X_s)\,\mathrm{e}^{\frac12\int_0^s K^-(X_r)\,\mathrm{d}r+\frac12\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s\,\mathrm{d}s.$$

With a similar argument, we have

$$\Big|\xi_t^{(3)}\Big|\le\mathrm{e}^{\frac12\int_0^t K^-(X_s)\,\mathrm{d}t+\frac12\int_0^t\sigma^-(X_s)\,\mathrm{d}l_s}\int_0^t\gamma(X_s)\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s\,\mathrm{d}l_s.$$

These estimates together imply

$$\mathbb{E}\left[\sup_{t\in[0,T]}\Big|\int_0^t h_s\langle W_s^{\tilde h}(v,v),\,//_s\mathrm{d}B_s\rangle\Big|\right]$$

$$\le 3C(h)^{1/2}\Bigg\{\big(3+\sqrt{10}\big)\left(\mathbb{E}\int_0^T\alpha(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}s\right)^{1/2}$$

$$+\frac12\left(\mathbb{E}\int_0^T\beta(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}r}\,\tilde h_s^2\,\mathrm{d}s\right)^{1/2}$$

$$+\frac12\left(\mathbb{E}\int_0^T\gamma(X_s)^2\,\mathrm{e}^{\int_0^s K^-(X_r)\,\mathrm{d}r+\int_0^s\sigma^-(X_r)\,\mathrm{d}l_r}\,\tilde h_s^2\,\mathrm{d}l_s\right)^{1/2}\Bigg\}.$$

□

Lemma 3.4. *Let D be an open relatively compact domain in M and $x\in D$. Fix $T>0$ and suppose that h is a bounded, non-negative and adapted process with paths in the Cameron-Martin space $L^{1,2}([0,T];\mathbb{R})$. Then for $f\in\mathcal{B}_b(M)$ and $v\in T_xM$,*

$$(\nabla\mathbf{d}P_{T-t}f)(\tilde Q_t(\tilde h_t v),\tilde Q_t(\tilde h_t v))+(\mathbf{d}P_{T-t}f)\big(W_t^{\tilde h}(v,\tilde h_t v)\big)$$

$$-2\mathbf{d}P_{T-t}f(\tilde Q_t(\tilde h_t v))\int_0^t\langle\tilde Q_s(h_s v),//_s\mathrm{d}B_s\rangle$$

$$-P_{T-t}f(X_t)\int_0^t\langle W_s^{\tilde h}(v,h_s v),//_s\mathrm{d}B_s\rangle$$

$$+ P_{T-t}f(X_t)\left(\left(\int_0^t \langle \tilde{Q}_s(h_s v), //_s \mathrm{d}B_s\rangle\right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2\,\mathrm{d}s\right) \tag{3.10}$$

is a local martingale, and in particular a true martingale on $[0, T\wedge\tau_D)$.

Proof. We first prove that for $f\in\mathcal{B}_b(M)$ and $v\in T_xM$,

$$M_t(v,v) = \nabla\mathbf{d}P_{T-t}f(\tilde{Q}_t(v),\tilde{Q}_t(v)) + (\mathbf{d}P_{T-t}f)(W_t(v,v)) \tag{3.11}$$

is a local martingale where

$$\begin{aligned} W_t(v,v) =& \tilde{Q}_t\int_0^t \tilde{Q}_s^{-1}R(//_s\mathrm{d}B_s,\tilde{Q}_s(v))\tilde{Q}_s(v)\\ &-\frac{1}{2}\tilde{Q}_t\int_0^t \tilde{Q}_s^{-1}(\mathbf{d}^*R - R(Z)+\nabla\mathrm{Ric}^\sharp_Z)(\tilde{Q}_s(v),\tilde{Q}_s(v))\,\mathrm{d}s\\ &-\frac{1}{2}\tilde{Q}_t\int_0^t \tilde{Q}_s^{-1}(\nabla(\nabla N)^\sharp - R(N))(\tilde{Q}_s(v),\tilde{Q}_s(v))\,\mathrm{d}l_s. \end{aligned} \tag{3.12}$$

Let us recall some commutation rules which will be helpful in the subsequent calculations:

$$\begin{aligned} &\mathbf{d}L = (\mathrm{tr}\,\nabla^2+\nabla_Z)\mathbf{d}f - \mathbf{d}f(\mathrm{Ric}^\sharp - (\nabla Z)^\sharp);\\ &\nabla\mathbf{d}(\Delta f) = \mathrm{tr}\,\nabla^2(\nabla\mathbf{d}f) - (\nabla\mathbf{d}f)(\mathrm{Ric}^\sharp\odot\mathrm{id}+\mathrm{id}\odot\mathrm{Ric}^\sharp - 2R^{\sharp,\sharp})\\ &\qquad\qquad - \mathbf{d}f(\mathbf{d}^*R+\nabla\mathrm{Ric}^\sharp);\\ &\nabla\mathbf{d}(Z(f)) = \nabla_Z(\nabla\mathbf{d}f) + (\nabla\mathbf{d}f)((\nabla Z)^\sharp\odot\mathrm{id}+\mathrm{id}\odot(\nabla Z)^\sharp)\\ &\qquad\qquad + \mathbf{d}f(\nabla(\nabla Z)^\sharp + R(Z));\\ &\nabla\mathbf{d}(Nf) = \nabla_N(\nabla\mathbf{d}f) + (\nabla\mathbf{d}f)((\nabla N)^\sharp\odot\mathrm{id}+\mathrm{id}\odot(\nabla N)^\sharp)\\ &\qquad\qquad + \mathbf{d}f(\nabla(\nabla N)^\sharp + R(N)) \end{aligned} \tag{3.13}$$

where $\nabla\mathbf{d}f(\nabla N\odot\mathrm{id}(v,v)) = \nabla\mathbf{d}f(\nabla_v N, v)$. Then by Itô's formula we have

$$\begin{aligned} \mathrm{d}M_t(v,v) =& (\nabla_{//_t\,\mathrm{d}B_t}\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v)) + (\nabla_{//_t\mathrm{d}B_t}\mathbf{d}P_{T-t}f)(W_t(v,v))\\ &+(\nabla\mathbf{d}P_{T-t}f)\left(\mathrm{D}\tilde{Q}_t(v),\tilde{Q}_t(v)\right) + (\nabla\mathbf{d}P_{T-t}f)\left(\tilde{Q}_t(v),\mathrm{D}\tilde{Q}_t(v)\right)\\ &+\partial_t(\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}t\\ &+\frac{1}{2}(\mathrm{tr}\,\nabla^2+\nabla_Z)(\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}t\\ &+\frac{1}{2}\nabla_N(\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}l_t + \frac{1}{2}\nabla_N(\mathbf{d}P_{T-t}f)(W_t(v,v))\,\mathrm{d}l_t\\ &+(\mathbf{d}P_{T-t}f)(\mathrm{D}W_t(v,v)) + \langle\mathrm{D}(\mathbf{d}P_{T-t}f),\mathrm{D}W_t(v,v)\rangle\\ &+\partial_t(\mathbf{d}P_{T-t}f)(W_t(v,v))\,\mathrm{d}t + \frac{1}{2}(\mathrm{tr}\,\nabla^2+\nabla_Z)(\mathbf{d}P_{T-t}f)(W_t(v,v))\,\mathrm{d}t. \end{aligned} \tag{3.14}$$

Taking into account the commutation properties (3.13) and according to the definition of $\tilde{Q}_t$, for the terms on the right side of (3.14), we observe that

$$\partial_t(\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}t + (\nabla\mathbf{d}P_{T-t}f)\left(\mathrm{D}\tilde{Q}_t(v),\tilde{Q}_t(v)\right)$$

$$
\begin{aligned}
&+ (\nabla \mathbf{d} P_{T-t} f)\left(\tilde{Q}_t(v), \mathrm{D}\tilde{Q}_t(v)\right)\\
&= -\frac{1}{2}\left((\operatorname{tr}\nabla^2 + \nabla_Z)\nabla \mathbf{d} P_{T-t} f\right)(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}t\\
&\quad + (\nabla \mathbf{d} P_{T-t} f)(\mathrm{Ric}_Z^\sharp(\tilde{Q}_t(v)), \tilde{Q}_t(v))\,\mathrm{d}t - (\nabla \mathbf{d} P_{T-t} f)(R^{\sharp,\sharp}(\tilde{Q}_t(v), \tilde{Q}_t(v)))\,\mathrm{d}t\\
&\quad + \frac{1}{2}\mathbf{d} P_{T-t} f\left((\mathbf{d}^* R - R(Z) + \nabla \mathrm{Ric}_Z)^\sharp(\tilde{Q}_t(v), \tilde{Q}_t(v))\right)\mathrm{d}t\\
&\quad + (\nabla \mathbf{d} P_{T-t} f)\left(-\mathrm{Ric}_Z^\sharp(\tilde{Q}_t(v))\,\mathrm{d}t + (\nabla N)^\sharp(\tilde{Q}_t(v))\,\mathrm{d}l_t, \tilde{Q}_t(v)\right)\\
&= -\frac{1}{2}\left((\operatorname{tr}\nabla^2 + \nabla_Z)\nabla \mathbf{d} P_{T-t} f\right)(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}t\\
&\quad - \nabla \mathbf{d} P_{T-t} f(R^{\sharp,\sharp}(\tilde{Q}_t(v), \tilde{Q}_t(v)))\,\mathrm{d}t\\
&\quad + \frac{1}{2}\mathbf{d} P_{T-t} f\left((\mathbf{d}^* R - R(Z) + \nabla \mathrm{Ric}_Z)^\sharp(\tilde{Q}_t(v), \tilde{Q}_t(v))\right)\mathrm{d}t\\
&\quad + \nabla \mathbf{d} P_{T-t} f\left((\nabla N)^\sharp(\tilde{Q}_t(v)), \tilde{Q}_t(v)\right)\mathrm{d}l_t.
\end{aligned}
$$

Then using the definition of W_t, we calculate the quadratic covariation of $\mathbf{d} P_{T-t} f$ and $W_t(v,v)$ as

$$
\begin{aligned}
\left[\mathrm{D}(\mathbf{d} P_{T-t} f), \mathrm{D}W_t(v,v)\right] &= \left[\nabla_{//_t \mathrm{d}B_t}\mathbf{d} P_{T-t} f, R(//_t \mathrm{d}B_t, \tilde{Q}_t(v))\tilde{Q}_t(v)\right]\\
&= \operatorname{tr}\langle \nabla_{\cdot} \mathbf{d} P_{T-t} f, R(\,\cdot\,, \tilde{Q}_t(v))\tilde{Q}_t(v)\rangle\,\mathrm{d}t\\
&= \nabla \mathbf{d} P_{T-t} f(R^{\sharp,\sharp}(\tilde{Q}_t(v), \tilde{Q}_t(v)))\,\mathrm{d}t.
\end{aligned}
$$

According to the definition of $W_t(v,v)$, we have

$$
\begin{aligned}
&(\mathbf{d} P_{T-t} f)(\mathrm{D}W_t(v,v)) + (\partial_t \mathbf{d} P_{T-t} f)(W_t(v,v))\,\mathrm{d}t\\
&\quad = (\mathbf{d} P_{T-t} f)\Big(R(//_t \mathrm{d}B_t, \tilde{Q}_t(v))\tilde{Q}_t(v)\\
&\qquad - \frac{1}{2}(\mathbf{d}^* R - R(Z) + \nabla \mathrm{Ric}_Z)^\sharp(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}t\\
&\qquad - \frac{1}{2}(\nabla^2 N - R(N))^\sharp(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}l_t + \frac{1}{2}(\nabla N)^\sharp(W_t(v,v))\,\mathrm{d}l_t\Big)\\
&\qquad - \frac{1}{2}(\operatorname{tr}\nabla^2 + \nabla_Z)\mathbf{d} P_{T-t} f(W_t(v,v))\,\mathrm{d}t.
\end{aligned}
$$

We conclude that

$$
\begin{aligned}
&(\nabla \mathbf{d} P_{T-t} f)\left(\mathrm{D}\tilde{Q}_t(v), \tilde{Q}_t(v)\right) + (\nabla \mathbf{d} P_{T-t} f)\left(\tilde{Q}_t(v), \mathrm{D}\tilde{Q}_t(v)\right)\\
&\quad + \partial_t(\nabla \mathbf{d} P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}t\\
&\quad + \frac{1}{2}(\operatorname{tr}\nabla^2 + \nabla_Z)(\nabla \mathbf{d} P_{T-t} f)(\tilde{Q}_t(v), \tilde{Q}_t(v))\,\mathrm{d}t\\
&\quad + (\mathbf{d} P_{T-t} f)(\mathrm{D}W_t(v,v)) + [\mathrm{D}(\mathbf{d} P_{T-t} f), \mathrm{D}W_t(v,v)]\\
&\quad + \partial_t(\mathbf{d} P_{T-t} f)(W_t(v,v))\,\mathrm{d}t + \frac{1}{2}(\operatorname{tr}\nabla^2 + \nabla_Z)(\mathbf{d} P_{T-t} f)(W_t(v,v))\,\mathrm{d}t
\end{aligned}
$$

$$
\begin{aligned}
&= -\frac{1}{2}(\mathbf{d}P_{T-t}f)(\nabla^2 N - R(N))^\sharp(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}l_t \\
&\quad + \frac{1}{2}(\mathbf{d}P_{T-t}f)((\nabla N)^\sharp(W_t(v,v)))\,\mathrm{d}l_t \\
&\quad + \frac{1}{2}\nabla\mathbf{d}P_{T-t}f((\nabla N)^\sharp(\tilde{Q}_t(v)),\tilde{Q}_t(v))\,\mathrm{d}l_t \\
&\quad + \frac{1}{2}\nabla\mathbf{d}P_{T-t}f(\tilde{Q}_t(v),(\nabla N)^\sharp(\tilde{Q}_t(v))\,\mathrm{d}l_t.
\end{aligned}
\tag{3.15}
$$

On the other hand, for the terms in (3.14) related to the normal vector on the boundary, we have

$$
\begin{aligned}
&\nabla_N(\nabla\mathbf{d}P_{T-t}f)(\tilde{Q}_t(v),\tilde{Q}_t(v))\,\mathrm{d}l_t + \nabla_N(\mathbf{d}P_{T-t}f)(W_t(v,v))\,\mathrm{d}l_t \\
&= -\nabla\mathbf{d}P_{T-t}f\big((\nabla N)^\sharp(\tilde{Q}_t(v)),\tilde{Q}_t(v)\big)\,\mathrm{d}l_t - \nabla\mathbf{d}P_{T-t}f(\tilde{Q}_t(v),(\nabla N)^\sharp(\tilde{Q}_t(v)))\,\mathrm{d}l_t \\
&\quad - \mathbf{d}P_{T-t}f((\nabla^2 N + R(N))(\tilde{Q}_t(v),\tilde{Q}_t(v)))\,\mathrm{d}l_t \\
&\quad - \mathbf{d}P_{T-t}f((\nabla N)^\sharp(W_t(v,v)))\,\mathrm{d}l_t.
\end{aligned}
$$

Combining this with (3.14) and (3.15), we obtain

$$
\begin{aligned}
&\mathrm{d}M_t(v,v) \\
&\overset{\mathrm{m}}{=} \frac{1}{2}(\mathbf{d}P_{T-t}f)\Big((\nabla^2 N + R(N))(\tilde{Q}_t(v),\tilde{Q}_t(v))(X_t)\,\mathrm{d}l_t - (\nabla N)^\sharp(W_t(v,v))(X_t)\,\mathrm{d}l_t\Big) \\
&\quad - \frac{1}{2}(\mathbf{d}P_{T-t}f)\,\Big((\nabla^2 N + R(N))(\tilde{Q}_t(v),\tilde{Q}_t(v))\Big)\,(X_t)\,\mathrm{d}l_t \\
&\quad + \frac{1}{2}(\mathbf{d}P_{T-t}f)\,\Big((\nabla N)^\sharp(W_t(v,v))\Big)\,(X_t)\,\mathrm{d}l_t = 0.
\end{aligned}
$$

In other words, $M_t(v,v)$ is a local martingale.

Let

$$
M_t^{\tilde{h}}(v,v) = \nabla\mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v),\tilde{Q}_t(v)) + (\mathbf{d}P_{T-t}f)(W_t^{\tilde{h}}(v,v)).
$$

From the definition of $W_t^{\tilde{h}}(v,v)$, resp. $W_t(v,v)$, and in view of the fact that $M_t(v,v)$ is a local martingale, we see that

$$
M_t^{\tilde{h}}(v,v) - \int_0^t (\nabla\mathbf{d}P_{T-s}f)(\tilde{Q}_s(h_s v),\tilde{Q}_s(v))\,\mathrm{d}s \tag{3.16}
$$

is a local martingale as well. Replacing in $M_t^{\tilde{h}}(v,v)$ the second argument v by $\tilde{h}_t v$, we further get that also

$$
\begin{aligned}
&M_t^{\tilde{h}}(v,\tilde{h}(t)v) - \int_0^t (\nabla\mathbf{d}P_{T-s}f)(\tilde{Q}_s(h_s v),\tilde{Q}_s(\tilde{h}_t v))\,\mathrm{d}s \\
&\quad - \int_0^t \nabla\mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v),\tilde{Q}_s(\tilde{h}_s v))\,\mathrm{d}s - \int_0^t (\mathbf{d}P_{T-s}f)(W_s^{\tilde{h}}(v,h_s v))\,\mathrm{d}s \\
&\quad + \int_0^t \int_0^s (\nabla\mathbf{d}P_{T-r}f)(\tilde{Q}_r(h_r v),\tilde{Q}_r(h_s v))\,\mathrm{d}r\,\mathrm{d}s
\end{aligned}
$$

(3.17)

is a local martingale. Note that $M_t^{\tilde h}(v,\tilde h_t v) = M_t^{\tilde h}(v,v)\,\tilde h_t$. Exchanging the order of integration in the last term shows that

$$\begin{aligned}
&M_t^{\tilde h}(v,\tilde h_t v) - \int_0^t (\nabla \mathbf{d} P_{T-s} f)(\tilde Q_s(h_s v), \tilde Q_s(\tilde h_t v))\,\mathrm{d}s\\
&\qquad - \int_0^t \nabla \mathbf{d} P_{T-s} f(\tilde Q_s(\tilde h_s v), \tilde Q_s(h_s v))\,\mathrm{d}s\\
&\qquad - \int_0^t (\mathbf{d} P_{T-s} f)(W_s^{\tilde h}(v, h_s v))\,\mathrm{d}s\\
&\qquad + \int_0^t (\nabla \mathbf{d} P_{T-r} f)(\tilde Q_r(h_r v), \tilde Q_r((\tilde h_t - \tilde h_r) v))\,\mathrm{d}r\\
&= M_t^{\tilde h}(v,\tilde h_t v) - \int_0^t (\mathbf{d} P_{T-s} f)(W_s^{\tilde h}(v, h_s v))\,\mathrm{d}s\\
&\qquad - 2\int_0^t \nabla \mathbf{d} P_{T-s} f(\tilde Q_s(h_s v), \tilde Q_s(\tilde h_s v))\,\mathrm{d}s
\end{aligned} \tag{3.18}$$

is a local martingale. Moreover, since $NP_{T-t}f(X_t)\mathbf{1}_{\{X_t\in\partial M\}} = 0$ and by the Itô formula, we have

$$P_{T-t} f(X_t) = P_T f(x) + \int_0^t \mathbf{d} P_{T-s} f(/\!/_s\,\mathrm{d}B_s). \tag{3.19}$$

The usual integration by parts yields

$$\int_0^t (\mathbf{d} P_{T-s} f)(W_s^{\tilde h}(v, h_s v))\,\mathrm{d}s - P_{T-t} f(X_t)\int_0^t \langle W_s^{\tilde h}(v, h_s v), /\!/_s\,\mathrm{d}B_s\rangle \tag{3.20}$$

is a local martingale.

On the other hand, from the Itô formula and the commutation rule (3.13), we obtain

$$\begin{aligned}
&\mathrm{d}(\mathbf{d} P_{T-t} f(\tilde Q_t(v)))\\
&= \nabla \mathbf{d} P_{T-t} f(/\!/_t\,\mathrm{d}B_t,\, \tilde Q_t(v)) - \frac{1}{2}\mathbf{d}(\Delta P_{T-t} f)(\tilde Q_t(v))\,\mathrm{d}t\\
&\quad + \frac{1}{2}(\mathrm{tr}\,\nabla^2 \mathbf{d} P_{T-t} f)(\tilde Q_t(v))\,\mathrm{d}t + \frac{1}{2}\nabla_N(\mathbf{d} P_{T-t} f)(\tilde Q_t(v))\,\mathrm{d}l_t\\
&\quad - \frac{1}{2}\mathbf{d} P_{T-t} f(\mathrm{Ric}^\sharp(\tilde Q_t(v)))\,\mathrm{d}t - \frac{1}{2}\mathbf{d} P_{T-t} f((\nabla N)^\sharp(\tilde Q_t(v)))\,\mathrm{d}l_t\\
&= \nabla \mathbf{d} P_{T-t} f(/\!/_t\,\mathrm{d}B_t,\, \tilde Q_t(v)) + \frac{1}{2}\nabla_N(\mathbf{d} P_{T-t} f)(\tilde Q_t(v))\,\mathrm{d}l_t\\
&\quad - \frac{1}{2}\mathbf{d} P_{T-t} f((\nabla N)^\sharp(\tilde Q_t(v)))\,\mathrm{d}l_t\\
&= \nabla \mathbf{d} P_{T-t} f(/\!/_t\,\mathrm{d}B_t,\, \tilde Q_t(v)) + \frac{1}{2}\mathbf{d}(N(P_{T-t} f))(\tilde Q_t(v))\,\mathrm{d}l_t\\
&= \nabla \mathbf{d} P_{T-t} f(/\!/_t\,\mathrm{d}B_t,\, \tilde Q_t(v)).
\end{aligned}$$

It thus follows that

$$\begin{aligned}\mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v)) = \mathbf{d}P_T f(v) + \int_0^t (\nabla \mathbf{d}P_{T-s}f)(/\!/_s \,\mathrm{d}B_s, \tilde{Q}_s(\tilde{h}_s v)) \\ + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v))\,\mathrm{d}s.\end{aligned}$$

Integration by parts yields that

$$\begin{aligned}&\int_0^t (\nabla \mathbf{d}P_{T-s}f)(\tilde{Q}_s(h_s v), \tilde{Q}_s(\tilde{h}_s v))\,\mathrm{d}s \\ &\quad - \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v)) \int_0^t \langle \tilde{Q}_s(h_s v), /\!/_s \,\mathrm{d}B_s\rangle \\ &\quad + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v))\,\mathrm{d}s \int_0^t \langle \tilde{Q}_s(h_s v)/\!/_s \,\mathrm{d}B_s\rangle \end{aligned} \tag{3.21}$$

is also a local martingale. Concerning the last term in (3.21), we note that

$$\begin{aligned}&\int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v))\,\mathrm{d}s \int_0^t \langle \tilde{Q}_s(h_s v), /\!/_s \,\mathrm{d}B_s\rangle \\ &\quad - \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \left(\int_0^s \langle \tilde{Q}_r(h_r v), /\!/_r \,\mathrm{d}B_r\rangle\right) \mathrm{d}s\end{aligned}$$

is a local martingale. Combining this with (3.21) we conclude that

$$\begin{aligned}&\int_0^t (\nabla \mathbf{d}P_{T-s}f)(\tilde{Q}_s(h_s v), \tilde{Q}_s(\tilde{h}_s v))\,\mathrm{d}s \\ &\quad - \mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v)) \int_0^t \langle \tilde{Q}_s(h_s v), /\!/_s \,\mathrm{d}B_s\rangle \\ &\quad + \int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \int_0^s \langle \tilde{Q}_r(h_r v), /\!/_r \,\mathrm{d}B_r\rangle\,\mathrm{d}s \end{aligned} \tag{3.22}$$

is a local martingale. Using the local martingales (3.20) and (3.22) to replace the last two terms in (3.18), we conclude that

$$\begin{aligned}&(\nabla \mathbf{d}P_{T-t}f)(\tilde{Q}_t(\tilde{h}_t v), \tilde{Q}_t(\tilde{h}_t v)) + (\mathbf{d}P_{T-t}f)(W_t^{\tilde{h}}(v, \tilde{h}_t v)) \\ &\quad - P_{T-t}f(X_t) \int_0^t \langle W_s^{\tilde{h}}(v, h_s v), /\!/_s \,\mathrm{d}B_s\rangle \\ &\quad - 2\mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v)) \int_0^t \langle \tilde{Q}_s(h_s v), /\!/_s \,\mathrm{d}B_s\rangle \\ &\quad + 2\int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \int_0^s \langle \tilde{Q}_r(h_r v), /\!/_r \,\mathrm{d}B_r\rangle\,\mathrm{d}s \end{aligned} \tag{3.23}$$

is a local martingale as well. On the other hand, by the product rule for martingales, we have

$$\left(\int_0^t \langle \tilde{Q}_s(h_s v), /\!/_s \,\mathrm{d}B_s\rangle\right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2\,\mathrm{d}s$$

$$= 2\int_0^t \left(\int_0^s \langle \tilde{Q}_r(h_r v), //_r \, \mathrm{d}B_r\rangle\right) \langle \tilde{Q}_s(h_s v), //_s \, \mathrm{d}B_s\rangle \tag{3.24}$$

which along with (3.19) implies that

$$P_{T-t}f(X_t)\left(\left(\int_0^t \langle \tilde{Q}_s(h_s v), //_s \, \mathrm{d}B_s\rangle\right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2 \, \mathrm{d}s\right)$$
$$- 2\int_0^t \mathbf{d}P_{T-s}f(\tilde{Q}_s(h_s v)) \int_0^s \langle \tilde{Q}_r(h_r v), //_r \, \mathrm{d}B_r\rangle \, \mathrm{d}s$$

is a local martingale. Applying this observation to (3.23), we finally see that

$$\begin{aligned}
&(\nabla \mathbf{d}P_{T-t}f)\big(\tilde{Q}_t(\tilde{h}_t v), \tilde{Q}_t(\tilde{h}_t v)\big) + (\mathbf{d}P_{T-t}f)(W_t^{\tilde{h}}(v, \tilde{h}_t v))\\
&- 2\mathbf{d}P_{T-t}f(\tilde{Q}_t(\tilde{h}_t v)) \int_0^t \langle \tilde{Q}_s(h_s v), //_s \, \mathrm{d}B_s\rangle\\
&- P_{T-t}f(X_t) \int_0^t \langle W_s^{\tilde{h}}(v, h_s v), //_s \, \mathrm{d}B_s\rangle\\
&+ P_{T-t}f(X_t)\left(\left(\int_0^t \langle \tilde{Q}_s(h_s v), //_s \, \mathrm{d}B_s\rangle\right)^2 - \int_0^t |\tilde{Q}_s(h_s v)|^2 \, \mathrm{d}s\right)
\end{aligned}$$

is a local martingale. This completes the proof. □

With the help of Lemma 3.3 and 3.4, we are now in position to prove Theorem 3.1.

Proof of Theorem 3.1. Let $h_s^\varepsilon = 0$ for $s \geq (T-\varepsilon) \wedge \tau_k$. Let $B_k := \{x : \rho_o(x) \leq k\}$ for $k \geq 1$. By the strong Markov property, the boundedness of $P_\cdot f$ on $[\varepsilon, T] \times B_k$ and the boundedness of $|\mathbf{d}P_\cdot f|$ and $|\mathrm{Hess}_{P_\cdot} f|$ on $[\varepsilon, T] \times B_k$ for $f \in \mathcal{B}_b(M)$, it follows from Lemma 3.4 that

$$\begin{aligned}
(\nabla \mathbf{d}P_T f)(v,v) &= -\mathbb{E}\left[f(X_T^x) \int_0^{(T-\varepsilon)\wedge\tau_k} \langle W_s^{\tilde{h}^\varepsilon}(h_s^\varepsilon v, v), //_s \mathrm{d}B_s\rangle\right]\\
&+ \mathbb{E}\left[f(X_T^x)\left(\left(\int_0^{(T-\varepsilon)\wedge\tau_k} \langle \tilde{Q}_s(h_s^\varepsilon v), //_s \mathrm{d}B_s\rangle\right)^2 - \int_0^{(T-\varepsilon)\wedge\tau_k} |\tilde{Q}_s(h_s^\varepsilon v)|^2 \, \mathrm{d}s\right)\right].
\end{aligned}$$

Letting $\varepsilon \downarrow 0$, we have

$$\begin{aligned}
&(\nabla \mathbf{d}P_T f)(v,v)\\
&= -\mathbb{E}\left[f(X_T^x) \int_0^{T\wedge\tau_k} \langle W_s^{\tilde{h}_s}(h_s v, v), //_s \mathrm{d}B_s\rangle\right]\\
&\quad + \mathbb{E}\left[f(X_T^x)\left(\left(\int_0^{T\wedge\tau_k} \langle \tilde{Q}_s(h_s v), //_s \mathrm{d}B_s\rangle\right)^2 - \int_0^{T\wedge\tau_k} |\tilde{Q}_s(h_s v)|^2 \, \mathrm{d}s\right)\right].
\end{aligned}$$

By Lemma 3.3 and the observation that there exists a constant $c > 0$ such that

$$\mathbb{E}\left[\sup_{t\in[0,T]}\left|\left(\left(\int_0^{t\wedge\tau_k}\langle\tilde{Q}_s(h_sv), //_s\mathrm{d}B_s\rangle\right)^2 - \int_0^{t\wedge\tau_k}|\tilde{Q}_s(h_sv)|^2\,\mathrm{d}s\right)\right|\right]$$
$$\leq c\,\mathbb{E}\left[\int_0^T \mathrm{e}^{\int_0^s K^-(X_s)\,\mathrm{d}s+\int_0^s\sigma^-(X_s)\,\mathrm{d}l_s}\,h_s^2\,\mathrm{d}s\right],$$

we complete the proof by Fatou's lemma. □

3.2. **Global Bismut type Hessian estimates of Neumann semigroup.**

In this subsection, we continue the discussion on explicit global estimates for Hess_{P_tf} under suitable conditions.

For $\varepsilon > 0$ and $\gamma \geq 0$, let

$$\mathcal{D}_{\gamma\varepsilon} := \{\phi \in C_b^2(M) : \inf\phi = 1,\ N\log\phi \geq \sigma^- + \gamma\varepsilon\},$$

and consider the following condition:

(C) The functions K, σ in (3.1) and α, β, γ in (3.2) are constant, and there exists $\phi \in \mathcal{D}_{\gamma\varepsilon}$ for some $\varepsilon > 0$ such that

$$K_{\phi,q} = \sup_{x\in M}\left\{-L\log\phi + 2q|\nabla\log\phi|^2\right\} < \infty$$

for some positive constant $q > 1$.

By [27, Section 3.2], such ϕ can be constructed if ∂M has strictly positive injectivity radius, the sectional curvature of M being bounded above and Z bounded. In particular, if the manifold is compact, this condition are met automatically. Under the global bounds of condition **(C)**, it has been explained above that $|\nabla P_\cdot f|$ is bounded on $[0,T]\times M$ for $f \in C_b^1(M)$. Next local Bismut formulae, as the one in Theorem 3.1 for Hess_{P_tf}, permit us to show that for any $\varepsilon > 0$,

$$|\mathrm{Hess}_{P_\cdot f}| \text{ is bounded on } [\varepsilon, T]\times M. \tag{3.25}$$

This requires for $x \in M$ and a given relatively compact open neighborhood D of x, the construction of an adapted real process h_t such that $h_t = 0$ for $t \geq T\wedge\tau_D$ and $\int_0^{T\wedge\tau_D} h_t\,\mathrm{d}t = -1$ with the property that

$$\sup_{x\in M}\mathbb{E}^x\left[\int_0^T h_t^{2p}\,\mathrm{d}t\right] < \infty, \text{ and } \sup_{x\in M}\mathbb{E}^x[\mathrm{e}^{q(\sigma^-+\varepsilon)l_t}] < \infty$$

for $1/p + 1/q = 1$ and $p, q > 1$, where $\tau_D := \inf\{t \geq 0\colon X_t^x \notin D\}$ denotes the first exit time of D, see estimate (3.5). In Appendix below we briefly sketch the construction of processes h satisfying the required properties. To this end, we also introduce the conformal change of the metric such that the boundary under the new metric is convex in Remark 5.1 below as well.

Theorem 3.5. *Assume that condition* **(C)** *holds. Let h be a non-positive and adapted process satisfying $\int_0^T h_s\,\mathrm{d}s = -1$ and*

$$\mathbb{E}^x\left[\int_0^T (h_s^2+\tilde{h}_s^2)\,\mathrm{e}^{\sigma^- l_s}\,\mathrm{d}s + \int_0^T \tilde{h}_s^2\,\mathrm{e}^{\sigma^- l_s}\,\mathrm{d}l_s\right] < \infty,$$

where $\tilde{h}_t = 1+\int_0^t h_s\,\mathrm{d}s$. Then for $f\in\mathcal{B}_b(M)$ and $v\in T_xM$,

$$\begin{aligned}&\mathrm{Hess}_{P_Tf}(v,v)(x)\\&= -\mathbb{E}^x\left[f(X_T)\int_0^T \langle W_s^{\tilde{h}}(v,h_sv), //_s\mathrm{d}B_s\rangle\right]\\&\quad + \mathbb{E}^x\left[f(X_T)\left(\left(\int_0^T \langle \tilde{Q}_s(h_sv), //_s\mathrm{d}B_s\rangle\right)^2 - \int_0^T |\tilde{Q}_s(h_sv)|^2\,\mathrm{d}s\right)\right].\end{aligned}$$

Moreover for $T>0$ and $f\in\mathcal{B}_b(M)$,

$$\begin{aligned}|\mathrm{Hess}_{P_Tf}|(x) &\le \left(\alpha+\frac{\beta}{2}\sqrt{T}+\frac{2}{T}\right)\mathrm{e}^{K^-T}\,\mathbb{E}^x[\mathrm{e}^{\sigma l_T}](P_Tf^2)^{1/2}(x)\\&\quad + \frac{\gamma}{2\sqrt{T}}\,\mathrm{e}^{K^-T}\,\mathbb{E}^x\left[\mathrm{e}^{\sigma l_T}\right]^{1/2}\left[\mathbb{E}^x\left(\int_0^T \mathrm{e}^{\frac{1}{2}\sigma l_s}\,\mathrm{d}l_s\right)^2\right]^{1/2}(P_Tf^2)^{1/2}(x).\end{aligned}$$

Proof. For the adapted process h, we see from Lemma 3.3 that

$$\begin{aligned}&\mathbb{E}^x\left[\sup_{t\in[0,T]}\left|\int_0^t h_s\langle W_s^{\tilde{h}}(v,v),\, //_s\mathrm{d}B_s\rangle\right|\right]\\&\le 3\,\mathrm{e}^{K^-T}\left(\mathbb{E}^x\int_0^T \mathrm{e}^{\sigma^- l_s}\,h_s^2\,\mathrm{d}s\right)^{1/2}\\&\quad\times\left\{\left[\alpha(3+\sqrt{10})+\frac{\beta}{2}\right]\left(\mathbb{E}^x\int_0^T \mathrm{e}^{\sigma^-\,l_s}\,\tilde{h}_s^2\,\mathrm{d}s\right)^{1/2} + \frac{\gamma}{2}\left(\mathbb{E}^x\int_0^T \mathrm{e}^{\sigma^-\,l_s}\,\tilde{h}_s^2\,\mathrm{d}l_s\right)^{1/2}\right\}\\&< \infty,\end{aligned}$$

and

$$\begin{aligned}&\mathbb{E}^x\left[\left|\left(\int_0^T \langle \tilde{Q}_s(h_sv), //_s\mathrm{d}B_s\rangle\right)^2 - \int_0^T |\tilde{Q}_s(h_sv)|^2\,\mathrm{d}s\right|\right]\\&\le 2\,\mathrm{e}^{K^-T}\,\mathbb{E}^x\left(\int_0^T \mathrm{e}^{\sigma^-\,l_s}\,\tilde{h}_s^2\,\mathrm{d}s\right) < \infty.\end{aligned}$$

Moreover, by (3.25) both $|\nabla P_\cdot f|$ and $|\mathrm{Hess}_{P_\cdot f}|$ are bounded on $[\varepsilon,T]\times M$. We complete the proof by following the steps as in the proof of Theorem 3.1 to obtain from (3.10),

$$\mathrm{Hess}_{P_Tf}(v,v)(x) = -\mathbb{E}^x\left[f(X_T)\int_0^T \langle W_s^{\tilde{h}}(v,h_sv), //_s\mathrm{d}B_s\rangle\right]$$

$$+\,\mathbb{E}^x\left[f(X_T)\left(\left(\int_0^T\langle\tilde Q_s(h_sv),//_s\mathrm{d}B_s\rangle\right)^2-\int_0^T|\tilde Q_s(h_sv)|^2\,\mathrm{d}s\right)\right].\tag{3.26}$$

Indeed, using the mentioned boundedness on $[\varepsilon,T]\times M$, we get (3.26) first for f replaced by $P_\varepsilon f$ and from this (3.26) is obtained by letting ε tend to zero. In particular, letting $h_s=-\frac{1}{T}$ when $s\in[0,T]$ and $\tilde h(s)=\frac{T-s}{T}$ for $s\in[0,T]$, then

$$\begin{aligned}
&|\mathrm{Hess}_{P_Tf}|(x)\\
&\le (P_T|f|^2)^{1/2}\left[\mathbb{E}^x\left(\int_0^T\langle W_s^{\tilde h}(v,h_sv),//_s\mathrm{d}B_s\rangle\right)^2\right]^{1/2}\\
&\qquad+2(P_T|f|^2)^{1/2}\int_0^T\mathbb{E}^x[\mathrm{e}^{\sigma l_s-Ks}]h^2(s)\,\mathrm{d}s\\
&\le\frac{1}{T}(P_T|f|^2)^{1/2}\left[\left(\mathbb{E}^x\left[\int_0^T\left|\tilde Q_s\int_0^s\tilde Q_r^{-1}R(//_r\mathrm{d}B_r,\tilde Q_r(\tilde h(r)v))\tilde Q_r(v)\right|^2\mathrm{d}s\right]\right)^{1/2}\right.\\
&+\frac12\left(\mathbb{E}^x\left[\int_0^T\left|\tilde Q_s\int_0^s\tilde Q_r^{-1}(\mathbf{d}^*R-R(Z)+\nabla\mathrm{Ric}_Z)^\sharp(\tilde Q_r(\tilde h(r)v),\tilde Q_r(v))\,\mathrm{d}r\right|^2\mathrm{d}s\right]\right)^{1/2}\\
&\left.+\frac12\left(\mathbb{E}^x\left[\int_0^T\left|\tilde Q_s\int_0^s\tilde Q_r^{-1}(\nabla^2N-R(N))^\sharp(\tilde Q_r(\tilde h(r)v),\tilde Q_r(v))\,\mathrm{d}l_r\right|^2\mathrm{d}s\right]\right)^{1/2}\right]\\
&+\frac{2}{T^2}(P_T|f|^2)^{1/2}(x)\,\mathrm{e}^{K^-T}\int_0^T\mathbb{E}^x[\mathrm{e}^{\sigma l_s}]\,\mathrm{d}s\\
&\le\left(\alpha+\frac{\beta}{2}\sqrt{T}+\frac{2}{T}\right)\mathrm{e}^{K^-T}\,\mathbb{E}^x[\mathrm{e}^{\sigma l_T}](P_T|f|^2)^{1/2}\\
&\qquad+\frac{\gamma}{2\sqrt{T}}\,\mathrm{e}^{K^-T}\,\mathbb{E}^x\left[\mathrm{e}^{\sigma l_T}\right]^{1/2}\left[\mathbb{E}^x\left(\int_0^T\mathrm{e}^{\frac12\sigma l_s}\,\mathrm{d}l_s\right)^2\right]^{1/2}(P_T|f|^2)^{1/2}.\qquad\square
\end{aligned}$$

The following is a direct consequence of the estimate in Theorem 3.5 by letting $\phi\equiv1$ in the condition (**C**).

Corollary 3.6. *Assume that condition* (**C**) *holds with* $\sigma=\gamma=0$. *Then*

$$|\mathrm{Hess}_{P_Tf}|\le\left(\alpha+\frac{\sqrt{T}}{2}\beta+\frac{2}{T}\right)\mathrm{e}^{K^-T}(P_T|f|^2)^{1/2}$$

for $T>0$ *and* $f\in\mathcal{B}_b(M)$.

3.3. Hessian formula with gradient terms for Neumann semigroup.

The main theorem in this section relies on the fact that under (**B**), along with suitable conditions, the local martingale M_t defined in (3.11) is a true martingale. This fact will be exploited for further applications.

Theorem 3.7. *Assume that condition* **(C)** *holds. For $T>0$ let $h\in C([0,T])$ such that $\int_0^T h_t\,\mathrm{d}t=-1$. Then for $v\in T_xM$ and $f\in C_b^1(M)$,*

(3.27)
$$\mathrm{Hess}_{P_Tf}(v,v)=\mathbb{E}\left[-\mathbf{d}f(\tilde Q_T(v))\int_0^T\langle\tilde Q_s(h_sv),//_s\mathrm{d}B_s\rangle+\mathbf{d}f(W_T^{\tilde h}(v,v))\right]$$

where $\tilde h_t=1+\int_0^t h_s\,\mathrm{d}s$. Moreover, for $T>0$,

$$|\mathrm{Hess}_{P_Tf}|\le\left(\alpha\sqrt{T}+\frac{\beta}{2}T+\frac{1}{\sqrt{T}}\right)\mathbb{E}\left[\mathrm{e}^{\sigma^-l_T}\right]\mathrm{e}^{K^-T}\,\|\nabla f\|_\infty$$
$$+\frac{\gamma}{2}\mathbb{E}\left[\mathrm{e}^{\frac12\sigma^-l_T}\int_0^T\mathrm{e}^{\frac12\sigma^-l_s}\;\mathrm{d}l_s\right]\mathrm{e}^{K^-T}\,\|\nabla f\|_\infty.$$

Proof. Recall that by (3.16)

$$\nabla\mathbf{d}P_{T-t}f(\tilde Q_t(\tilde h_tv),\tilde Q_t(v))+(\mathbf{d}P_{T-t}f)(W_t^{\tilde h}(v,v))$$
$$-\int_0^t(\nabla\mathbf{d}P_{T-s}f)(\tilde Q_s(h_sv),\tilde Q_s(v))\,\mathrm{d}s$$

is a local martingale. On the other hand, we know from the proof of Lemma 3.4 that

$$\int_0^t(\nabla\mathbf{d}P_{T-s}f)(\tilde Q_s(h_sv),\tilde Q_s(v))\,\mathrm{d}s-\mathbf{d}P_{T-t}f(\tilde Q_t(v))\int_0^t\langle\tilde Q_s(h_sv),//_s\mathrm{d}B_s\rangle$$

is a local martingale as well. We conclude that

$$\nabla\mathbf{d}P_{T-t}f(\tilde Q_t(\tilde h_tv),\tilde Q_t(v))+(\mathbf{d}P_{T-t}f)(W_t^{\tilde h}(v,v))$$
$$-\mathbf{d}P_{T-t}f(\tilde Q_t(v))\int_0^t\langle\tilde Q_s(h_sv),//_s\mathrm{d}B_s\rangle$$

is a local martingale. As $\|R\|_\infty<\infty$, $\mathrm{Ric}\ge K$ for some constant K, and $\mathrm{II}\ge\sigma$ for some non-positive constant σ,

$$\left\|\mathbf{d}^*R+\nabla\mathrm{Ric}_Z^\sharp-R(Z)\right\|_\infty<\infty\quad\text{and}\quad\left\|\nabla^2N+R(N)\right\|_\infty<\infty,$$

we first get

$$\sup_{s\in[0,T]}\mathbb{E}|\tilde Q_s(v)|^2\le\sup_{s\in[0,T]}\mathrm{e}^{-Ks}\,\mathbb{E}[\mathrm{e}^{\sigma^-l_T}]<\infty,$$

and then

$$\mathbb{E}\left[|W_{t\wedge\tau_k}^{\tilde h}(v,v)|\right]\le\mathbb{E}\left[\mathrm{e}^{K^-t\wedge\tau_k+\sigma^-l_{t\wedge\tau_k}}\right]^{1/2}\mathbb{E}\left[\mathrm{e}^{-K^-t\wedge\tau_k-\sigma^-l_{t\wedge\tau_k}}\,|\xi_{t\wedge\tau_k}^{(1)}|^2\right]^{1/2}$$
$$+\frac12\mathbb{E}\left[|\xi_{t\wedge\tau_k}^{(2)}|\right]+\frac12\mathbb{E}\left[|\xi_{t\wedge\tau_k}^{(3)}|\right]$$
$$\le\alpha\mathbb{E}\left[\mathrm{e}^{K^-t+\sigma^-l_t}\right]^{1/2}\left[\int_0^t\mathbb{E}[\mathrm{e}^{-K^-s-\sigma^-l_s}]\tilde h_s^2\,\mathrm{d}s\right]^{1/2}$$
$$+\frac12\mathbb{E}\left[\mathrm{e}^{\frac{K^-}{2}t+\frac{\sigma^-}{2}l_t}\int_0^t\mathrm{e}^{\frac{K^-s}{2}+\frac{\sigma^-l_s}{2}}\,\tilde h_s\,(\beta\mathrm{d}s+\gamma\mathrm{d}l_s)\right],\tag{3.28}$$

where $\xi^{(1)}$, $\xi^{(2)}$ and $\xi^{(3)}$ are defined as above. Letting k tend to ∞ then yields

$$\mathbb{E}\left[|W_t^{\tilde h}(v,v)|\right] < \infty.$$

Recall that $|\nabla P_\cdot f|$ is bounded on $[0,T]\times M$ and $|\nabla \mathbf{d} P_\cdot f|$ is bounded on $[\varepsilon, T]\times M$ for $0<\varepsilon<T$ for $f\in C_b^1(M)$, see Remark 5.4. Hence we may again the claimed formulas show first for f replaced by $f_\varepsilon := P_\varepsilon f$ and then take the limit as $\varepsilon\downarrow 0$ in the final formulas. Hence we may assume that $|\nabla P_\cdot f|$ and $|\nabla \mathbf{d} P_\cdot f|$ are bounded on $[0,T]\times M$, so that (3.16) is a true martingale. By taking expectations and passing to the limit as $\varepsilon\downarrow 0$, inequality (3.27) is obtained.

Let now $\tilde h_s = (T-s)/T$ for $s\in[0,T]$. It is straightforward to deduce from (3.27) and (3.28) that

$$\begin{aligned}
|\mathrm{Hess}_{P_T f}| &\le \|\nabla f\|_\infty\, \mathrm{e}^{-KT/2}\,\mathbb{E}[\mathrm{e}^{\sigma l_T/2}]\mathbb{E}\left[\int_0^T |\tilde Q_s|^2 h_s^2\,\mathrm{d}s\right]^{1/2}\\
&\quad + \|\nabla f\|_\infty \mathbb{E}\left[|W_T^{\tilde h}(v,v)|\right]\\
&\le \|\nabla f\|_\infty\left(\alpha\sqrt{T}+\frac{\beta}{2}T+\frac{1}{\sqrt{T}}\right)\mathbb{E}\left[\mathrm{e}^{\sigma l_T}\right]\mathrm{e}^{K^-T}\\
&\quad + \frac{\gamma}{2}\|\nabla f\|_\infty \mathbb{E}\left(\mathrm{e}^{\frac12\sigma l_T}\int_0^T \mathrm{e}^{\frac12 \sigma l_s}\,\mathrm{d}l_s\right)\mathrm{e}^{K^-T}
\end{aligned}$$

which shows the second claim. □

For manifolds with specific boundary properties, more refined results can be derived.

Corollary 3.8. *Assume that the boundary ∂M is empty or $\mathrm{II}\ge 0$ and $\nabla^2 N + R(N) = 0$. Moreover, suppose that $\mathrm{Ric}_V \ge K > 0$, $\alpha := \|R\|_\infty < \infty$ and $\beta := \|\nabla \mathrm{Ric}_V^\sharp + \mathrm{d}^* R + R(\nabla V)\|_\infty < \infty$.*

(i) *If $\mathrm{Ric}_V\ge K$, $\mathrm{II}\ge 0$, then for $f\in C_b^1(M)$,*

$$|\mathrm{Hess}_{P_t f}| \le \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)\mathrm{e}^{-Kt/2}(P_t|\nabla f|^2)^{1/2}.$$

(ii) *If $\mathrm{Ric}_V = K$, $\mathrm{II}=0$, then for $f\in C_b^1(M)$,*

$$|\mathrm{Hess}_{P_t f}|_{\mathrm{HS}} \le \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}} + \frac{d\alpha}{\sqrt{K}} + \frac{d\beta}{K}\right)\mathrm{e}^{-Kt/2}(P_t|\nabla f|^2)^{1/2}.$$

Proof. If $\mathrm{II}\ge 0$, and $\mathrm{Ric}_Z\ge K$, then by [27, Corollary 3.2.6] we know that $|\nabla P_\cdot f|$ is bounded on $[0,t]\times M$. Moreover, $\nabla^2 N + R(N) = 0$, we choose $\tilde h$

such that $|\tilde{h}| \le 1$ and

$$\left(\mathbb{E}|W_t^{\tilde{h}}(v,v)|^2\right)^{1/2} \le \alpha\,\mathrm{e}^{-Kt/2}\left(\int_0^t \mathrm{e}^{-Ks}\,\mathrm{d}s\right)^{1/2} + \frac{\beta}{2}\,\mathrm{e}^{-Kt/2}\int_0^t \mathrm{e}^{-Ks/2}\,\mathrm{d}s$$
$$\le \frac{\alpha}{\sqrt{K}}\,\mathrm{e}^{-Kt/2} + \frac{\beta}{K}\,\mathrm{e}^{-Kt/2}.$$

Combining this with Theorem 3.7, we conclude that

$$|\mathrm{Hess}_{P_tf}| \le (P_t|\nabla f|^2)^{1/2}\,\mathrm{e}^{-Kt/2}\left(\int_0^t \mathrm{e}^{-Ks}\,h^2(s)\,\mathrm{d}s\right)^{1/2}$$
$$+ (P_t|\nabla f|^2)^{1/2}\left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)\mathrm{e}^{-Kt/2}.$$

The following choice of h:

$$h_s = -\frac{\mathrm{e}^{Ks}}{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}, \quad s \in [0,t], \tag{3.29}$$

then leads to the first inequality.

If $\mathrm{II} = 0$ and $\mathrm{Ric}_V = K$, then $\tilde{Q}_t = \mathrm{e}^{-Kt/2}\,/\!/_t$ and from the conditions, the local martingale in (3.11) is a true martingale, we then obtain

$$\mathrm{Hess}_{P_tf}(v,w) = \mathbb{E}\Bigg[\mathrm{e}^{-Kt}\,\mathrm{Hess}_f(/\!/_tv, /\!/_tw)$$
$$+ \mathrm{e}^{-Kt/2}\,\mathbf{d}f\left(/\!/_t\int_0^t /\!/_s^{-1}\,\mathrm{e}^{-Ks/2}\,R(/\!/_s\mathrm{d}B_s, /\!/_sv)(/\!/_sw)\right)$$
$$- \frac{1}{2}\,\mathrm{e}^{-Kt/2}\,\mathbf{d}f\left(/\!/_t\int_0^t \mathrm{e}^{-Ks/2}\,/\!/_s^{-1}(\mathbf{d}^*R - R(\nabla V) + \nabla\mathrm{Ric}_V)^\sharp(/\!/_sv, /\!/_sw)\,\mathrm{d}s\right)\Bigg].$$

This implies

$$|\mathrm{Hess}_{P_tf}|_{\mathrm{HS}} \le \mathrm{e}^{-Kt}\,P_t|\mathrm{Hess}_f|_{\mathrm{HS}} + \left(d\alpha\,\mathrm{e}^{-Kt/2}\left(\int_0^t \mathrm{e}^{-Ks}\,\mathrm{d}s\right)^{1/2}\right.$$
$$\left. + \frac{d\beta}{2}\,\mathrm{e}^{-Kt/2}\int_0^t \mathrm{e}^{-Ks/2}\,\mathrm{d}s\right)(P_t|\nabla f|^2)^{1/2}. \tag{3.30}$$

On the other hand, by Itô's formula and the condition $\mathrm{II} = 0$ we have

$$\mathrm{d}|\nabla P_{t-s}f|^2(X_s) = \frac{1}{2}\left(L|\nabla P_{t-s}f|^2(X_s) - \langle\nabla P_{t-s}f, \nabla LP_{t-s}f\rangle(X_s)\right)\mathrm{d}s$$
$$+ \langle\nabla|\nabla P_{t-s}f|^2(X_s), /\!/_s\mathrm{d}B_s\rangle, \quad s \in [0,t].$$

Using the Bochner-Weitzenböck formula and the assumption $\mathrm{Ric}_V = K$, we obtain

$$\mathrm{d}|\nabla P_{t-s}f|^2(X_s) \ge \left(\mathrm{Ric}_V(\nabla P_{t-s}f, \nabla P_{t-s}f) + |\mathrm{Hess}_{P_{t-s}f}|^2_{\mathrm{HS}}\right)(X_s)\,\mathrm{d}s$$
$$+ \langle\nabla|\nabla P_{t-s}f|^2(X_s), /\!/_s\mathrm{d}B_s\rangle$$

$$
\begin{aligned}
&= K|\nabla P_{t-s}f|^2(X_s)\,\mathrm{d}s + |\mathrm{Hess}_{P_{t-s}f}|_{\mathrm{HS}}^2(X_s)\,\mathrm{d}s\\
&\quad + \langle \nabla|\nabla P_{t-s}f|^2(X_s), //_s \mathrm{d}B_s\rangle.
\end{aligned}
$$

From this, we conclude that

$$
P_t|\nabla f|^2 - \mathrm{e}^{Kt}\,|\nabla P_t f|^2 \geq \int_0^t \mathrm{e}^{K(t-s)}\,P_s|\mathrm{Hess}_{P_{t-s}f}|_{\mathrm{HS}}^2\,\mathrm{d}s.
$$

By the inequality of Cauchy-Schwarz, this yields

$$
\begin{aligned}
&\mathrm{e}^{-Kt/2}(P_t|\nabla f|^2)^{1/2}\\
&\geq \left(\int_0^t \mathrm{e}^{-Ks}(P_s|\mathrm{Hess}_{P_{t-s}f}|_{\mathrm{HS}})^2\,\mathrm{d}s\right)^{1/2}\\
&\geq \left(\frac{K}{\mathrm{e}^{Kt}-1}\right)^{1/2}\int_0^t P_s|\mathrm{Hess}_{P_{t-s}f}|_{\mathrm{HS}}\,\mathrm{d}s.
\end{aligned}
$$

Using inequality (3.30) obtained before, we have

$$
\begin{aligned}
\mathrm{e}^{-Kt/2}(P_t|\nabla f|^2)^{1/2} &\geq \left(\int_0^t \mathrm{e}^{Ks}\,\mathrm{d}s\right)^{1/2}|\mathrm{Hess}_{P_tf}|_{\mathrm{HS}}\\
&\quad - \left(\frac{d\alpha\int_0^t \mathrm{e}^{\frac{1}{2}Ks}\left(\int_0^s \mathrm{e}^{-Kr}\,\mathrm{d}r\right)^{1/2}\mathrm{d}s}{\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}} + \frac{d\beta\int_0^t \mathrm{e}^{\frac{1}{2}Ks}\int_0^s \mathrm{e}^{-Kr/2}\,\mathrm{d}r\mathrm{d}s}{2\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}}\right)\\
&\qquad\qquad \times (P_t|\nabla f|^2)^{1/2},
\end{aligned}
$$

which implies

$$
\begin{aligned}
|\mathrm{Hess}_{P_tf}|_{\mathrm{HS}} &\leq (P_t|\nabla f|^2)^{1/2}\left[\frac{\mathrm{e}^{-Kt/2}}{\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}} + \frac{d\alpha\int_0^t \mathrm{e}^{\frac{1}{2}Ks}\left(\int_0^s \mathrm{e}^{-Kr}\,\mathrm{d}r\right)^{1/2}\mathrm{d}s}{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}\right.\\
&\qquad\left. + \frac{d\beta\int_0^t \mathrm{e}^{\frac{1}{2}Ks}\left(\int_0^s \mathrm{e}^{-Kr/2}\,\mathrm{d}r\right)\mathrm{d}s}{2\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}\right]\\
&\leq (P_t|\nabla f|^2)^{1/2}\,\mathrm{e}^{-Kt/2}\left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\,\mathrm{d}r}} + \frac{d\alpha}{\sqrt{K}} + \frac{d\beta}{K}\right). \qquad \square
\end{aligned}
$$

4. Stein method and log-Sobolev inequality

In this section, we consider $L = \Delta - \nabla V$ for $V \in C^2(M)$ such that

$$
\mu(\mathrm{d}x) = \mathrm{e}^{-V(x)}\,\mathrm{vol}(\mathrm{d}x)
$$

is a probability measure where $\mathrm{vol}(\mathrm{d}x)$ denotes the volume measure on M. Let $P_t = \mathrm{e}^{\frac{1}{2}Lt}$ be the contraction semigroup generated by L on $L^2(\mu)$ with Neumann boundary conditions. In [9], we used the Hessian formula to establish an HSI inequality on manifolds without boundary, which contains the new quantity called Stein discrepancy and in a certain sense improves the classical log-Sobolev inequality.

To establish such log-Sobolev inequalities on manifolds with boundary, we first adapt the definition of Stein kernel and Stein discrepancy to manifolds with boundary. A symmetric 2-tensor $\tau_\nu\colon M \to T^*M \times T^*M$ on M is said to be a Stein kernel for a probability measure ν on M if $\tau_\nu(v,w) \in L^1(\nu)$ for every $v, w \in T_xM$, $x \in M$, and

$$\int \langle \nabla V, \nabla f\rangle \, \mathrm{d}\nu = \int \langle \tau_\nu, \mathrm{Hess} f\rangle_{\mathrm{HS}} \, \mathrm{d}\nu, \quad f \in \mathcal{C}_N^\infty(L),$$

where ∇V is the first order part of the operator L and where

$$\mathcal{C}_N^\infty(L) = \big\{ f \in C^\infty(M) \colon Nf|_{\partial M} = 0,\ Lf \in \mathcal{B}_b(M)\big\}.$$

Since

$$\int Lf \, \mathrm{d}\mu = \int_{\partial M} N(f) \, \mathrm{d}\mu = 0$$

for $f \in \mathcal{C}_N^\infty(L)$, it is easy to see that the identity map id is a Stein kernel for μ.

Definition 4.1. Let τ_ν be a Stein kernel for ν. The Stein discrepancy is defined as

$$S(\nu \,|\, \mu)^2 = \inf \int_M |\tau_\nu - \mathrm{id}|^2_{\mathrm{HS}} \, \mathrm{d}\nu,$$

where the infimum is taken over all Stein kernels of ν, and takes the value $+\infty$ if no Stein kernel exists.

Let us first recall the classical log-Sobolev inequality on Riemannian manifolds when the boundary is convex. Assume that

$$\mathrm{Ric}_V := \mathrm{Ric} + \mathrm{Hess}_V \geq K, \quad \mathrm{II} \geq 0$$

holds for some positive constant K. Then the classical logarithmic Sobolev inequality with respect to the measure μ indicates that for every probability measure $\mathrm{d}\nu = h \, \mathrm{d}\mu$ with smooth density $h\colon M \to \mathbb{R}_+$,

$$H(\nu \,|\, \mu) \leq \frac{1}{2K} I(\nu \,|\, \mu),$$

where

$$H(\nu \,|\, \mu) = \int h \log h \, \mathrm{d}\mu = \mathrm{Ent}_\mu(h)$$

is the relative entropy of $\mathrm{d}\nu = h \, \mathrm{d}\mu$ with respect to μ and

$$I(\nu \,|\, \mu) = \int \frac{|\nabla h|^2}{h} \, \mathrm{d}\mu = I_\mu(h)$$

the Fisher information of ν (or h) with respect to μ. This result is known as the Bakry-Émery criterion due to [2] for the logarithmic Sobolev inequality. Let us recall the following observations.

Lemma 4.2. *Assume that*

$$\mathrm{Ric}_V \geq K \text{ and } \quad \mathrm{II} \geq 0$$

for some positive constant K, and let τ_ν be a Stein kernel for $\mathrm{d}\nu = h\,\mathrm{d}\mu$ where $h \in C_0^\infty(M)$. For $t > 0$ let $\mathrm{d}\nu^t = P_t h\,\mathrm{d}\mu$. Then

(i) *(Integrated de Bruijn's formula)*

$$H(\nu\,|\,\mu) = \mathrm{Ent}_\mu(h) = \frac{1}{2}\int_0^\infty I_\mu(P_t h)\,\mathrm{d}t;$$

(ii) *(Exponential decay of Fisher information)*

$$I_\mu(P_t h) = I(\nu^t\,|\,\mu) \leq \mathrm{e}^{-Kt}\, I(\nu\,|\,\mu) = \mathrm{e}^{-Kt}\, I_\mu(h), \quad t \geq 0.$$

Proof. Since $N(P_t f \log P_t f) = 0$ and $\left(\frac{1}{2}L - \frac{\partial}{\partial t}\right)(P_t h \log P_t h) = \frac{|\nabla P_t h|^2}{2P_t h}$, we have

$$\begin{aligned} H(\nu\,|\,\mu) &= \int_M h\log h\,\mathrm{d}\mu = -\int_M\int_0^\infty \frac{\mathrm{d}\,(P_t h\log P_t h)}{\mathrm{d}t}\,\mathrm{d}t\,\mathrm{d}\mu \\ &= \int_0^\infty \left(\int_M \left(\frac{1}{2}L - \frac{\partial}{\partial t}\right)(P_t h\log P_t h)\,\mathrm{d}\mu\right)\mathrm{d}t \\ &= \frac{1}{2}\int_0^\infty\int_M \frac{|\nabla P_t h|^2}{P_t h}\,\mathrm{d}\mu\,\mathrm{d}t. \end{aligned}$$

The second assertion can be checked by observing first from the derivative formula that

$$|\nabla P_t h|^2 \leq \mathrm{e}^{-Kt}\left(P_t\big|\nabla(\sqrt{h}\,)^2\big|\right)^2 \leq 4\,\mathrm{e}^{-Kt}(P_t h)\,P_t\big|\nabla\sqrt{h}\big|^2$$

which implies

$$\begin{aligned} I_\mu(P_t h) &= \int_M \frac{|\nabla P_t h|^2}{P_t h}\,\mathrm{d}\mu \leq 4\int_M \mathrm{e}^{-Kt}\,\frac{(P_t h)P_t|\nabla\sqrt{h}|^2}{P_t h}\,\mathrm{d}\mu \\ &= 4\int_M \mathrm{e}^{-Kt}\,P_t|\nabla\sqrt{h}|^2\,\mathrm{d}\mu = 4\,\mathrm{e}^{-Kt}\int_M |\nabla\sqrt{h}|^2\,\mathrm{d}\mu \\ &= \mathrm{e}^{-Kt}\,I(\nu\,|\,\mu) = \mathrm{e}^{-Kt}\,I_\mu(h). \end{aligned}$$

□

All expressions should be considered for $h + \varepsilon$ as $\varepsilon \downarrow 0$. We continue our discussion under the condition that $\nabla^2 N + R(N) = 0$ and $-\nabla N \geq 0$. The following assertions describe the relationship between the relative entropy and Stein discrepancy.

Lemma 4.3. *Assume that $\alpha := \|R\|_\infty < \infty$, $\beta := \|\nabla \mathrm{Ric}_V^\sharp + \mathrm{d}^*R + R(\nabla V)\|_\infty < \infty$ and*

$$\nabla^2 N + R(N) = 0.$$

Let $\mathrm{d}\nu = h\,\mathrm{d}\mu$ for $h \in C_0^\infty(M)$.

(i) *If* $\mathrm{Ric}_V \geq K,\ \mathrm{II} \geq 0,$ *then*

$$I_\mu(P_t h) \leq d^2 \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\, \mathrm{d}r}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 \mathrm{e}^{-Kt}\, S^2(\nu \,|\, \mu).$$

(ii) *If* $\mathrm{Ric}_V = K,\ \mathrm{II} = 0,$ *then*

$$I_\mu(P_t h) \leq \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\, \mathrm{d}r}} + \frac{d\alpha}{\sqrt{K}} + \frac{d\beta}{K} \right)^2 \mathrm{e}^{-Kt}\, S^2(\nu \,|\, \mu).$$

Proof. Let $g_t = \log P_t h$. By the symmetry of $(P_t)_{t\geq 0}$ in $L^2(\mu)$,

$$I_\mu(P_t h) = -\int (Lg_t) P_t h \,\mathrm{d}\mu = -\int (LP_t g_t) h \,\mathrm{d}\mu = -\int LP_t g_t \,\mathrm{d}\nu.$$

Hence according to the definition of Stein kernel and since $P_t g_t \in \mathcal{C}_N^\infty(L)$, we have

$$\begin{aligned} I_\mu(P_t h) &= -\int \langle \mathrm{id}, \mathrm{Hess}_{P_t g_t} \rangle_{\mathrm{HS}} \,\mathrm{d}\nu - \int \langle \nabla V, \nabla P_t g_t \rangle \,\mathrm{d}\nu \\ &= \int \langle \tau_\nu - \mathrm{id}, \mathrm{Hess}_{P_t g_t} \rangle_{\mathrm{HS}} \,\mathrm{d}\nu. \end{aligned}$$

This argument is due to [14] and connects the Fisher information to the Stein discrepancy. We first prove assertion (i). By the Cauchy-Schwarz inequality,

$$\begin{aligned} I_\mu(P_t h) &= \int \langle \tau_\nu - \mathrm{id}, \mathrm{Hess}_{P_t g_t} \rangle_{\mathrm{HS}} \,\mathrm{d}\nu \\ &\leq \left(\int |\tau_\nu - \mathrm{id}|_{\mathrm{HS}}^2 \,\mathrm{d}\nu \right)^{1/2} \left(\int |\mathrm{Hess}_{P_t g_t}|_{\mathrm{HS}}^2 \,\mathrm{d}\nu \right)^{1/2} \\ &\leq d \left(\int |\tau_\nu - \mathrm{id}|_{\mathrm{HS}}^2 \,\mathrm{d}\nu \right)^{1/2} \left(\int |\mathrm{Hess}_{P_t g_t}|^2 \,\mathrm{d}\nu \right)^{1/2} \\ &\leq d \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\, \mathrm{d}r}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right) \mathrm{e}^{-\frac{K}{2}t} \left(\int |\tau_\nu - \mathrm{id}|_{\mathrm{HS}}^2 \,\mathrm{d}\nu \right)^{\frac{1}{2}} \left(\int P_t |\nabla g_t|^2 \,\mathrm{d}\nu \right)^{\frac{1}{2}} \end{aligned}$$

where Corollary 3.8 is used for the function $g_t = \log P_t h$. Since

$$\begin{aligned} \int P_t |\nabla g_t|^2 \,\mathrm{d}\nu = \int P_t |\nabla g_t|^2 h \,\mathrm{d}\mu &= \int |\nabla g_t|^2 P_t h \,\mathrm{d}\mu \\ &= \int \frac{|\nabla P_t h|^2}{P_t h} \,\mathrm{d}\mu = I_\mu(P_t h), \end{aligned}$$

it then follows that

$$I_\mu(P_t h) \leq d^2 \left(\frac{1}{\sqrt{\int_0^t \mathrm{e}^{Kr}\, \mathrm{d}r}} + \frac{\alpha}{\sqrt{K}} + \frac{\beta}{K} \right)^2 \mathrm{e}^{-Kt} \int |\tau_\nu - \mathrm{id}|_{\mathrm{HS}}^2 \,\mathrm{d}\nu.$$

Taking the infimum over all Stein kernels of ν, we finish the proof of (i). Along the same steps, item (ii) can be proved by means of Corollary 3.8 as well. □

Using the lemmata above, we are now in position to establish the following result.

Theorem 4.4. *Assume that* $\alpha := \|R\|_\infty < \infty$, $\beta := \|\nabla \mathrm{Ric}_V^\sharp + \mathrm{d}^*R + R(\nabla V)\|_\infty < \infty$ *and*

$$\nabla^2 N + R(N) = 0.$$

Let $\mathrm{d}\nu = h\,\mathrm{d}\mu$ *with* $h \in C_0^\infty(M)$.

(i) *If* $\mathrm{Ric}_V \geq K$, $\mathrm{II} \geq 0$, *then*

$$H(\nu\,|\,\mu) \leq \frac{1}{2K}\Big(d^2(1+\varepsilon)\Big(\frac{\alpha}{\sqrt{K}}+\frac{\beta}{K}\Big)^2 S^2(\nu\,|\,\mu)\Big) \wedge I(\nu\,|\,\mu) - \frac{d^2(1+\varepsilon)}{2\varepsilon} S^2(\nu\,|\,\mu)$$
$$\times \ln\left(\frac{d^2(1+\frac{1}{\varepsilon})KS^2(\nu\,|\,\mu)}{\Big(I(\nu\,|\,\mu) - d^2(1+\varepsilon)\Big(\frac{\alpha}{\sqrt{K}}+\frac{\beta}{K}\Big)^2 S^2(\nu\,|\,\mu)\Big)^+ + d^2(1+\frac{1}{\varepsilon})KS^2(\nu\,|\,\mu)}\right)$$

for every $\varepsilon > 0$. *Moreover, if* $\alpha = 0$ *and* $\beta = 0$, *then*

$$H(\nu\,|\,\mu) \leq \frac{d^2}{2} S^2(\nu\,|\,\mu) \ln\left(1 + \frac{I}{d^2KS^2(\nu\,|\,\mu)}\right).$$

(ii) *If* $\mathrm{Ric}_V = K$, $\mathrm{II} = 0$, *then*

$$H(\nu\,|\,\mu) \leq \frac{1}{2K}\Big(d^2(1+\varepsilon)\left(\frac{\alpha}{\sqrt{K}}+\frac{\beta}{K}\right)^2 S^2(\nu\,|\,\mu)\Big) \wedge I(\nu\,|\,\mu)$$
$$- \frac{1}{2}\Big(1+\frac{1}{\varepsilon}\Big) S^2(\nu\,|\,\mu)$$
$$\times \ln\left(\frac{(1+\frac{1}{\varepsilon})KS^2(\nu\,|\,\mu)}{\Big(I(\nu\,|\,\mu) - d^2(1+\varepsilon)\Big(\frac{\alpha}{\sqrt{K}}+\frac{\beta}{K}\Big)^2 S^2(\nu\,|\,\mu)\Big) \vee 0 + (1+\frac{1}{\varepsilon})KS^2(\nu\,|\,\mu)}\right)$$

for every $\varepsilon > 0$. *Moreover, if* $\alpha = \beta = 0$, *then*

$$H(\nu\,|\,\mu) \leq \frac{1}{2} S^2(\nu\,|\,\mu) \ln\left(1 + \frac{I}{KS^2(\nu\,|\,\mu)}\right).$$

Proof. We only need to prove the first estimate. To this end, we write $I = I(\nu\,|\,\mu)$ and $S = S(\nu\,|\,\mu)$ for simplicity. By Theorem 4.3 and Lemma 4.2, we have that for every $\varepsilon > 0$,

$$\begin{aligned}
H(\nu\,|\,\mu) &= \frac{1}{2}\int_0^u I_\mu(P_t h)\,\mathrm{d}t + \frac{1}{2}\int_u^\infty I_\mu(P_t h)\,\mathrm{d}t \\
&\leq \frac{1}{2}\inf_{u>0}\left\{A\int_0^u \mathrm{e}^{-Kt}\,\mathrm{d}t + B\int_u^\infty \frac{K}{\mathrm{e}^{Kt}(\mathrm{e}^{Kt}-1)}\,\mathrm{d}t + C\int_u^\infty \mathrm{e}^{-Kt}\,\mathrm{d}t\right\} \\
&= \frac{1}{2}\inf_{u>0}\left\{\frac{A(1-\mathrm{e}^{-Ku}) + C\,\mathrm{e}^{-Ku}}{K} + B\int_0^{\mathrm{e}^{-\alpha u}} \frac{r}{1-r}\,\mathrm{d}r\right\}
\end{aligned}$$

where

$$A = I(\nu \,|\, \mu); \quad B = d^2 \left(1 + \frac{1}{\varepsilon}\right) S^2(\nu \,|\, \mu);$$

$$C = d^2(1+\varepsilon)\left(\frac{\alpha}{\sqrt{K}} + \frac{\beta}{K}\right)^2 S^2(\nu \,|\, \mu).$$

It is easy to see that if $A \leq C$, then inf is reached when u tends to ∞; if $A > C$, then inf is reached for $\mathrm{e}^{\alpha u} = \frac{A-C+BK}{A-C}$ so that

$$H(\nu \,|\, \mu) \leq \frac{C}{2K} + \frac{1}{2} B \ln\left(1 + \frac{A-C}{BK}\right).$$

We conclude that

$$H(\nu \,|\, \mu) \leq \frac{C \wedge A}{2K} + \frac{1}{2} B \ln\left(1 + \frac{(A-C) \vee 0}{BK}\right).$$

The rest of the proof is the same replacing B by

$$\left(1 + \frac{1}{\varepsilon}\right) S^2(\nu \,|\, \mu).$$

The details are omitted here. □

Let (M, g) be a connected complete Riemannian manifold M. Considering the specific case that $\mathrm{Hess}_V = K > 0$, then by Obata's Rigidity Theorem (see [20, Theorem 2] or [30, Theorem 3.4]), M is isometric to $\mathbb{R}^n$. The following corollary shows that the result is consistent with Ledoux-Nourdin-Peccati [14] for the Gaussian measure on the Euclidean space $\mathbb{R}^n$.

Corollary 4.5. *Let (M, g) be a connected complete Riemannian manifold with boundary. Assume that $\mathrm{Hess}_V = K > 0$, $\mathrm{II} = 0$, and $\nabla^2 N = 0$. Let $\mathrm{d}\nu = h\,\mathrm{d}\mu$ with $h \in C_0^\infty(M)$. Then,*

$$I(\nu \,|\, \mu) \leq \frac{1}{2} S^2(\nu \,|\, \mu) \log\left(1 + \frac{I(\nu \,|\, \mu)}{K S^2(\nu \,|\, \mu)}\right).$$

Proof. From the condition $\mathrm{Hess}_V = K > 0$, we know that the manifold M is isometric to $\mathbb{R}^n$, i.e. $\|R\|_\infty = 0$, $\nabla \mathrm{Ric}_Z = 0$ and $\mathbf{d}^* R = 0$. Then by Theorem 4.3 (ii),

$$I_\mu(P_t h) \leq \frac{K}{\mathrm{e}^{2Kt} - \mathrm{e}^{Kt}} S^2(\nu \,|\, \mu).$$

The assertion can be obtained by a same arguments as in the proof of Theorem 4.4. □

5. Appendix

In this section, we introduce the ways to construct a sequence of h_k such that when k tends to ∞, the limit of h_k is a deterministic function which belongs to $C^1([0, T])$. Before this, let us first introduce the way to make conformal change of the metric such that the boundary is convex under the new metric and estimate the local time as well(see [27]).

Remark 5.1 (Conformal change of the metric)**.** We start with a conformal change of the metric g. Since $\phi \in \mathcal{D}_\varepsilon$, we have $\mathrm{II} \geq \sigma \geq -(\sigma^- + \varepsilon) \geq -N \log \phi$ and the boundary ∂M is convex under the metric $g' := \phi^{-2} g$. Let Δ' and ∇' be the Laplacian and gradient operator associated to the metric g'. Then

$$L = \phi^{-2}(\Delta' + \phi^2(Z + (d-2)\nabla \log \phi)) = \phi^{-2}(\Delta' + Z')$$

where $Z' := \phi^2(Z + (d-2)\nabla \log \phi)$. Let $\rho'(x,y)$ be the geodesic distance from x to y with respect to the metric g' on M.

Furthermore, let

$$U_i = \phi^{-1}(\gamma(s)) P'_{\gamma(0),\gamma(s)} V_i, \quad J_i(s) = f(s) U_i, \quad 1 \leq i \leq d,$$

where $\{V_i\}_{i=1}^d$ is a g'-orthonormal basis of $T_x M$, $P'_{\gamma(0),\gamma(s)}$ denotes parallel displacement from x to y with respect to the metric g' and $f(s) = 1 \wedge \frac{s}{\rho(x,y)\wedge 1}$. Then $J_i(0) = 0$ and $J_i(\rho') = \phi^{-1}(y) P'_{x,y} V_i$, $1 \leq i \leq d$,

$$\begin{aligned}
&\phi^{-2}(\Delta' + Z')\rho'(x,\cdot)(y) \\
&\leq \sum_{i=1}^d \int_0^{\rho'} \Big\{(|\nabla'_{\dot\gamma} J_i|')^2 - \langle R'(\dot\gamma, J_i)J_i, \dot\gamma\rangle'\Big\}(s)\,\mathrm{d}s + \phi^{-2}(y) Z'\rho'(x,\cdot)(y) \\
&\leq \sum_{i=1}^d \int_0^{\rho'} \Big\{f'(s)^2 \phi^{-2}(\gamma(s)) + f(s)^2 (|\nabla'_{\dot\gamma} U_i|')^2 - f(s)^2 \langle R'(\dot\gamma, U_i)U_i, \dot\gamma\rangle'\Big\}(s)\,\mathrm{d}s \\
&\qquad + \phi^{-2}(y) Z'\rho'(x,\cdot)(y).
\end{aligned} \tag{5.1}$$

On the other hand,

$$\begin{aligned}
&\phi^{-2}(y) Z'\rho'(x,\cdot)(y) \\
&= \int_0^{\rho'} \frac{\mathrm{d}}{\mathrm{d}s}\left\{f(s)^2 \phi^{-2}(\gamma(s)) \langle Z'(\gamma(s)), \dot\gamma(s)\rangle'\right\}\,\mathrm{d}s \\
&= 2\int_0^{\rho'} f'(s) f(s) \phi^{-2}(\gamma(s)) \langle Z'(\gamma), \dot\gamma\rangle'(s) \\
&\quad + f(s)^2 \frac{\mathrm{d}}{\mathrm{d}s}\left\{\phi^{-2}(\gamma)\langle Z'(\gamma), \dot\gamma\rangle'\right\}(s)\,\mathrm{d}s \\
&= 2\int_0^{\rho'} f'(s) f(s) \phi^{-2}(\gamma(s)) \langle Z'(\gamma), \dot\gamma\rangle'(s)\,\mathrm{d}s \\
&\quad + \int_0^{\rho'} f(s)^2 \phi^{-2}(\gamma(s)) \langle (\nabla'_{\dot\gamma} Z')\circ\gamma, \dot\gamma\rangle'(s)\,\mathrm{d}s \\
&\quad - 2\int_0^{\rho'} f(s)^2 \phi^{-2}(\gamma(s)) \langle \nabla \log\phi(\gamma(s)), \dot\gamma(s)\rangle \langle Z'(\gamma(s)), \dot\gamma(s)\rangle'\,\mathrm{d}s.
\end{aligned} \tag{5.2}$$

Note that $|\dot\gamma| = \phi$.

We then conclude from (5.1) and (5.2) that

$$\begin{aligned}
&\phi^{-2}(y)(\Delta' + Z')\rho'(x,\cdot)(y)\\
&\le -\int_0^{\rho'} f(s)^2\phi^{-2}(\gamma(s))\Big\{(\mathrm{Ric}^Z)'(\dot\gamma(s),\dot\gamma(s)) + (d-4)\langle\nabla\log\phi,\dot\gamma(s)\rangle^2\\
&\qquad\qquad + 2\langle Z,\dot\gamma(s)\rangle\langle\nabla\log\phi,\dot\gamma(s)\rangle\Big\}\,\mathrm{d}s\\
&\quad + 2\int_0^{\rho'} f'(s)f(s)\phi^{-2}(\gamma(s))\langle Z'(\gamma),\dot\gamma\rangle'(s)\,\mathrm{d}s\\
&\quad + d\int_0^{\rho'} f'(s)^2\phi^{-2}(\gamma(s))\,\mathrm{d}s\\
&\le -(K-K_\phi)\rho'(x,y) + d\int_0^{\rho'(x,y)\wedge 1}\frac{1}{(\rho'(x,y)\wedge 1)^2}\phi^{-2}(\gamma(s))\,\mathrm{d}s\\
&\quad + \frac{2}{\rho'(x,y)\wedge 1}\int_0^{\rho'(x,y)\wedge 1}\phi^{-2}(\gamma(s))\\
&\qquad\qquad \times \Big|\langle Z(\gamma(s)),\dot\gamma(s)\rangle + (d-2)\langle\nabla\log\phi,\dot\gamma(s)\rangle\Big|\,\mathrm{d}s\\
&\le -(K-K_\phi)\rho'(x,y) + 2\sup_{z\in B'(x,1)}(|Z| + (d-2)|\nabla\phi|)(z) + \frac{d}{\rho'(x,y)\wedge 1}.
\end{aligned}$$

Remark 5.2 (Estimate of local time)**.** The next step is to check that for $\alpha > 0$,

$$\sup_{x\in M}\mathbb{E}^x\big[\,\mathrm{e}^{\alpha\sigma^- l_t}\,\big] < \|\phi\|_\infty^{2\alpha}\exp\Big(\alpha K_{\phi,\alpha}t\Big) < \infty, \tag{5.3}$$

$$\sup_{x\in M}\mathbb{E}^x\big[\,\mathrm{e}^{(\sigma^-+\varepsilon)l_t}\,\big] < \|\phi\|_\infty^{2}\exp\Big(K_{\phi}t\Big) < \infty, \tag{5.4}$$

for $\phi\in\mathcal{D}$, where

$$K_{\phi,\alpha} = \sup_M\left\{-L\log\phi + 2\alpha|\nabla\log\phi|^2\right\}$$

and $K_\phi := K_{\phi,1}$ for simplicity. By Itô's formula,

$$\begin{aligned}
\mathrm{d}\phi^{-2\alpha}(X_t) &= \langle\nabla\phi^{-2\alpha}(X_t), //_t\mathrm{d}B_t\rangle + \frac{1}{2}L\phi^{-2\alpha}(X_t)\,\mathrm{d}t + \frac{1}{2}N\phi^{-2\alpha}(X_t)\,\mathrm{d}l_t\\
&\le \langle\nabla\phi^{-2\alpha}(X_t), //_t\mathrm{d}B_t\rangle - \alpha\phi^{-2\alpha}(X_t)\left(-K_{\phi,\alpha}\,\mathrm{d}t + N\log\phi(X_t)\,\mathrm{d}l_t\right)\\
&\le \langle\nabla\phi^{-2\alpha}(X_t), //_t\mathrm{d}B_t\rangle - \alpha\phi^{-2\alpha}(X_t)\left(-K_{\phi,\alpha}\,\mathrm{d}t + \sigma^-\,\mathrm{d}l_t\right),
\end{aligned}$$

then

$$\phi^{-2\alpha}(X_t)\exp\left(-\alpha K_{\phi,\alpha}t + \alpha\sigma^-\,l_t\right)$$

is a local submartingale. Therefore, by Fatou's lemma and taking into account that $\phi\ge 1$, we get

$$\mathbb{E}\left[\phi^{-2\alpha}(X_t)\exp\left(-\alpha K_{\phi,\alpha}t + \alpha\sigma^-\,l_t\right)\right] \le 1,$$

which proves (5.3) and (5.4).

Remark 5.3 (Construction of ϕ)**.** We fist introduce the following condition from [26] and give the estimate of $\|\phi\|_\infty$ and $K_{\phi,\alpha}$. Using Condition **(B)**, F.-Y. Wang constructed a function $\phi \in \mathcal{D}$ (see [26, p.1436] or [28, Theorem 3.2.9] for the notation and result). Modifying his construction one defines

$$\log \phi(x) = \frac{\sigma^-}{\Lambda_0} \int_0^{\rho_\partial(x)} (\ell(s) - \ell(r_1))^{1-d}\, ds \int_{s\wedge r_1}^{r_1} (\ell(u) - \ell(r_1))^{d-1}\, du$$

where

$$\ell(t) := \begin{cases} \cos\sqrt{k}t - \frac{\theta}{\sqrt{k}} \sin\sqrt{k}t, & k > 0, \\ 1 - \theta t, & k = 0, \\ \cosh\sqrt{-k}t - \frac{\theta}{\sqrt{-k}} \sinh\sqrt{-k}t, & k < 0, \end{cases} \tag{5.5}$$

and $r_1 := r_0 \wedge \ell^{-1}(0)$ and

$$\Lambda_0 := (1 - \ell(r_1))^{1-d} \int_0^{r_1} (\ell(s) - \ell(r_1))^{d-1}\, ds.$$

Then from the proof of [25, Theorem 1.1], we get:

$$K_{\phi,\alpha} \le K_\alpha := \frac{d\sigma^-}{r_1} + 2(\sigma^-)^2\alpha \quad \text{and} \quad \|\phi\|_\infty \le \mathrm{e}^{\frac{\sigma^-}{2} dr_1}. \tag{5.6}$$

Remark 5.4 (Construction of h and applications to bound $|\mathrm{Hess}_{P.f}|$)**.** Let $D = B'(x,k)$ where $B'(x,k) := \{y \in M \colon \rho'(x,y) \le k\}$ for some $k > 0$. We search for an adapted real process $h = h_k$ satisfying $\int_0^t (h_k)_s\, \mathrm{d}s = -1$ for $t \ge T \wedge \tau_k$ and

$$\mathbb{E}^x \left[\int_0^T (h_k^{2p})_s\, \mathrm{d}s \right] < \infty$$

where τ_k is the first exit time from $B(x,k)$. To h_k we then consider

$$(\tilde{h}_k)_t = 1 + \int_0^t (h_k)_s\, \mathrm{d}s$$

so that $(\tilde{h}_k)_0 = 1$ and $(\tilde{h}_k)_t = 0$ for $t \ge T \wedge \tau_k$. For $k > 0$ let

$$\theta_k(p) = \cos\left(\frac{\pi\rho'(x,p)}{2k}\right), \quad p \in B(x,k).$$

Then set $(\tilde{h}_k)_s = (\tilde{h} \circ \ell_k)_s$ where a function $\tilde{h} \in C^1([0,T])$ is chosen so that $\tilde{h}_0 = 1$, $\tilde{h}_t = 0$ with $(\tilde{h})' = h$ and

$$\ell_k(s) = \int_0^s \theta_k^{-2}(X_r(x)) \mathbf{1}_{\{r < \sigma_k(T)\}}\, \mathrm{d}r,$$

$$\sigma_k(s) = \inf\left\{ r \ge 0 : \int_0^r \theta_k^{-2}(X_u(x))\, \mathrm{d}u \ge s \right\}.$$

This construction is due to [22], the claim follows from [23, 22], see the proof of [7, Lemma 2.1] for the details. For this $\tilde{h}_k$, we have

$$\begin{aligned}\mathbb{E}\left[\int_0^{t\wedge\tau_k} h_k^{2p}(s)\,\mathrm{d}s\right] &= \mathbb{E}\left[\int_0^{\sigma(t)} (h\circ\ell_k)^{2p}(s)\theta_k^{-4p}(X_s(x))\,\mathrm{d}s\right]\\ &= \int_0^t h^{2p}(s)\mathbb{E}\big[\theta_k^{-4p+2}(X_s'(x))\big]\,\mathrm{d}s\end{aligned}$$

where $X'(x)$ denotes the diffusion starting at x with generator $\frac{1}{2}\theta_k^2 L$ which almost surely doesn't not exit $B'(x,k)$ by [22, Proposition 2.3.]. To estimate the integration we use

$$\frac{1}{2}\theta_k^2 L\theta_k^{-4p+2} = (2p-1)\theta_k^{-4p+2}\left[\frac{4p-1}{2}|\nabla\theta_k|^2 - \theta_k L\theta_k\right]$$

to obtain, via Ito's formula, Gronwall's lemma and the fact $N\rho'(x,\cdot)\le 0$, that

$$\mathbb{E}[\theta_k^{-4p+2}(X_s'(x))] \le \theta_k(x)^{-4p+2}\,\mathrm{e}^{c(\theta_k)s},$$

where

$$c(\theta_k) = (2p-1)\sup_{B'(x,k)}\left\{\frac{(4p-1)}{2}|\nabla\theta_k|^2 - \theta_k L\theta_k\right\}.$$

Using $\theta_k(x)=1$ and taking

$$\tilde{h}_t = 1 - \frac{c(\theta_k)}{p(1-\mathrm{e}^{-c(\theta_k)T/p})}\int_0^t \mathrm{e}^{-c(\theta_k)r/p}\,\mathrm{d}r$$

we obtain

$$\begin{aligned}\mathbb{E}\left[\int_0^{T\wedge\tau} h_k^{2p}(s)\,\mathrm{d}s\right] &\le \int_0^T \left(\frac{c(\theta_k)}{p}\right)^{2p}\frac{\mathrm{e}^{-c(\theta_k)s}}{(1-\mathrm{e}^{-c(\theta_k)T/p})^{2p}}\,\mathrm{d}s\\ &\le \left(\frac{c(\theta_k)}{p}\right)^{2p}\frac{T}{(1-\mathrm{e}^{-c(\theta_k)T/p})^{2p}} \le \frac{\mathrm{e}^{2c(\theta_k)T}}{T^{2p-1}}.\end{aligned}$$

Indeed, according to the definition of θ_k, we have

$$|\nabla\theta_k| \le \frac{\pi}{2k},$$

and by the Laplacian comparison theorem

$$\begin{aligned}&-(\theta_k L\theta_k)(p)\\ &\le \cos\left(\frac{\pi\rho'(x,p)}{2k}\right)\sin\left(\frac{\pi\rho'(x,p)}{2k}\right)\frac{\pi}{2k}L\rho'(x,\cdot)(p) + \cos\left(\frac{\pi\rho'(x,p)}{2k}\right)^2\frac{\pi^2}{4k^2}\\ &\le \frac{\pi^2\rho'(x,p)}{4k^2}\left(\frac{(d-1)}{\rho'(x,p)\wedge 1} + (K-K_\phi)\rho'(x,p)\right) + \frac{\pi^2}{4k^2}\\ &\le \frac{\pi^2}{4k} + \frac{(d+1)\pi^2}{4k^2} + \frac{(K-K_\phi)\pi^2}{4}, \qquad \rho'(x,p)\le k,\end{aligned}$$

where

$$\mathrm{Ric}_Z + L\log\phi - 2|\nabla \log\phi|^2 \geq K - K_\phi.$$

We then conclude that

$$c(\theta_k) \leq (2p-1)\left(\frac{\pi^2}{2k} + \frac{(2d+4p+1)\pi^2}{4k^2} + \frac{(K-K_\phi)\pi^2}{2}\right).$$

Then by the local version of the Bismut type Hessian formula, we have

$$\begin{aligned}
&|\mathrm{Hess}_{P_T f}|(x)\\
&\leq 3\,\mathrm{e}^{K^- T}\,\|f\|_\infty \left[\mathbb{E}^x \int_0^T h_k^2(s)\,\mathrm{e}^{\sigma^- l_s}\,\mathrm{d}s\right]^{1/2}\\
&\quad \times \Bigg\{ \left[(3+\sqrt{10})\alpha + \frac{\beta}{2}\right]\left(\mathbb{E}^x \int_0^T \mathrm{e}^{\sigma^- l_s}\,\mathrm{d}s\right)^{1/2}\\
&\qquad + \frac{\gamma}{2}\left(\mathbb{E}^x \int_0^T \mathrm{e}^{\sigma^- l_s}\,\mathrm{d}l_s\right)^{1/2} + \frac{2}{3}\left(\mathbb{E}^x \int_0^T h_k^2(s)\,\mathrm{e}^{\sigma^- l_s}\,\mathrm{d}s\right)^{1/2}\Bigg\}\\
&\leq 3\,\mathrm{e}^{K^- T}\,\|f\|_\infty\|\phi\|_\infty \left(\mathrm{e}^{K_{\phi,q}T}\,T^{1/q}\left(\frac{\mathrm{e}^{2c(\theta_k)T}}{T^{2p-1}}\right)^{1/p}\right)^{1/2}\\
&\qquad \times \Bigg\{ \left((3+\sqrt{10})\alpha + \frac{\beta}{2}\right)\left(\mathrm{e}^{K_\phi T}\,T\right)^{1/2} + \frac{\sqrt{\gamma}}{2}\left(\frac{\mathrm{e}^{K_\phi T}}{\sigma^- + \gamma\epsilon}\right)^{1/2}\\
&\qquad\quad + \frac{2}{3}\left[\mathrm{e}^{K_{\phi,q}T}\,T^{1/q}\left(\frac{\mathrm{e}^{2c(\theta_k)T}}{T^{2p-1}}\right)^{1/p}\right]^{1/2}\Bigg\},
\end{aligned}$$

where $\phi \in \mathcal{D}_{\gamma\varepsilon}$ for small $\varepsilon > 0$. When the manifold is non-compact, letting k tend to ∞ yields

$$\begin{aligned}
|\mathrm{Hess}_{P_T f}|(x) &\leq 3\,\mathrm{e}^{K^- T}\,\|\phi\|_\infty\|f\|_\infty \left(\mathrm{e}^{K_{\phi,q}T + \frac{2p-1}{p}(K-K_\phi)\pi^2}\,T^{-1}\right)^{1/2}\\
&\quad \times \Bigg\{ \left((3+\sqrt{10})\alpha + \frac{\beta}{2}\right)\left(\mathrm{e}^{K_\phi T}\,T\right)^{\frac{1}{2}} + \frac{1}{2}\left(\frac{\gamma\,\mathrm{e}^{K_\phi T}}{\sigma^- + \gamma\epsilon}\right)^{1/2}\\
&\qquad + \frac{2}{3}\left(\mathrm{e}^{K_{\phi,q}T + \frac{2p-1}{p}(K-K_\phi)\pi^2}\,T^{-1}\right)^{1/2}\Bigg\} < \infty
\end{aligned}$$

for $T > 0$. We can use the same strategy to construct $\phi \in \mathcal{D}_{\gamma\varepsilon}$ by replacing σ^- with $\sigma^- + \gamma\varepsilon$ in Remark 5.3, where the estimates of $\|\phi\|_\infty$ and K_ϕ then are modified as follows

$$K_\phi \leq \frac{d(\sigma^- + \gamma\varepsilon)}{r_1} + 2(\sigma^- + \gamma\varepsilon)^2, \quad \text{and} \quad \|\phi\|_\infty \leq \mathrm{e}^{\frac{1}{2}(\sigma^- + \gamma\varepsilon)dr_1}.$$

Conflict of Interest and Ethics Statements. The authors declare that there is no conflict of interest. Data sharing is not applicable to this article as no data-sets were created or analyzed in this study.

Acknowledgement. The authors would like thank the referee for helpful comments. This work was supported in part by the National Key R&D Program of China (No. 2020YFA0712900)

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